



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:38 PM GMT

PDB ID : 1PPJ
Title : Bovine cytochrome bc1 complex with stigmatellin and antimycin
Authors : Huang, L.S.; Cobessi, D.; Tung, E.Y.; Berry, E.A.
Deposited on : 2003-06-16
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

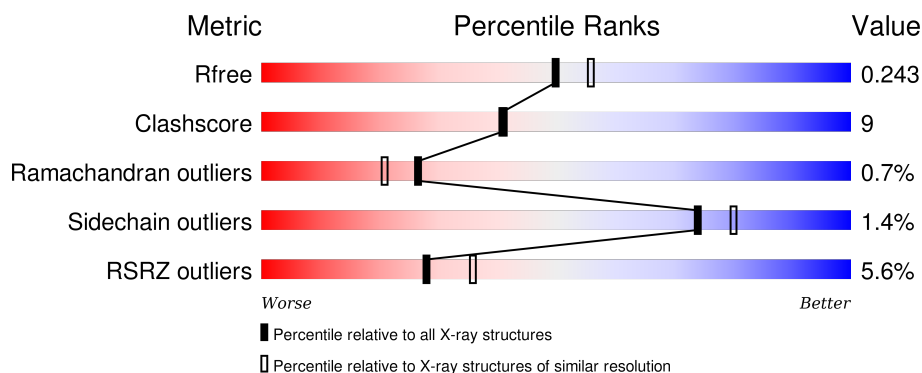
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	<div> <div>2%</div> <div>82% 16% ..</div> </div>
1	N	446	<div> <div>6%</div> <div>80% 18% ..</div> </div>
2	B	439	<div> <div>2%</div> <div>80% 16% .</div> </div>
2	O	439	<div> <div>3%</div> <div>84% 13% .</div> </div>
3	C	379	<div> <div>%</div> <div>84% 11% . .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	379	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	78	
8	U	78	
9	I	78	
9	V	78	
10	J	62	
10	W	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	BHG	A	4004	X	-	-	-
11	BHG	C	2010	X	-	-	X
11	BHG	C	4002	X	-	-	X
11	BHG	D	4003	X	-	-	X
11	BHG	F	3011	X	-	-	X
11	BHG	F	4001	X	-	-	X
11	BHG	P	3010	X	-	-	X
11	BHG	R	4007	X	-	-	X
11	BHG	S	2011	X	-	-	X
12	AZI	A	4011	-	-	-	X
12	AZI	C	2005	-	-	-	X
12	AZI	G	4009	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	FES	R	501	-	-	-	X
18	CDL	G	2004	-	-	-	X
18	CDL	T	3004	-	-	-	X
19	PEE	C	2007	-	-	-	X
19	PEE	D	2006	-	-	-	X
19	PEE	P	3007	-	-	-	X
19	PEE	Q	3006	-	-	-	X
20	ANY	P	3002	X	-	-	-
21	GOL	B	2009	-	-	-	X
21	GOL	C	2008	-	-	-	X
21	GOL	O	3009	-	-	-	X
21	GOL	P	3008	-	-	-	X

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 33549 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	1
			3396	2117	601	658	20			
1	N	442	Total	C	N	O	S	10	0	1
			3396	2117	601	658	20			

- Molecule 2 is a protein called Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	1
			3178	1997	562	612	7			
2	O	424	Total	C	N	O	S	0	0	1
			3156	1984	558	607	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	365	Total	C	N	O	S	0	0	0
			2892	1940	450	485	17			
3	P	365	Total	C	N	O	S	0	0	0
			2891	1940	449	485	17			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			
4	Q	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

- Molecule 5 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1510	954	263	285	8			
5	R	196	Total	C	N	O	S	0	0	0
			1517	956	263	290	8			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			
6	S	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	2
			621	406	117	97	1			
7	T	76	Total	C	N	O	S	0	0	2
			626	409	118	98	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			
8	U	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			

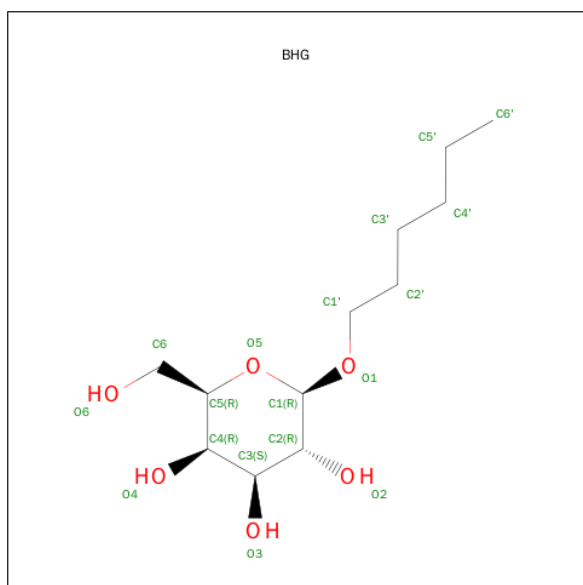
- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	43	Total	C	N	O	S	0	0	0
			285	175	53	56	1			
9	V	43	Total	C	N	O	S	0	0	0
			285	175	53	56	1			

- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

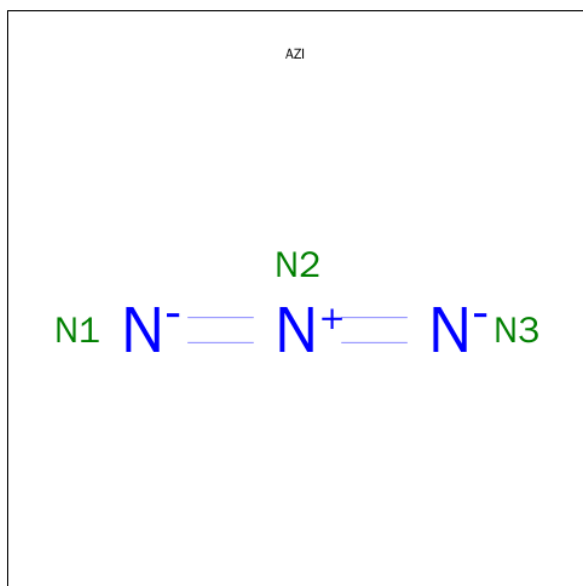
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	33	Total	C	N	O	0	0	1
			284	185	50	49			
10	W	62	Total	C	N	O	0	0	1
			506	332	88	86			

- Molecule 11 is SUGAR (2-HEXYLOXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-3,4,5-TRIOL) (three-letter code: BHG) (formula: $C_{12}H_{24}O_6$).



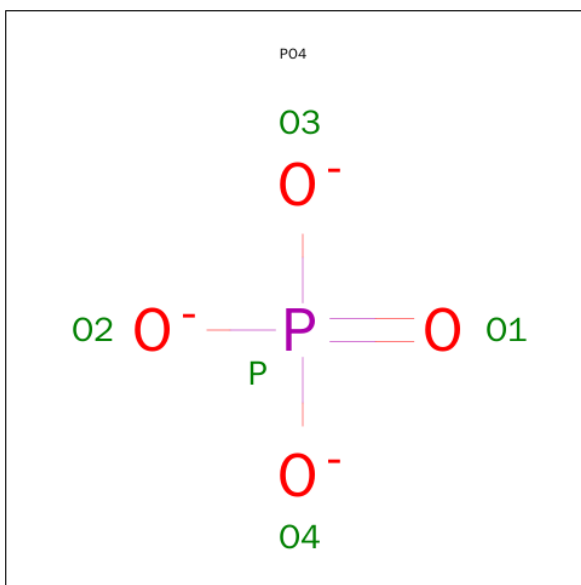
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			18	12	6		
11	S	1	Total	C	O	0	0
			18	12	6		
11	P	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	C	1	Total	C	O	0	0
			18	12	6		
11	D	1	Total	C	O	0	0
			18	12	6		
11	A	1	Total	C	O	0	0
			18	12	6		
11	R	1	Total	C	O	0	0
			18	12	6		

- Molecule 12 is AZIDE ION (three-letter code: AZI) (formula: N_3).



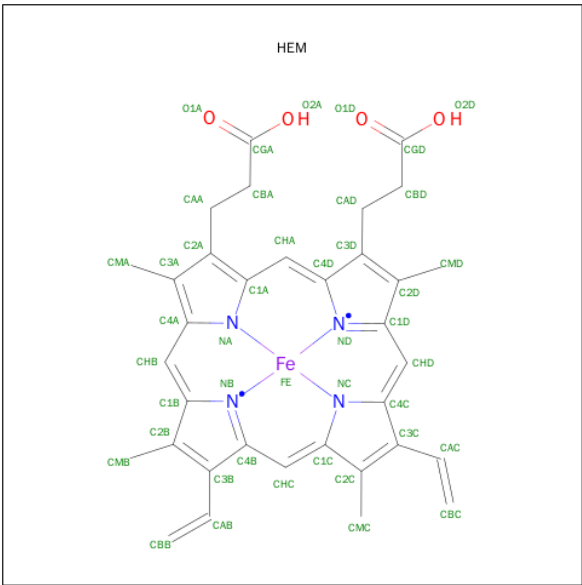
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total N 3 3	0	0
12	P	1	Total N 3 3	0	0
12	G	1	Total N 3 3	0	0
12	O	1	Total N 3 3	0	0
12	A	1	Total N 3 3	0	0

- Molecule 13 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



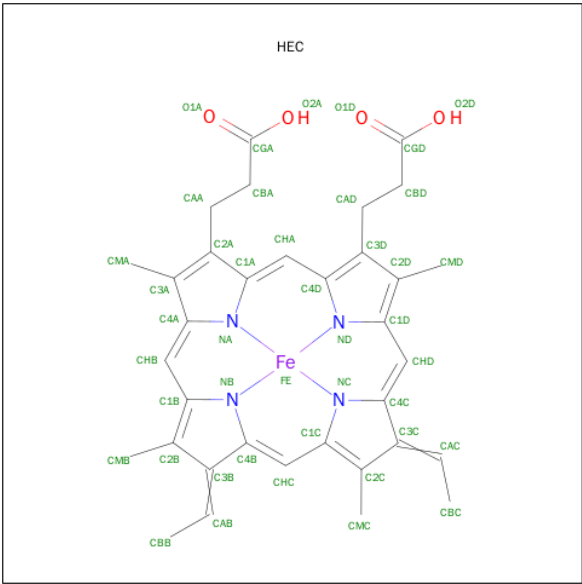
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	F	1	Total	O	P	0	0
			5	4	1		
13	A	1	Total	O	P	0	0
			5	4	1		
13	S	1	Total	O	P	0	0
			5	4	1		
13	P	1	Total	O	P	0	0
			5	4	1		
13	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



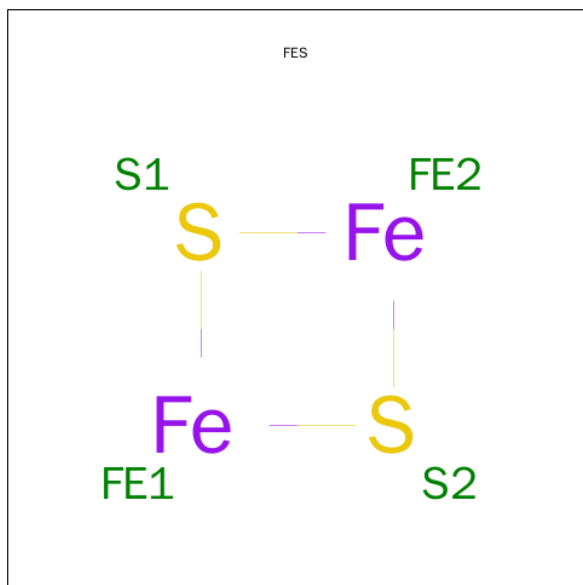
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 15 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



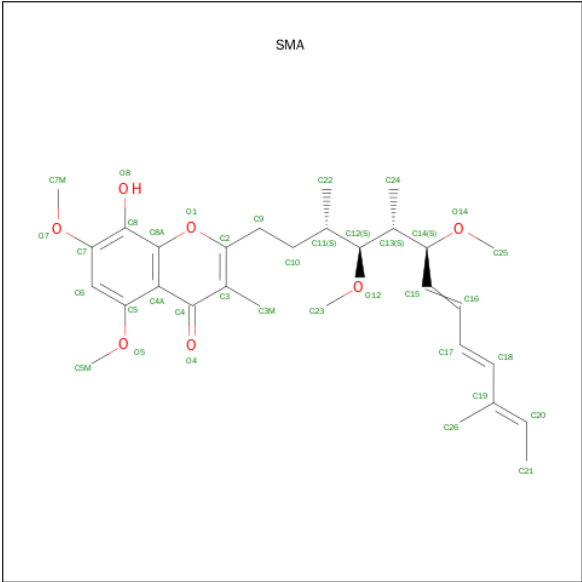
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



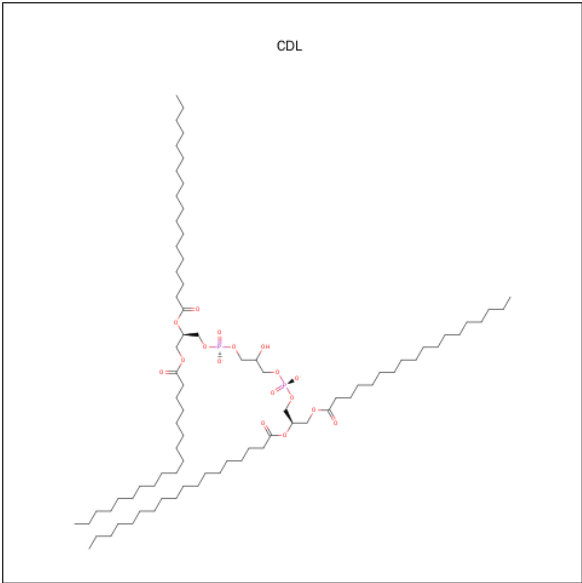
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	E	1	Total	Fe	S	0	0
			4	2	2		
16	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 17 is STIGMATELLIN A (three-letter code: SMA) (formula: $\text{C}_{30}\text{H}_{42}\text{O}_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			37	30	7		
17	P	1	Total	C	O	0	0
			37	30	7		

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



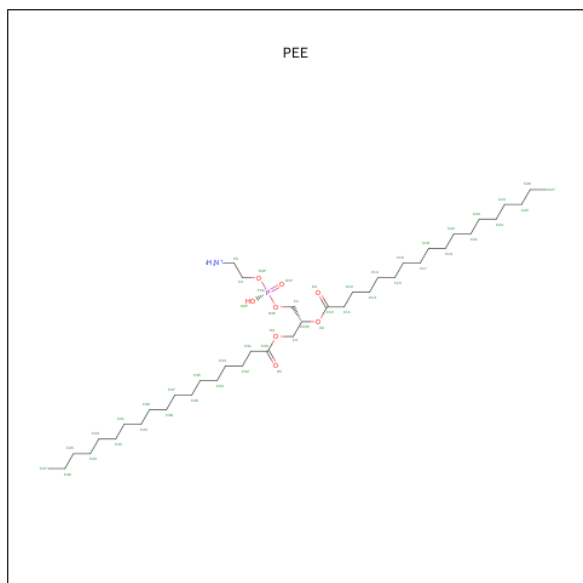
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	P	0	0
			39	24	13	2		
18	G	1	Total	C	O	P	0	0
			44	25	17	2		

Continued on next page...

Continued from previous page...

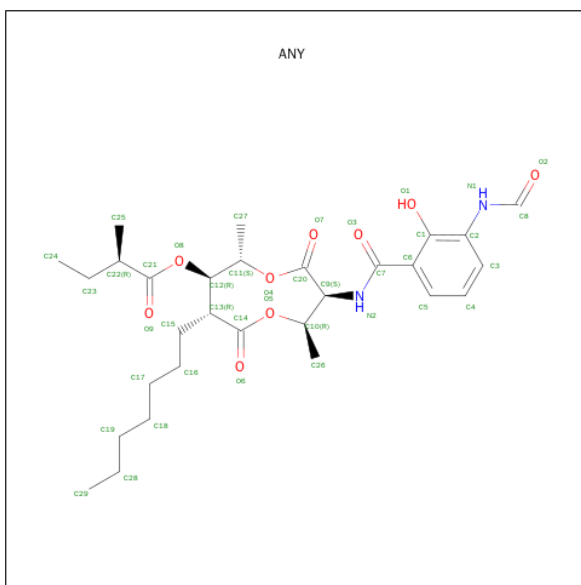
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	P	1	Total	C	O	P	0	0
			39	24	13	2		
18	T	1	Total	C	O	P	0	0
			49	30	17	2		

- Molecule 19 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



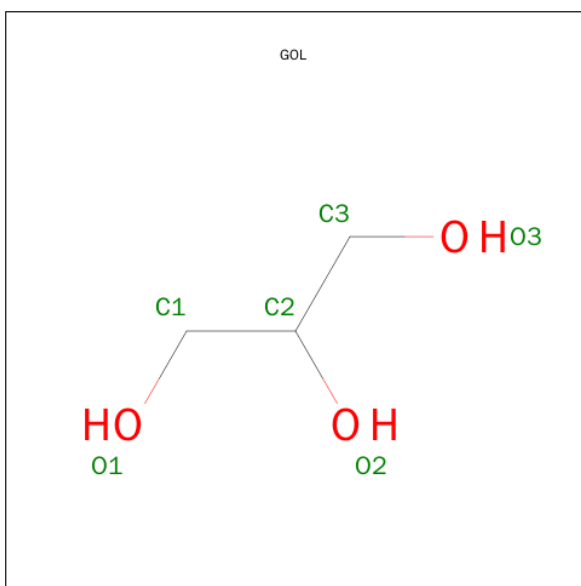
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
19	D	1	Total	C	N	O	P	0	0
			26	16	1	8	1		
19	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
19	Q	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 20 is 2-METHYL-BUTYRIC ACID 3-(3-FORMYLAMINO-2-HYDROXY-BENZOYLAMINO)-8-HEPTYL-2,6-DIMETHYL-4,9-DIOXO-[1,5]DIOXONAN-7-YL ESTER (three-letter code: ANY) (formula: $C_{29}H_{42}N_2O_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	C	1	Total 37	C 26	N 2	O 9	0	0
20	P	1	Total 37	C 26	N 2	O 9	0	0

- Molecule 21 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	C	1	Total C O 6 3 3	0	0
21	B	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	P	1	Total	C	O	0	0
			6	3	3		
21	O	1	Total	C	O	0	0
			6	3	3		
21	R	1	Total	C	O	0	0
			6	3	3		
21	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 22 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	219	Total	O	0	0
			219	219		
22	B	167	Total	O	0	0
			167	167		
22	C	123	Total	O	0	0
			123	123		
22	D	96	Total	O	0	0
			96	96		
22	E	50	Total	O	0	0
			50	50		
22	F	63	Total	O	0	0
			63	63		
22	G	17	Total	O	0	0
			17	17		
22	H	17	Total	O	0	0
			17	17		
22	I	16	Total	O	0	0
			16	16		
22	J	4	Total	O	0	0
			4	4		
22	N	98	Total	O	0	0
			98	98		
22	O	127	Total	O	0	0
			127	127		
22	P	115	Total	O	0	0
			115	115		
22	Q	89	Total	O	0	0
			89	89		
22	R	63	Total	O	0	0
			63	63		

Continued on next page...

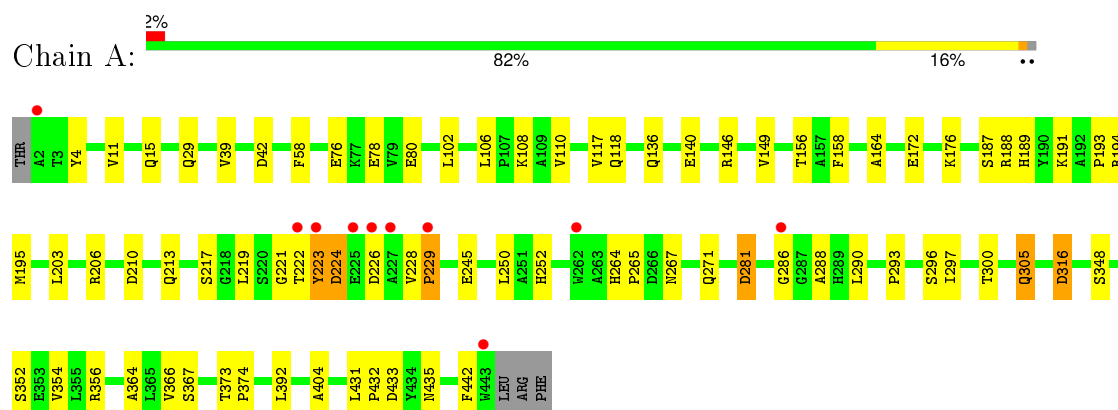
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	S	63	Total 63	O 63	0	0
22	T	20	Total 20	O 20	0	0
22	U	6	Total 6	O 6	0	0
22	V	8	Total 8	O 8	0	0
22	W	9	Total 9	O 9	0	0

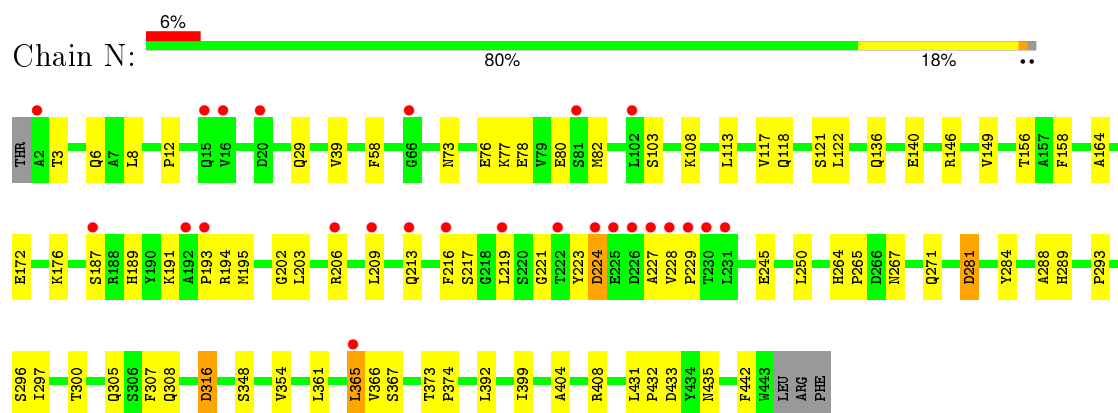
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

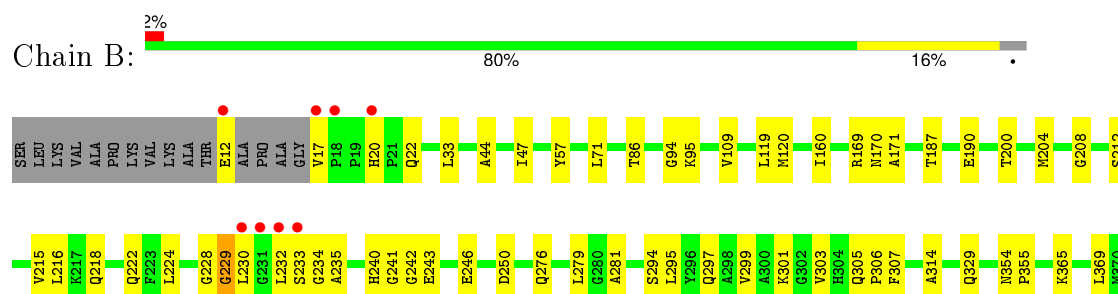
- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

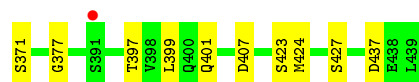


- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

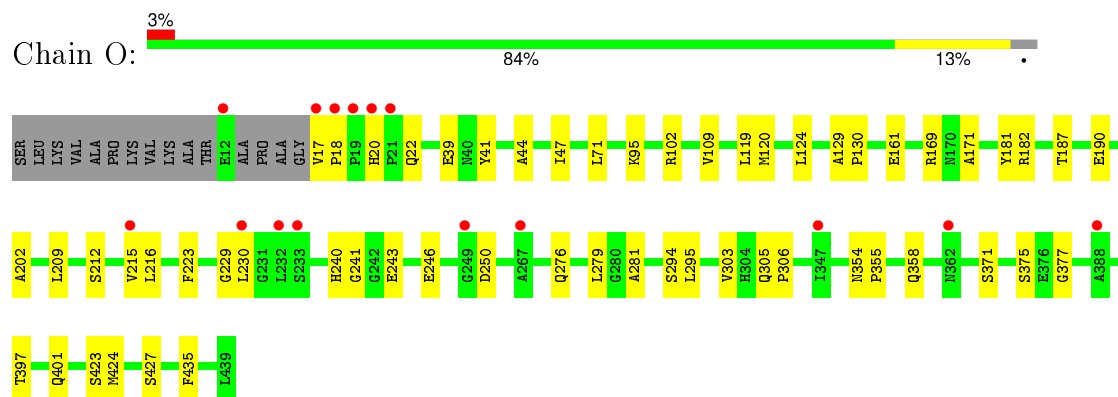


- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

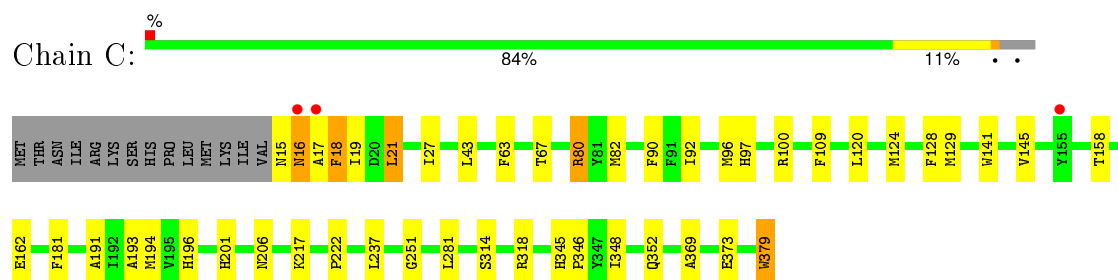




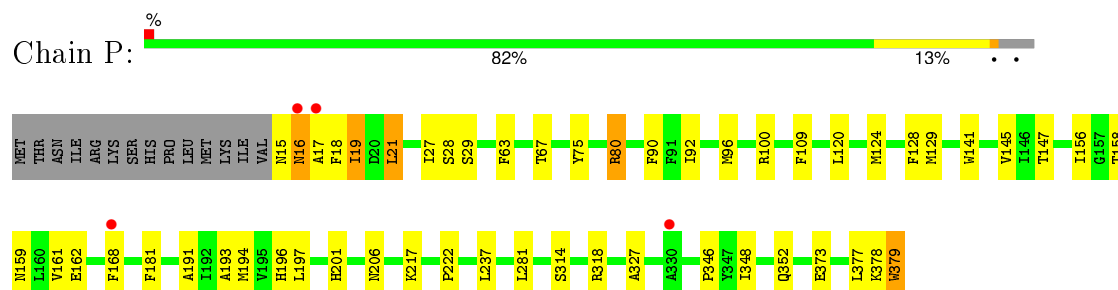
- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial



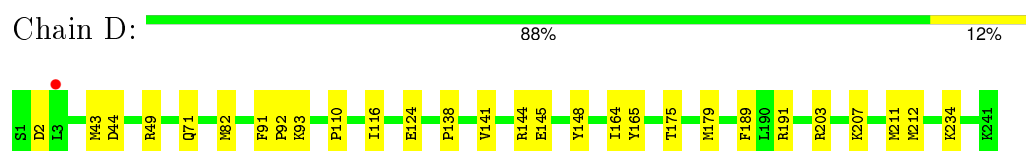
- Molecule 3: Cytochrome b



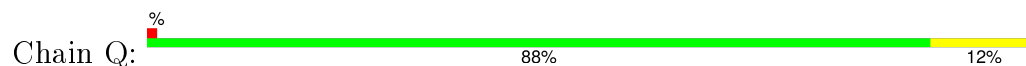
- Molecule 3: Cytochrome b

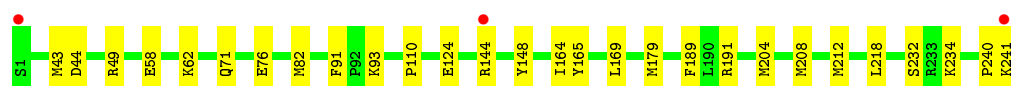


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

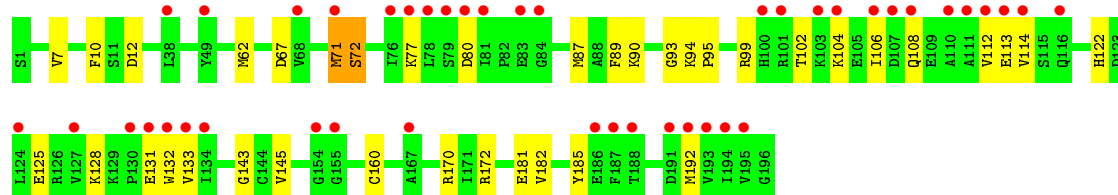
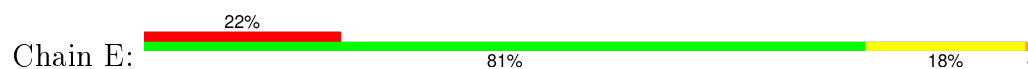


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

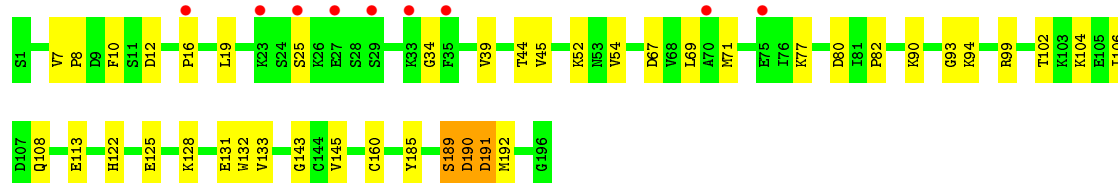
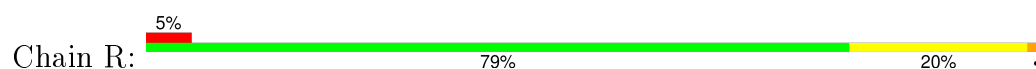




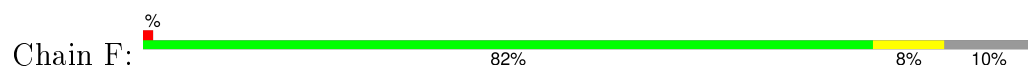
- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein



- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein



- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C



- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

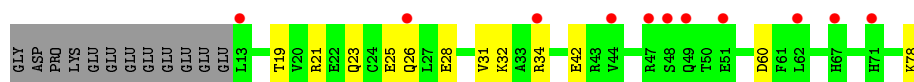




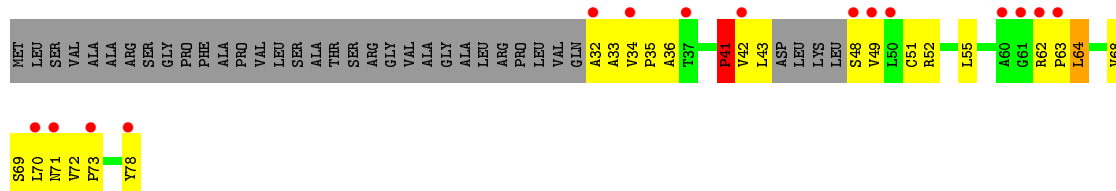
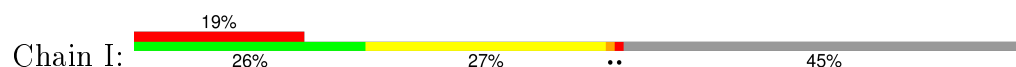
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein



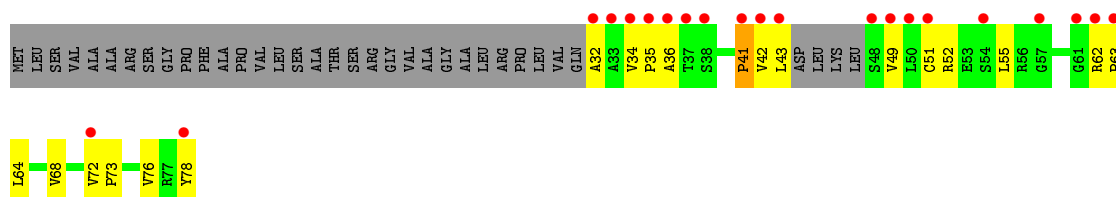
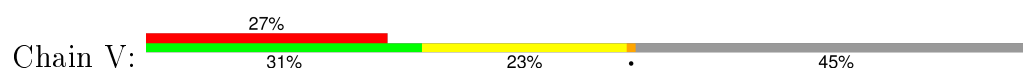
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein



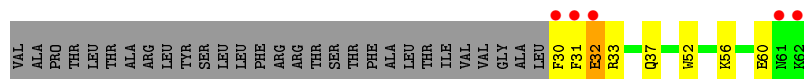
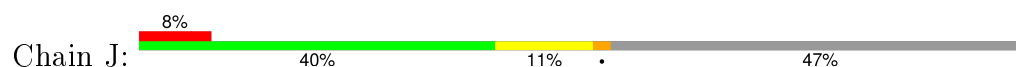
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

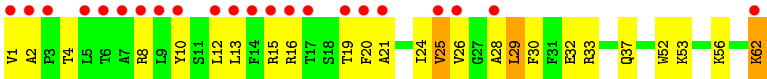


- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein



- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.53Å 168.75Å 231.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.53 – 2.10 93.53 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (93.53-2.10) 97.8 (93.53-2.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.260 0.226 , 0.243	Depositor DCC
R_{free} test set	14181 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 65.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 285060 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33549	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, GOL, CDL, PO4, BHG, FES, HEC, HEM, PEE, ANY, SMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/3465	0.64	0/4704
1	N	0.30	0/3465	0.63	1/4704 (0.0%)
2	B	0.32	0/3236	0.63	0/4388
2	O	0.31	0/3213	0.62	0/4354
3	C	0.34	0/2986	0.64	1/4089 (0.0%)
3	P	0.33	0/2985	0.64	1/4087 (0.0%)
4	D	0.30	0/1978	0.61	0/2684
4	Q	0.29	0/1978	0.59	0/2684
5	E	0.29	0/1544	0.64	1/2087 (0.0%)
5	R	0.30	0/1551	0.66	1/2097 (0.0%)
6	F	0.32	0/878	0.63	0/1175
6	S	0.30	0/878	0.61	0/1175
7	G	0.31	0/642	0.61	0/869
7	T	0.31	0/647	0.61	0/876
8	H	0.30	0/544	0.56	0/729
8	U	0.27	0/544	0.55	0/729
9	I	0.35	0/286	0.87	2/387 (0.5%)
9	V	0.34	0/286	0.84	1/387 (0.3%)
10	J	0.33	0/292	0.53	0/386
10	W	0.31	0/518	0.55	0/696
All	All	0.31	0/31916	0.63	8/43287 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	35	PRO	N-CA-CB	5.84	110.31	103.30
9	I	64	LEU	CA-CB-CG	5.72	128.47	115.30
5	R	143	GLY	N-CA-C	5.70	127.35	113.10
1	N	365	LEU	CA-CB-CG	5.68	128.36	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	143	GLY	N-CA-C	5.58	127.06	113.10
9	V	35	PRO	N-CA-CB	5.36	109.73	103.30
3	C	109	PHE	N-CA-C	-5.26	96.79	111.00
3	P	109	PHE	N-CA-C	-5.12	97.17	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3396	0	3292	65	0
1	N	3396	0	3292	57	0
2	B	3178	0	3153	72	0
2	O	3156	0	3123	44	0
3	C	2892	0	2938	36	0
3	P	2891	0	2937	43	0
4	D	1919	0	1868	27	0
4	Q	1919	0	1868	28	0
5	E	1510	0	1495	30	0
5	R	1517	0	1499	33	0
6	F	861	0	854	12	0
6	S	861	0	854	19	0
7	G	621	0	626	15	0
7	T	626	0	631	15	0
8	H	539	0	524	11	0
8	U	539	0	524	10	0
9	I	285	0	280	50	0
9	V	285	0	280	24	0
10	J	284	0	264	5	0
10	W	506	0	512	30	0
11	A	18	0	24	0	0
11	C	36	0	48	2	0
11	D	18	0	24	3	0
11	F	36	0	48	3	0
11	P	18	0	24	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	R	18	0	24	1	0
11	S	18	0	24	3	0
12	A	3	0	0	0	0
12	C	3	0	0	0	0
12	G	3	0	0	0	0
12	O	3	0	0	0	0
12	P	3	0	0	0	0
13	A	5	0	0	0	0
13	C	5	0	0	0	0
13	F	5	0	0	0	0
13	P	5	0	0	0	0
13	S	5	0	0	0	0
14	C	86	0	60	3	0
14	P	86	0	60	2	0
15	D	43	0	30	3	0
15	Q	43	0	30	1	0
16	E	4	0	0	0	0
16	R	4	0	0	0	0
17	C	37	0	42	2	0
17	P	37	0	42	2	0
18	D	39	0	39	0	0
18	G	44	0	32	0	0
18	P	39	0	39	2	0
18	T	49	0	42	2	0
19	C	49	0	72	0	0
19	D	26	0	26	3	0
19	P	49	0	72	1	0
19	Q	51	0	82	3	0
20	C	37	0	28	1	0
20	P	37	0	29	2	0
21	B	6	0	8	0	0
21	C	12	0	16	1	0
21	O	6	0	8	0	0
21	P	6	0	8	0	0
21	R	6	0	8	1	0
22	A	219	0	0	7	0
22	B	167	0	0	5	0
22	C	123	0	0	1	0
22	D	96	0	0	0	0
22	E	50	0	0	0	0
22	F	63	0	0	0	0
22	G	17	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	H	17	0	0	0	0
22	I	16	0	0	2	0
22	J	4	0	0	0	0
22	N	98	0	0	1	0
22	O	127	0	0	2	0
22	P	115	0	0	5	0
22	Q	89	0	0	0	0
22	R	63	0	0	5	0
22	S	63	0	0	1	0
22	T	20	0	0	0	0
22	U	6	0	0	0	0
22	V	8	0	0	1	0
22	W	9	0	0	0	0
All	All	33549	0	31803	551	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (551) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:LYS:HE2	9:I:32:ALA:HB3	1.47	0.94
10:W:16:ARG:HB2	10:W:19:THR:HG22	1.48	0.94
2:O:95:LYS:HE2	9:V:32:ALA:N	1.82	0.94
1:A:136:GLN:HE21	9:I:51:CYS:HB3	1.30	0.93
1:A:146:ARG:HA	22:A:4191:HOH:O	1.69	0.92
9:I:32:ALA:HA	9:I:71:ASN:CB	1.99	0.91
6:S:13:LEU:H	6:S:13:LEU:HD23	1.32	0.91
2:B:200:THR:HG21	2:B:228:GLY:HA3	1.51	0.90
1:N:136:GLN:HE21	9:V:51:CYS:HB3	1.38	0.88
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.56	0.88
8:H:25:GLU:HB2	8:H:34:ARG:HH22	1.38	0.88
2:B:95:LYS:HE2	9:I:32:ALA:CB	2.03	0.88
8:U:25:GLU:HB2	8:U:34:ARG:HH22	1.37	0.87
1:N:136:GLN:NE2	9:V:51:CYS:HB3	1.93	0.83
2:B:204:MET:HE1	2:B:224:LEU:HD22	1.58	0.83
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.57	0.83
1:N:39:VAL:HG11	1:N:195:MET:HE3	1.60	0.81
9:V:36:ALA:HB2	9:V:73:PRO:HD2	1.63	0.81
9:V:49:VAL:HG11	9:V:55:LEU:HD13	1.62	0.81
6:F:13:LEU:O	6:F:16:ILE:HG12	1.80	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:20:HIS:HB2	2:O:22:GLN:HG2	1.62	0.80
1:A:136:GLN:NE2	9:I:51:CYS:HB3	1.96	0.80
5:R:44:THR:HG21	10:W:24:ILE:HD13	1.65	0.78
9:I:49:VAL:HG11	9:I:55:LEU:HD13	1.65	0.77
2:B:71:LEU:HD23	9:I:68:VAL:HG21	1.68	0.74
6:F:95:LYS:HB2	6:F:95:LYS:NZ	2.02	0.74
5:R:34:GLY:CA	10:W:10:TYR:HB2	2.17	0.74
10:W:21:ALA:O	10:W:25:VAL:HG23	1.88	0.74
5:R:34:GLY:HA2	10:W:10:TYR:HB2	1.70	0.74
2:O:71:LEU:HD23	9:V:68:VAL:HG21	1.70	0.74
4:D:110:PRO:HG3	15:D:501:HEC:HMD3	1.71	0.73
6:S:95:LYS:HB2	6:S:95:LYS:NZ	2.04	0.72
7:T:63:THR:O	7:T:67:GLU:HG2	1.90	0.72
8:U:28:GLU:O	8:U:31:VAL:HG22	1.91	0.71
5:E:112:VAL:HG21	5:E:170:ARG:NH2	2.05	0.71
8:H:28:GLU:O	8:H:31:VAL:HG22	1.91	0.71
3:P:17:ALA:HA	3:P:201:HIS:HE1	1.55	0.70
3:C:129:MET:CE	3:C:181:PHE:HD2	2.05	0.70
7:G:63:THR:O	7:G:67:GLU:HG2	1.91	0.70
9:I:72:VAL:HG13	9:I:73:PRO:HD2	1.74	0.69
3:P:129:MET:CE	3:P:181:PHE:HD2	2.05	0.69
3:C:17:ALA:HA	3:C:201:HIS:HE1	1.57	0.69
9:I:62:ARG:HB3	9:I:63:PRO:HD2	1.74	0.69
1:N:209:LEU:O	1:N:213:GLN:HG3	1.93	0.69
5:R:104:LYS:O	5:R:108:GLN:HG3	1.91	0.69
9:V:62:ARG:HB3	9:V:63:PRO:HD2	1.74	0.69
2:B:204:MET:CE	2:B:224:LEU:HD22	2.23	0.68
5:E:104:LYS:O	5:E:108:GLN:HG3	1.92	0.68
2:B:200:THR:CG2	2:B:228:GLY:HA3	2.23	0.68
1:A:293:PRO:O	1:A:297:ILE:HG12	1.93	0.68
1:N:293:PRO:O	1:N:297:ILE:HG12	1.94	0.68
9:I:32:ALA:HA	9:I:71:ASN:HB3	1.76	0.68
2:B:20:HIS:HB2	2:B:22:GLN:HG2	1.74	0.67
8:U:25:GLU:CB	8:U:34:ARG:HH22	2.08	0.67
22:A:4203:HOH:O	9:I:73:PRO:HG3	1.94	0.67
8:U:28:GLU:O	8:U:32:LYS:HG2	1.95	0.67
8:H:25:GLU:CB	8:H:34:ARG:HH22	2.07	0.67
2:B:95:LYS:HE2	9:I:32:ALA:N	2.10	0.67
1:A:39:VAL:HG11	1:A:195:MET:HE3	1.75	0.67
8:H:28:GLU:O	8:H:32:LYS:HG2	1.95	0.66
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:358:GLN:HB2	22:O:4120:HOH:O	1.95	0.66
3:C:129:MET:HE1	3:C:181:PHE:HD2	1.61	0.66
8:H:21:ARG:O	8:H:25:GLU:HG2	1.96	0.66
3:P:379:TRP:CZ3	6:S:33:ARG:HD3	2.29	0.66
6:F:95:LYS:HB2	6:F:95:LYS:HZ2	1.61	0.66
4:Q:110:PRO:HG3	15:Q:501:HEC:HMD3	1.78	0.66
1:A:316:ASP:OD1	1:A:316:ASP:N	2.26	0.66
3:P:129:MET:HE1	3:P:181:PHE:HD2	1.60	0.65
10:W:33:ARG:O	10:W:37:GLN:HG3	1.96	0.65
5:R:189:SER:O	5:R:190:ASP:C	2.33	0.65
3:C:16:ASN:HD22	3:C:16:ASN:N	1.93	0.65
1:A:136:GLN:O	1:A:140:GLU:HG3	1.97	0.65
7:T:34:ILE:HB	7:T:35:PRO:HD3	1.79	0.65
9:I:32:ALA:N	9:I:72:VAL:HG23	2.13	0.64
4:Q:144:ARG:HH11	4:Q:144:ARG:HG2	1.62	0.64
3:C:379:TRP:CZ3	6:F:33:ARG:HD3	2.32	0.64
10:W:16:ARG:HH11	10:W:19:THR:HG21	1.63	0.64
1:N:113:LEU:O	1:N:117:VAL:HG12	1.97	0.64
2:O:306:PRO:HA	9:V:52:ARG:HG3	1.80	0.64
9:I:36:ALA:HB2	9:I:73:PRO:HD2	1.79	0.64
9:V:72:VAL:HG13	9:V:73:PRO:HD2	1.78	0.64
1:A:172:GLU:OE2	1:A:176:LYS:HE3	1.98	0.64
5:E:112:VAL:HG21	5:E:170:ARG:HH22	1.61	0.64
4:D:144:ARG:HG2	4:D:144:ARG:HH11	1.64	0.63
4:D:71:GLN:HA	4:D:82:MET:HE2	1.81	0.63
1:A:305:GLN:HA	1:A:305:GLN:HE21	1.62	0.63
2:B:94:GLY:O	9:I:32:ALA:HB2	1.99	0.63
8:U:21:ARG:O	8:U:25:GLU:HG2	1.98	0.62
9:I:32:ALA:CA	9:I:71:ASN:CB	2.74	0.62
1:N:136:GLN:O	1:N:140:GLU:HG3	2.00	0.62
2:B:299:VAL:HG12	2:B:303:VAL:CG1	2.30	0.62
1:A:352:SER:HB3	6:S:110:LYS:OXT	1.99	0.62
2:B:95:LYS:CE	9:I:32:ALA:HB3	2.25	0.61
1:N:316:ASP:N	1:N:316:ASP:OD1	2.33	0.61
14:P:501:HEM:HMC1	14:P:501:HEM:HBC2	1.83	0.61
5:R:44:THR:CG2	10:W:24:ILE:HG21	2.30	0.61
1:N:224:ASP:OD1	1:N:227:ALA:HB3	1.99	0.61
2:O:202:ALA:HB3	2:O:229:GLY:O	2.00	0.61
9:I:32:ALA:N	9:I:71:ASN:HB2	2.16	0.61
4:Q:218:LEU:HD13	22:R:4057:HOH:O	1.99	0.61
1:N:172:GLU:OE2	1:N:176:LYS:HE3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:250:ASP:HB3	22:O:4111:HOH:O	1.99	0.60
1:A:288:ALA:HB2	1:A:300:THR:HG22	1.84	0.60
22:A:4157:HOH:O	9:I:41:PRO:HB3	2.00	0.60
14:C:501:HEM:HMC1	14:C:501:HEM:HBC2	1.82	0.60
6:F:13:LEU:HD12	6:F:16:ILE:HD11	1.84	0.60
3:P:16:ASN:HD22	3:P:16:ASN:N	1.99	0.60
5:E:71:MET:O	5:E:72:SER:HB3	2.01	0.60
6:S:95:LYS:HB2	6:S:95:LYS:HZ2	1.66	0.60
5:E:94:LYS:HE3	3:P:168:PHE:O	2.01	0.59
1:N:193:PRO:HD3	1:N:221:GLY:HA2	1.84	0.59
9:I:32:ALA:HA	9:I:71:ASN:HB2	1.84	0.59
9:V:36:ALA:CB	9:V:73:PRO:HD2	2.32	0.59
1:N:288:ALA:HB2	1:N:300:THR:HG22	1.85	0.59
6:S:13:LEU:N	6:S:13:LEU:HD23	2.12	0.59
10:W:15:ARG:HG3	10:W:15:ARG:HH11	1.67	0.59
2:B:33:LEU:HD12	2:B:204:MET:HE2	1.85	0.58
5:R:39:VAL:HG13	22:R:4057:HOH:O	2.02	0.58
4:Q:218:LEU:HD22	22:R:4057:HOH:O	2.01	0.58
1:N:117:VAL:HG13	1:N:118:GLN:HG3	1.85	0.58
1:A:305:GLN:HB3	9:I:41:PRO:HA	1.85	0.58
1:A:252:HIS:ND1	22:A:4191:HOH:O	2.32	0.58
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.38	0.58
2:O:169:ARG:HG3	2:O:240:HIS:HB2	1.85	0.58
3:P:15:ASN:OD1	3:P:19:ILE:HB	2.03	0.58
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.39	0.57
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.86	0.57
9:I:42:VAL:HG12	9:I:43:LEU:CG	2.35	0.57
3:C:129:MET:HE1	3:C:181:PHE:CD2	2.40	0.57
2:B:12:GLU:HG2	2:B:17:VAL:N	2.19	0.57
4:D:145:GLU:HA	11:D:4003:BHG:H2	1.87	0.57
10:W:13:LEU:O	10:W:19:THR:HG23	2.05	0.56
4:Q:165:TYR:HA	4:Q:179:MET:HE2	1.86	0.56
3:C:251:GLY:HA2	21:C:2008:GOL:H11	1.87	0.56
1:A:118:GLN:HG2	1:A:219:LEU:HD13	1.88	0.56
2:B:299:VAL:O	2:B:303:VAL:HG12	2.05	0.56
2:B:354:ASN:HB2	2:B:355:PRO:HD3	1.85	0.56
7:T:71:ARG:HH22	8:U:60:ASP:CG	2.08	0.56
2:B:299:VAL:HG12	2:B:303:VAL:HG12	1.87	0.56
1:N:3:THR:OG1	1:N:6:GLN:HG3	2.05	0.56
1:A:188:ARG:NH1	1:A:229:PRO:HD3	2.20	0.56
9:I:32:ALA:HA	9:I:71:ASN:CG	2.25	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.88	0.56
7:G:42:ARG:HG3	7:G:42:ARG:HH11	1.71	0.56
4:Q:44:ASP:OD1	4:Q:93:LYS:HE2	2.05	0.56
10:J:56:LYS:HG2	10:J:60:GLU:CD	2.26	0.56
1:N:228:VAL:HG13	1:N:228:VAL:O	2.06	0.56
19:Q:3006:PEE:H18	5:R:54:VAL:HG22	1.88	0.56
5:R:128:LYS:HE3	5:R:185:TYR:O	2.05	0.56
1:A:191:LYS:HE2	1:A:223:TYR:CB	2.36	0.56
11:F:3011:BHG:H1	1:N:289:HIS:NE2	2.21	0.55
5:R:44:THR:HG22	10:W:24:ILE:HG21	1.89	0.55
10:J:32:GLU:HG3	10:J:33:ARG:N	2.20	0.55
2:B:305:GLN:HB3	2:B:329:GLN:OE1	2.06	0.55
1:N:39:VAL:CG1	1:N:195:MET:HE3	2.33	0.55
1:N:361:LEU:O	1:N:365:LEU:HG	2.07	0.55
1:N:281:ASP:OD2	9:V:73:PRO:HG3	2.07	0.55
2:O:202:ALA:HB1	2:O:230:LEU:HD23	1.89	0.55
2:B:212:SER:O	2:B:215:VAL:HG22	2.07	0.55
1:A:267:ASN:O	1:A:271:GLN:HG2	2.07	0.54
4:D:44:ASP:OD1	4:D:93:LYS:HE2	2.07	0.54
1:A:193:PRO:HD3	1:A:221:GLY:HA2	1.88	0.54
1:A:228:VAL:O	1:A:228:VAL:HG13	2.06	0.54
3:P:100:ARG:C	3:P:100:ARG:HD2	2.27	0.54
5:R:44:THR:CG2	10:W:24:ILE:HD13	2.37	0.54
9:V:42:VAL:HG12	9:V:43:LEU:CG	2.38	0.54
1:A:136:GLN:NE2	9:I:51:CYS:CB	2.70	0.54
3:P:18:PHE:O	3:P:21:LEU:HB2	2.07	0.54
10:W:10:TYR:OH	10:W:15:ARG:NH1	2.41	0.54
3:P:314:SER:O	3:P:318:ARG:HD3	2.08	0.54
9:V:36:ALA:HB3	9:V:73:PRO:HG2	1.90	0.54
10:W:15:ARG:HG3	10:W:15:ARG:NH1	2.23	0.54
1:A:296:SER:O	1:A:300:THR:HG23	2.08	0.54
1:N:78:GLU:OE2	1:N:108:LYS:HD3	2.08	0.54
3:C:17:ALA:HA	3:C:201:HIS:CE1	2.42	0.53
4:D:144:ARG:NH1	4:D:144:ARG:HG2	2.23	0.53
1:A:78:GLU:OE2	1:A:108:LYS:HD3	2.08	0.53
9:I:32:ALA:CA	9:I:71:ASN:HB3	2.38	0.53
6:F:95:LYS:NZ	6:F:95:LYS:CB	2.69	0.53
3:P:129:MET:HE1	3:P:181:PHE:CD2	2.41	0.53
6:S:106:GLU:HG2	22:S:3048:HOH:O	2.06	0.53
1:N:373:THR:HB	1:N:374:PRO:HD3	1.90	0.53
4:D:165:TYR:HA	4:D:179:MET:HE2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:71:ARG:NH2	8:U:60:ASP:OD1	2.42	0.53
10:J:33:ARG:O	10:J:37:GLN:HG3	2.09	0.53
4:Q:208:MET:HA	19:Q:3006:PEE:H49	1.88	0.53
5:E:95:PRO:HG2	5:E:145:VAL:HG22	1.90	0.53
3:C:158:THR:O	3:C:162:GLU:HG3	2.09	0.53
3:C:18:PHE:O	3:C:21:LEU:HB2	2.08	0.53
2:O:279:LEU:HB3	2:O:295:LEU:HG	1.89	0.53
4:Q:144:ARG:NH1	4:Q:144:ARG:HG2	2.21	0.53
2:B:20:HIS:HB2	2:B:22:GLN:CG	2.39	0.53
9:I:70:LEU:HB3	22:I:1016:HOH:O	2.09	0.53
1:N:195:MET:SD	1:N:219:LEU:HD21	2.49	0.53
2:O:305:GLN:N	2:O:306:PRO:HD3	2.23	0.53
1:A:366:VAL:HG21	2:B:44:ALA:HB2	1.89	0.52
1:N:146:ARG:NH2	1:N:308:GLN:HE22	2.06	0.52
10:W:4:THR:O	10:W:8:ARG:HG2	2.09	0.52
2:B:169:ARG:HG3	2:B:240:HIS:HB2	1.91	0.52
1:N:365:LEU:HD11	1:N:399:ILE:HD11	1.91	0.52
1:N:267:ASN:O	1:N:271:GLN:HG2	2.09	0.52
2:O:212:SER:O	2:O:215:VAL:HG22	2.08	0.52
9:I:32:ALA:CA	9:I:71:ASN:HB2	2.40	0.52
7:T:41:THR:O	7:T:45:ILE:HG12	2.09	0.52
4:Q:164:ILE:O	4:Q:179:MET:HE2	2.10	0.52
7:G:41:THR:O	7:G:45:ILE:HG12	2.09	0.52
1:A:4:TYR:HB2	22:B:2124:HOH:O	2.10	0.52
4:D:148:TYR:OH	11:D:4003:BHG:H61	2.08	0.52
9:I:36:ALA:HB3	9:I:73:PRO:HG2	1.90	0.52
2:B:86:THR:HG23	9:I:70:LEU:HD11	1.92	0.52
10:W:52:TRP:O	10:W:56:LYS:HB2	2.09	0.52
1:N:158:PHE:O	1:N:164:ALA:HB2	2.10	0.52
3:P:206:ASN:HB3	14:P:502:HEM:O2D	2.10	0.52
5:R:94:LYS:HE3	21:R:4005:GOL:O3	2.09	0.52
8:U:19:THR:O	8:U:23:GLN:HG3	2.10	0.52
2:B:187:THR:OG1	2:B:190:GLU:HG3	2.10	0.52
1:A:364:ALA:HB2	9:I:33:ALA:HB1	1.92	0.52
4:Q:71:GLN:HA	4:Q:82:MET:HE2	1.90	0.51
6:F:19:TRP:CD1	11:F:4001:BHG:H1	2.46	0.51
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.92	0.51
1:N:354:VAL:HG21	1:N:404:ALA:HA	1.92	0.51
3:P:158:THR:O	3:P:162:GLU:HG3	2.11	0.51
3:P:80:ARG:C	3:P:80:ARG:HD3	2.31	0.51
1:A:191:LYS:HZ3	1:A:223:TYR:HA	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.41	0.51
3:P:17:ALA:HA	3:P:201:HIS:CE1	2.42	0.51
7:T:32:LYS:C	7:T:35:PRO:HD2	2.31	0.51
1:N:296:SER:O	1:N:300:THR:HG23	2.10	0.51
2:B:208:GLY:HA3	2:B:216:LEU:HD11	1.91	0.51
5:E:114:VAL:O	5:E:114:VAL:HG12	2.10	0.51
7:G:48:VAL:O	7:G:51:PRO:HD2	2.10	0.51
2:B:397:THR:O	2:B:401:GLN:HG3	2.11	0.51
3:C:16:ASN:ND2	3:C:16:ASN:N	2.59	0.51
2:O:202:ALA:HB3	2:O:229:GLY:C	2.30	0.51
3:C:206:ASN:HB3	14:C:502:HEM:O2D	2.11	0.51
4:D:2:ASP:OD1	7:G:70:LYS:HE3	2.11	0.51
9:I:36:ALA:CB	9:I:73:PRO:HD2	2.41	0.50
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.92	0.50
2:B:94:GLY:O	9:I:32:ALA:CB	2.59	0.50
6:S:12:TRP:N	6:S:13:LEU:HD23	2.27	0.50
6:S:95:LYS:CB	6:S:95:LYS:NZ	2.72	0.50
2:B:95:LYS:NZ	9:I:34:VAL:HG22	2.27	0.50
4:D:116:ILE:HG12	15:D:501:HEC:HMA3	1.92	0.50
7:T:48:VAL:O	7:T:51:PRO:HD2	2.12	0.50
10:J:52:TRP:O	10:J:56:LYS:HB2	2.12	0.50
1:N:366:VAL:HG21	2:O:44:ALA:HB2	1.94	0.50
9:I:32:ALA:HA	9:I:71:ASN:ND2	2.26	0.50
6:F:13:LEU:O	6:F:16:ILE:CG1	2.56	0.50
8:H:19:THR:O	8:H:23:GLN:HG3	2.11	0.49
2:B:279:LEU:HB3	2:B:295:LEU:HG	1.93	0.49
7:G:71:ARG:HH22	8:H:60:ASP:CG	2.15	0.49
2:O:95:LYS:NZ	9:V:34:VAL:HG22	2.26	0.49
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.94	0.49
3:C:15:ASN:C	3:C:17:ALA:H	2.15	0.49
5:R:25:SER:HA	22:R:4016:HOH:O	2.12	0.49
1:A:158:PHE:O	1:A:164:ALA:HB2	2.12	0.49
2:B:71:LEU:CD2	9:I:68:VAL:HG21	2.38	0.49
3:C:129:MET:HE2	3:C:181:PHE:HD2	1.78	0.49
5:R:90:LYS:HE3	5:R:93:GLY:O	2.12	0.49
1:A:140:GLU:HB3	9:I:48:SER:O	2.12	0.49
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.12	0.49
5:E:71:MET:O	5:E:72:SER:CB	2.60	0.49
3:C:80:ARG:C	3:C:80:ARG:HD3	2.33	0.49
3:P:378:LYS:HE3	6:S:17:ARG:HD3	1.95	0.49
2:B:246:GLU:O	2:B:427:SER:HA	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:56:TYR:O	7:G:60:THR:HG23	2.12	0.49
10:W:16:ARG:NH1	10:W:19:THR:HG21	2.25	0.49
7:G:32:LYS:C	7:G:35:PRO:HD2	2.32	0.49
4:D:234:LYS:HE2	5:E:10:PHE:CE1	2.48	0.49
18:P:3003:CDL:H721	18:P:3003:CDL:H511	1.95	0.49
2:O:215:VAL:HG23	2:O:216:LEU:N	2.28	0.48
5:E:102:THR:O	5:E:106:ILE:HG13	2.12	0.48
2:O:39:GLU:OE2	2:O:41:TYR:N	2.44	0.48
1:N:408:ARG:HD2	22:N:522:HOH:O	2.12	0.48
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.96	0.48
4:D:165:TYR:HA	4:D:179:MET:CE	2.44	0.48
3:P:29:SER:HB3	18:P:3003:CDL:H722	1.94	0.48
1:A:281:ASP:OD2	9:I:73:PRO:HG3	2.13	0.48
4:Q:124:GLU:OE2	4:Q:191:ARG:CD	2.62	0.48
9:V:32:ALA:HB1	22:V:1505:HOH:O	2.13	0.48
6:F:72:GLN:HA	6:F:72:GLN:OE1	2.14	0.48
2:B:297:GLN:O	2:B:301:LYS:HG3	2.14	0.48
1:N:76:GLU:HG2	1:N:80:GLU:OE2	2.14	0.48
1:A:76:GLU:HG2	1:A:80:GLU:OE2	2.13	0.48
3:C:191:ALA:HA	3:C:194:MET:CE	2.43	0.47
3:C:217:LYS:HE3	22:C:4101:HOH:O	2.14	0.47
1:N:366:VAL:HG23	1:N:367:SER:N	2.28	0.47
6:S:100:GLU:HB3	11:S:2011:BHG:H62	1.94	0.47
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.44	0.47
4:D:124:GLU:OE2	4:D:191:ARG:HD3	2.13	0.47
3:C:27:ILE:HD12	20:C:2002:ANY:H3	1.96	0.47
3:C:63:PHE:O	3:C:67:THR:HG23	2.14	0.47
2:B:95:LYS:HE2	9:I:32:ALA:CA	2.45	0.47
2:O:187:THR:OG1	2:O:190:GLU:HG3	2.14	0.47
3:C:120:LEU:O	3:C:124:MET:HG3	2.13	0.47
2:O:279:LEU:HA	2:O:294:SER:HB3	1.97	0.47
5:E:62:MET:HG2	22:P:3114:HOH:O	2.14	0.47
7:T:39:ARG:HH11	7:T:39:ARG:HG2	1.79	0.47
2:O:95:LYS:NZ	9:V:34:VAL:CG2	2.78	0.47
5:R:77:LYS:HA	5:R:192:MET:HG2	1.96	0.47
7:G:39:ARG:HG2	7:G:39:ARG:HH11	1.78	0.47
1:A:102:LEU:CD2	2:B:369:LEU:HD12	2.45	0.47
10:W:62:LYS:HD2	10:W:62:LYS:C	2.35	0.47
9:I:72:VAL:HG13	9:I:73:PRO:CD	2.43	0.47
9:I:72:VAL:CG1	9:I:73:PRO:HD2	2.44	0.47
1:A:223:TYR:O	1:A:224:ASP:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:56:TYR:O	7:T:60:THR:HG23	2.14	0.47
3:P:156:ILE:HA	3:P:159:ASN:HD22	1.80	0.47
3:C:314:SER:O	3:C:318:ARG:HD3	2.14	0.47
2:B:250:ASP:HB3	22:B:2139:HOH:O	2.14	0.47
2:O:209:LEU:HD23	2:O:375:SER:HB2	1.96	0.47
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.14	0.47
2:O:241:GLY:HA2	2:O:423:SER:OG	2.14	0.47
1:A:11:VAL:HG21	1:A:392:LEU:HD12	1.97	0.47
1:N:250:LEU:HD13	1:N:305:GLN:HG3	1.98	0.47
5:R:44:THR:HG21	10:W:24:ILE:HG21	1.97	0.46
5:E:112:VAL:CG2	5:E:170:ARG:HH22	2.28	0.46
4:Q:165:TYR:HA	4:Q:179:MET:CE	2.44	0.46
10:W:20:PHE:CE1	10:W:24:ILE:HD11	2.51	0.46
1:A:213:GLN:O	1:A:217:SER:OG	2.25	0.46
6:S:72:GLN:OE1	6:S:72:GLN:HA	2.15	0.46
3:P:237:LEU:HD13	4:Q:212:MET:HG3	1.98	0.46
2:B:95:LYS:CE	9:I:32:ALA:N	2.76	0.46
5:E:160:CYS:HB3	17:P:3001:SMA:H4	1.95	0.46
1:N:29:GLN:O	2:O:18:PRO:HG3	2.15	0.46
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.64	0.46
1:N:206:ARG:HH11	1:N:206:ARG:HG3	1.80	0.46
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.96	0.46
2:O:305:GLN:N	2:O:305:GLN:C	2.68	0.46
2:B:187:THR:HB	22:B:2093:HOH:O	2.14	0.46
6:S:16:ILE:HG13	6:S:17:ARG:N	2.30	0.46
4:Q:124:GLU:OE2	4:Q:191:ARG:HD3	2.15	0.46
4:D:138:PRO:HG2	4:D:141:VAL:CG2	2.46	0.46
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.97	0.46
9:I:69:SER:HB2	22:I:1441:HOH:O	2.14	0.46
3:P:191:ALA:HA	3:P:194:MET:CE	2.46	0.46
1:A:195:MET:HE2	1:A:195:MET:HB3	1.79	0.46
1:N:224:ASP:OD2	1:N:227:ALA:N	2.49	0.46
3:P:120:LEU:O	3:P:124:MET:HG3	2.16	0.46
17:C:2001:SMA:H4	5:R:160:CYS:HB3	1.97	0.46
7:T:28:HIS:CG	7:T:32:LYS:HE2	2.51	0.46
3:P:348:ILE:O	3:P:352:GLN:HG3	2.16	0.46
3:C:379:TRP:CE3	6:F:33:ARG:HD3	2.50	0.45
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.63	0.45
1:A:373:THR:HB	1:A:374:PRO:HD3	1.96	0.45
2:O:71:LEU:CD2	9:V:68:VAL:HG21	2.44	0.45
1:A:366:VAL:HG23	1:A:367:SER:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:8:ARG:O	10:W:12:LEU:HB2	2.16	0.45
3:C:97:HIS:CD2	14:C:502:HEM:NC	2.83	0.45
3:C:43:LEU:HD11	3:C:82:MET:HE2	1.97	0.45
3:P:158:THR:HB	22:P:3127:HOH:O	2.17	0.45
3:C:345:HIS:NE2	11:C:4002:BHG:H3	2.32	0.45
4:Q:240:PRO:O	4:Q:241:LYS:HB2	2.16	0.45
1:A:29:GLN:HB3	2:B:12:GLU:O	2.17	0.45
4:Q:204:MET:HE3	19:Q:3006:PEE:C10	2.46	0.45
1:A:102:LEU:HD21	2:B:369:LEU:HD12	1.98	0.45
4:D:207:LYS:HZ2	19:D:2006:PEE:H11	1.81	0.45
7:G:28:HIS:CG	7:G:32:LYS:HE2	2.51	0.45
9:V:72:VAL:HG13	9:V:73:PRO:CD	2.46	0.45
6:S:49:ARG:HH22	11:S:2011:BHG:H4	1.81	0.45
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.80	0.45
5:R:52:LYS:HE3	10:W:32:GLU:OE2	2.17	0.45
6:S:13:LEU:H	6:S:13:LEU:CD2	2.07	0.45
2:O:102:ARG:HH22	2:O:161:GLU:CD	2.20	0.45
3:P:281:LEU:HD23	3:P:281:LEU:C	2.37	0.45
9:V:64:LEU:HB3	9:V:78:TYR:OXT	2.17	0.45
9:I:32:ALA:N	9:I:71:ASN:CB	2.79	0.45
2:O:109:VAL:HB	2:O:119:LEU:HD12	1.98	0.45
2:B:240:HIS:CE1	2:O:435:PHE:CD1	3.05	0.45
5:R:102:THR:O	5:R:106:ILE:HG13	2.17	0.45
3:P:129:MET:HE2	3:P:181:PHE:HD2	1.78	0.45
3:C:191:ALA:HA	3:C:194:MET:HE2	1.98	0.45
3:C:145:VAL:HG21	17:C:2001:SMA:H6	1.98	0.45
1:A:108:LYS:HE3	1:A:108:LYS:HA	1.99	0.44
1:A:206:ARG:HG3	1:A:206:ARG:NH1	2.31	0.44
2:B:241:GLY:HA2	2:B:423:SER:OG	2.17	0.44
3:C:141:TRP:CH2	5:R:145:VAL:HG23	2.52	0.44
3:C:281:LEU:HD23	3:C:281:LEU:C	2.37	0.44
3:P:327:ALA:HA	7:T:51:PRO:HB3	1.98	0.44
1:N:206:ARG:NH1	1:N:206:ARG:HG3	2.32	0.44
1:A:213:GLN:HG2	22:A:4063:HOH:O	2.16	0.44
2:O:246:GLU:O	2:O:427:SER:HA	2.17	0.44
2:B:160:ILE:HG22	22:B:2146:HOH:O	2.16	0.44
15:D:501:HEC:HMB1	15:D:501:HEC:HBB3	1.99	0.44
2:O:354:ASN:HB3	2:O:355:PRO:HD3	2.00	0.44
10:W:25:VAL:O	10:W:28:ALA:HB3	2.17	0.44
2:O:181:TYR:CE1	2:O:182:ARG:HG2	2.53	0.44
5:E:145:VAL:HG23	3:P:141:TRP:CH2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:124:GLU:OE2	4:D:191:ARG:CD	2.65	0.44
3:C:237:LEU:HD13	4:D:212:MET:HG3	1.99	0.44
3:P:197:LEU:CD1	20:P:3002:ANY:H12	2.48	0.44
1:N:431:LEU:HD12	1:N:432:PRO:HD2	1.99	0.44
4:Q:43:MET:CE	4:Q:91:PHE:HE2	2.31	0.44
7:G:71:ARG:NH2	8:H:60:ASP:OD1	2.50	0.44
3:P:145:VAL:HG21	17:P:3001:SMA:H6	1.99	0.44
3:P:191:ALA:HA	3:P:194:MET:HE2	1.99	0.44
1:N:103:SER:HB3	1:N:202:GLY:O	2.18	0.44
2:O:397:THR:O	2:O:401:GLN:HG3	2.18	0.44
2:B:437:ASP:OD2	2:O:240:HIS:CD2	2.71	0.43
1:A:15:GLN:NE2	2:B:12:GLU:HB2	2.33	0.43
3:C:100:ARG:C	3:C:100:ARG:HD2	2.37	0.43
4:Q:148:TYR:CD1	4:Q:148:TYR:N	2.86	0.43
2:B:218:GLN:O	2:B:222:GLN:HG3	2.18	0.43
5:E:77:LYS:HA	5:E:192:MET:HG2	1.99	0.43
1:A:195:MET:SD	1:A:219:LEU:HD21	2.58	0.43
1:A:223:TYR:O	1:A:224:ASP:CB	2.66	0.43
6:F:104:ARG:HH21	11:F:3011:BHG:H6'3	1.83	0.43
1:N:213:GLN:O	1:N:217:SER:OG	2.29	0.43
1:N:82:MET:CE	1:N:108:LYS:HG2	2.48	0.43
2:B:279:LEU:HA	2:B:294:SER:HB3	2.00	0.43
1:A:222:THR:O	1:A:223:TYR:CB	2.66	0.43
1:A:356:ARG:NH1	22:A:4058:HOH:O	2.51	0.43
3:P:21:LEU:HD13	22:P:3100:HOH:O	2.18	0.43
4:D:49:ARG:NH2	5:E:67:ASP:HB3	2.33	0.43
5:R:69:LEU:O	5:R:71:MET:HG3	2.18	0.43
1:N:8:LEU:HD22	1:N:392:LEU:HB3	2.01	0.43
2:B:299:VAL:HG12	2:B:303:VAL:HG11	1.98	0.43
5:E:90:LYS:HE2	5:E:93:GLY:HA2	2.00	0.43
2:O:305:GLN:N	2:O:306:PRO:CD	2.82	0.43
2:B:12:GLU:CG	2:B:17:VAL:N	2.82	0.43
5:R:16:PRO:HA	5:R:19:LEU:HD12	2.00	0.43
1:N:288:ALA:CB	1:N:300:THR:HG22	2.48	0.43
22:B:2146:HOH:O	9:I:64:LEU:CG	2.66	0.43
9:I:64:LEU:HB3	9:I:78:TYR:OXT	2.18	0.43
1:A:281:ASP:HA	1:A:305:GLN:O	2.18	0.42
9:V:34:VAL:O	9:V:34:VAL:HG23	2.19	0.42
1:A:149:VAL:CG1	22:A:4191:HOH:O	2.66	0.42
6:S:95:LYS:HB2	6:S:95:LYS:HZ3	1.82	0.42
4:D:145:GLU:HG2	11:D:4003:BHG:O3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:ILE:O	3:C:96:MET:HG2	2.19	0.42
1:A:187:SER:O	1:A:191:LYS:HD3	2.18	0.42
2:B:232:LEU:HB3	2:B:235:ALA:CB	2.49	0.42
1:A:288:ALA:CB	1:A:300:THR:HG22	2.48	0.42
10:W:1:VAL:O	10:W:2:ALA:HB2	2.19	0.42
6:F:40:ASN:O	6:F:44:LYS:HG3	2.19	0.42
5:E:122:HIS:HB3	5:E:125:GLU:HG3	2.02	0.42
8:H:31:VAL:HG23	8:H:32:LYS:N	2.33	0.42
2:B:305:GLN:NE2	2:B:305:GLN:HA	2.35	0.42
7:G:39:ARG:HG2	7:G:39:ARG:NH1	2.34	0.42
1:A:286:GLY:HA3	1:A:290:LEU:HD21	2.01	0.42
4:D:211:MET:HE1	10:J:31:PHE:CZ	2.54	0.42
3:P:217:LYS:HG3	7:T:7:LEU:HD13	2.01	0.42
4:D:175:THR:HG23	8:H:78:LYS:HE3	2.01	0.42
1:N:156:THR:HA	5:R:7:VAL:HG21	2.01	0.42
1:A:156:THR:HA	5:E:7:VAL:HG21	2.00	0.42
1:N:264:HIS:HA	1:N:265:PRO:HD3	1.81	0.42
3:P:92:ILE:O	3:P:96:MET:HG2	2.19	0.42
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.84	0.42
9:V:42:VAL:HG12	9:V:43:LEU:N	2.34	0.42
8:U:31:VAL:HG23	8:U:32:LYS:N	2.34	0.42
2:O:202:ALA:HB3	2:O:230:LEU:HA	2.01	0.42
1:A:42:ASP:O	1:A:194:ARG:CZ	2.68	0.42
4:D:203:ARG:HD2	19:D:2006:PEE:N	2.34	0.42
4:Q:43:MET:HE1	4:Q:91:PHE:HE2	1.85	0.42
7:G:33:GLY:O	7:G:37:VAL:HG23	2.20	0.42
2:O:371:SER:O	2:O:377:GLY:HA3	2.20	0.42
3:P:193:ALA:O	3:P:196:HIS:HB3	2.19	0.42
1:A:117:VAL:HG11	1:A:195:MET:CE	2.50	0.42
2:B:303:VAL:HG13	2:B:303:VAL:O	2.20	0.42
5:E:99:ARG:HB3	5:E:133:VAL:HG12	2.01	0.42
4:D:207:LYS:NZ	19:D:2006:PEE:H11	2.35	0.42
4:Q:43:MET:HE1	4:Q:189:PHE:HZ	1.83	0.42
2:B:57:TYR:HD1	2:B:233:SER:HA	1.85	0.42
3:P:147:THR:HG22	3:P:161:VAL:HG13	2.00	0.42
3:C:193:ALA:O	3:C:196:HIS:HB3	2.19	0.42
10:W:8:ARG:HG2	10:W:8:ARG:HH11	1.84	0.42
3:C:345:HIS:CD2	11:C:4002:BHG:H3	2.55	0.42
2:B:230:LEU:N	2:B:230:LEU:HD12	2.35	0.42
2:O:17:VAL:HA	2:O:18:PRO:HD3	1.78	0.42
5:E:77:LYS:HD3	5:E:80:ASP:OD1	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:72:VAL:CG1	9:V:73:PRO:HD2	2.48	0.41
1:N:117:VAL:HG11	1:N:216:PHE:HE2	1.85	0.41
5:E:77:LYS:HB2	5:E:192:MET:HE3	2.02	0.41
2:B:243:GLU:HA	2:B:424:MET:O	2.20	0.41
2:O:243:GLU:HA	2:O:424:MET:O	2.21	0.41
3:C:369:ALA:O	3:C:373:GLU:HG3	2.20	0.41
8:U:26:GLN:HA	8:U:26:GLN:OE1	2.19	0.41
8:H:25:GLU:HB2	8:H:34:ARG:NH2	2.20	0.41
2:B:200:THR:O	2:B:204:MET:HG3	2.20	0.41
4:Q:218:LEU:HB3	22:R:4057:HOH:O	2.19	0.41
6:S:49:ARG:NH2	11:S:2011:BHG:H4	2.35	0.41
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.83	0.41
2:B:371:SER:O	2:B:377:GLY:HA3	2.20	0.41
5:E:172:ARG:HH11	5:E:172:ARG:HB3	1.85	0.41
3:P:63:PHE:O	3:P:67:THR:HG23	2.21	0.41
5:R:34:GLY:HA3	10:W:10:TYR:HB2	1.97	0.41
1:N:117:VAL:HG11	1:N:216:PHE:CE2	2.56	0.41
2:B:229:GLY:C	2:B:230:LEU:HD12	2.41	0.41
5:E:87:MET:CG	5:E:89:PHE:CZ	3.03	0.41
5:R:122:HIS:HB3	5:R:125:GLU:HG3	2.01	0.41
1:N:187:SER:O	1:N:191:LYS:HD3	2.20	0.41
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.56	0.41
2:O:95:LYS:O	2:O:109:VAL:HA	2.20	0.41
9:I:62:ARG:CB	9:I:63:PRO:HD2	2.49	0.41
3:P:28:SER:HB2	18:T:3004:CDL:HA21	2.01	0.41
1:N:12:PRO:HG3	2:O:18:PRO:HA	2.02	0.41
4:Q:43:MET:CE	4:Q:91:PHE:CE2	3.04	0.41
4:Q:58:GLU:O	4:Q:62:LYS:HG3	2.21	0.41
3:P:377:LEU:HD11	22:P:3086:HOH:O	2.21	0.41
4:Q:43:MET:CE	4:Q:189:PHE:HZ	2.34	0.41
5:E:87:MET:HG2	5:E:89:PHE:CZ	2.56	0.41
9:I:36:ALA:HB3	9:I:73:PRO:CG	2.51	0.41
4:D:43:MET:HE1	4:D:91:PHE:HE2	1.85	0.41
2:O:124:LEU:HD13	2:O:223:PHE:CB	2.50	0.41
1:A:250:LEU:HD13	1:A:305:GLN:HG3	2.03	0.41
1:N:284:TYR:HE1	9:V:73:PRO:HG3	1.85	0.41
3:P:379:TRP:CE3	6:S:33:ARG:HD3	2.55	0.41
2:B:354:ASN:ND2	2:B:407:ASP:OD2	2.54	0.41
5:R:80:ASP:O	5:R:82:PRO:HD3	2.20	0.41
1:N:73:ASN:O	1:N:77:LYS:HG3	2.20	0.41
2:O:129:ALA:N	2:O:130:PRO:CD	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:ALA:HA	9:I:63:PRO:HD3	2.02	0.41
4:D:164:ILE:O	4:D:179:MET:HE2	2.21	0.41
4:Q:71:GLN:HG3	4:Q:82:MET:CE	2.51	0.41
1:N:264:HIS:ND1	1:N:265:PRO:HD2	2.36	0.41
3:C:348:ILE:O	3:C:352:GLN:HG3	2.20	0.41
4:Q:232:SER:O	5:R:10:PHE:HE1	2.04	0.41
7:T:39:ARG:HG2	7:T:39:ARG:NH1	2.35	0.40
10:W:26:VAL:O	10:W:30:PHE:HD1	2.04	0.40
5:E:128:LYS:HE3	5:E:185:TYR:O	2.21	0.40
1:A:15:GLN:HE21	2:B:12:GLU:HB2	1.86	0.40
3:P:159:ASN:ND2	22:P:3127:HOH:O	2.54	0.40
2:B:170:ASN:HD22	2:B:232:LEU:HD23	1.86	0.40
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.97	0.40
19:P:3007:PEE:H2	18:T:3004:CDL:OB3	2.21	0.40
2:B:109:VAL:HB	2:B:119:LEU:HD12	2.03	0.40
5:R:77:LYS:HB2	5:R:192:MET:HE3	2.02	0.40
2:B:242:GLY:O	2:B:423:SER:HA	2.21	0.40
2:B:365:LYS:HB3	2:B:399:LEU:HD22	2.03	0.40
1:A:106:LEU:O	1:A:110:VAL:HG23	2.20	0.40
1:N:307:PHE:CD1	1:N:307:PHE:C	2.94	0.40
1:N:121:SER:O	1:N:122:LEU:HB2	2.22	0.40
4:Q:49:ARG:NH2	5:R:67:ASP:HB3	2.36	0.40
2:B:95:LYS:HB2	9:I:32:ALA:HB2	2.02	0.40
2:B:120:MET:HE2	2:B:120:MET:HA	2.04	0.40
5:E:112:VAL:O	5:E:114:VAL:N	2.54	0.40
3:P:318:ARG:HB3	3:P:373:GLU:OE2	2.21	0.40
2:B:232:LEU:HB3	2:B:235:ALA:HB3	2.04	0.40
2:B:307:PHE:CD1	2:B:307:PHE:C	2.94	0.40
9:V:76:VAL:HG13	9:V:76:VAL:O	2.21	0.40
2:B:95:LYS:O	2:B:109:VAL:HA	2.21	0.40
1:A:224:ASP:OD2	1:A:226:ASP:OD1	2.40	0.40
1:N:146:ARG:O	1:N:149:VAL:HG12	2.21	0.40
3:P:27:ILE:HD12	20:P:3002:ANY:H3	2.03	0.40
3:P:75:TYR:CE2	11:R:4007:BHG:H61	2.56	0.40
4:Q:234:LYS:HD2	5:R:8:PRO:HB2	2.04	0.40
7:T:54:ALA:O	7:T:58:VAL:HG23	2.22	0.40
10:W:29:LEU:HD12	10:W:29:LEU:HA	1.86	0.40
10:W:53:LYS:HE3	10:W:53:LYS:HB2	1.90	0.40
5:E:181:GLU:HG2	5:E:182:VAL:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/446 (99%)	425 (97%)	11 (2%)	4 (1%)	21	15
1	N	440/446 (99%)	425 (97%)	11 (2%)	4 (1%)	21	15
2	B	418/439 (95%)	405 (97%)	10 (2%)	3 (1%)	26	21
2	O	419/439 (95%)	404 (96%)	13 (3%)	2 (0%)	34	30
3	C	363/379 (96%)	352 (97%)	9 (2%)	2 (1%)	30	24
3	P	363/379 (96%)	352 (97%)	10 (3%)	1 (0%)	46	45
4	D	239/241 (99%)	233 (98%)	6 (2%)	0	100	100
4	Q	239/241 (99%)	232 (97%)	7 (3%)	0	100	100
5	E	194/196 (99%)	181 (93%)	10 (5%)	3 (2%)	13	7
5	R	194/196 (99%)	183 (94%)	8 (4%)	3 (2%)	13	7
6	F	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
6	S	97/110 (88%)	94 (97%)	1 (1%)	2 (2%)	9	3
7	G	73/81 (90%)	70 (96%)	3 (4%)	0	100	100
7	T	74/81 (91%)	69 (93%)	5 (7%)	0	100	100
8	H	64/78 (82%)	63 (98%)	1 (2%)	0	100	100
8	U	64/78 (82%)	64 (100%)	0	0	100	100
9	I	39/78 (50%)	37 (95%)	1 (3%)	1 (3%)	7	2
9	V	39/78 (50%)	36 (92%)	2 (5%)	1 (3%)	7	2
10	J	30/62 (48%)	28 (93%)	2 (7%)	0	100	100
10	W	59/62 (95%)	54 (92%)	4 (7%)	1 (2%)	11	5
All	All	3945/4220 (94%)	3803 (96%)	115 (3%)	27 (1%)	26	21

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	19	ILE
5	E	71	MET
5	E	72	SER
9	I	41	PRO
1	N	224	ASP
2	O	171	ALA
2	O	303	VAL
3	P	19	ILE
5	R	191	ASP
9	V	41	PRO
2	B	171	ALA
2	B	229	GLY
5	E	113	GLU
5	R	189	SER
5	R	190	ASP
6	S	13	LEU
1	A	223	TYR
3	C	18	PHE
1	N	223	TYR
1	A	229	PRO
1	A	442	PHE
1	N	229	PRO
1	N	442	PHE
6	S	14	GLU
10	W	25	VAL
2	B	234	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/370 (98%)	355 (98%)	8 (2%)	60	64
1	N	363/370 (98%)	357 (98%)	6 (2%)	68	74
2	B	332/343 (97%)	332 (100%)	0	100	100
2	O	328/343 (96%)	328 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	312/327 (95%)	304 (97%)	8 (3%)	54	58
3	P	311/327 (95%)	303 (97%)	8 (3%)	54	58
4	D	206/206 (100%)	206 (100%)	0	100	100
4	Q	206/206 (100%)	204 (99%)	2 (1%)	82	87
5	E	165/168 (98%)	164 (99%)	1 (1%)	90	94
5	R	167/168 (99%)	164 (98%)	3 (2%)	66	72
6	F	90/98 (92%)	90 (100%)	0	100	100
6	S	90/98 (92%)	87 (97%)	3 (3%)	45	47
7	G	66/71 (93%)	66 (100%)	0	100	100
7	T	66/71 (93%)	66 (100%)	0	100	100
8	H	63/74 (85%)	63 (100%)	0	100	100
8	U	63/74 (85%)	61 (97%)	2 (3%)	46	48
9	I	27/60 (45%)	26 (96%)	1 (4%)	41	41
9	V	27/60 (45%)	26 (96%)	1 (4%)	41	41
10	J	27/52 (52%)	25 (93%)	2 (7%)	17	13
10	W	51/52 (98%)	49 (96%)	2 (4%)	39	39
All	All	3323/3538 (94%)	3276 (99%)	47 (1%)	74	80

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	PHE
1	A	203	LEU
1	A	210	ASP
1	A	245	GLU
1	A	281	ASP
1	A	305	GLN
1	A	316	ASP
1	A	348	SER
3	C	16	ASN
3	C	21	LEU
3	C	80	ARG
3	C	90	PHE
3	C	128	PHE
3	C	222	PRO
3	C	346	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	379	TRP
5	E	12	ASP
9	I	41	PRO
10	J	30	PHE
10	J	32	GLU
1	N	58	PHE
1	N	203	LEU
1	N	245	GLU
1	N	281	ASP
1	N	316	ASP
1	N	348	SER
3	P	16	ASN
3	P	21	LEU
3	P	80	ARG
3	P	90	PHE
3	P	128	PHE
3	P	222	PRO
3	P	346	PRO
3	P	379	TRP
4	Q	76	GLU
4	Q	169	LEU
5	R	12	ASP
5	R	113	GLU
5	R	191	ASP
6	S	13	LEU
6	S	33	ARG
6	S	58	ARG
8	U	42	GLU
8	U	78	LYS
9	V	41	PRO
10	W	29	LEU
10	W	62	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	136	GLN
1	A	165	GLN
1	A	213	GLN
1	A	271	GLN
1	A	289	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	305	GLN
2	B	22	GLN
2	B	104	ASN
2	B	240	HIS
2	B	305	GLN
2	B	412	ASN
3	C	16	ASN
3	C	159	ASN
3	C	201	HIS
3	C	341	GLN
5	E	57	GLN
6	F	79	GLN
9	I	71	ASN
1	N	136	GLN
1	N	165	GLN
1	N	215	HIS
1	N	271	GLN
1	N	311	ASN
2	O	104	ASN
2	O	218	GLN
2	O	240	HIS
2	O	412	ASN
3	P	16	ASN
3	P	159	ASN
3	P	201	HIS
4	Q	225	HIS
5	R	57	GLN
6	S	38	HIS
6	S	79	GLN
8	U	71	HIS
8	U	75	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

45 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	PO4	A	2013	-	4,4,4	0.69	0	6,6,6	0.30	0
11	BHG	A	4004	-	18,18,18	1.54	3 (16%)	23,23,23	0.67	0
12	AZI	A	4011	-	0,2,2	0.00	-	0,1,1	0.00	-
21	GOL	B	2009	-	5,5,5	1.13	0	5,5,5	0.59	0
17	SMA	C	2001	-	35,38,38	1.97	7 (20%)	40,52,52	1.55	4 (10%)
20	ANY	C	2002	-	38,38,41	1.81	10 (26%)	32,52,55	1.71	6 (18%)
12	AZI	C	2005	-	0,2,2	0.00	-	0,1,1	0.00	-
19	PEE	C	2007	-	48,48,50	1.16	5 (10%)	49,53,55	0.83	4 (8%)
21	GOL	C	2008	-	5,5,5	1.36	0	5,5,5	0.78	0
11	BHG	C	2010	-	18,18,18	1.74	4 (22%)	23,23,23	0.72	0
11	BHG	C	4002	-	18,18,18	1.80	4 (22%)	23,23,23	0.76	1 (4%)
21	GOL	C	4006	-	5,5,5	1.24	0	5,5,5	0.64	0
13	PO4	C	4008	-	4,4,4	0.72	0	6,6,6	0.30	0
14	HEM	C	501	3	30,50,50	2.62	11 (36%)	24,82,82	2.08	6 (25%)
14	HEM	C	502	3	30,50,50	2.62	9 (30%)	24,82,82	2.36	9 (37%)
18	CDL	D	2003	-	38,38,99	1.02	1 (2%)	41,47,111	0.99	2 (4%)
19	PEE	D	2006	-	25,25,50	1.48	6 (24%)	26,30,55	0.76	1 (3%)
11	BHG	D	4003	-	18,18,18	1.77	4 (22%)	23,23,23	0.74	0
15	HEC	D	501	4	24,50,50	1.88	4 (16%)	19,82,82	2.47	2 (10%)
16	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
13	PO4	F	2012	-	4,4,4	0.63	0	6,6,6	0.30	0
11	BHG	F	3011	-	18,18,18	1.73	4 (22%)	23,23,23	0.70	0
11	BHG	F	4001	-	18,18,18	1.78	4 (22%)	23,23,23	0.75	1 (4%)
18	CDL	G	2004	-	43,43,99	1.09	3 (6%)	45,55,111	1.25	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	AZI	G	4009	-	0,2,2	0.00	-	0,1,1	0.00	-
21	GOL	O	3009	-	5,5,5	1.08	0	5,5,5	0.52	0
12	AZI	O	4010	-	0,2,2	0.00	-	0,1,1	0.00	-
17	SMA	P	3001	-	35,38,38	1.97	8 (22%)	40,52,52	1.59	4 (10%)
20	ANY	P	3002	-	38,38,41	1.80	11 (28%)	32,52,55	1.58	7 (21%)
18	CDL	P	3003	-	38,38,99	0.99	1 (2%)	41,47,111	0.99	2 (4%)
12	AZI	P	3005	-	0,2,2	0.00	-	0,1,1	0.00	-
19	PEE	P	3007	-	48,48,50	1.17	5 (10%)	49,53,55	0.83	4 (8%)
21	GOL	P	3008	-	5,5,5	1.20	0	5,5,5	0.59	0
11	BHG	P	3010	-	18,18,18	1.75	5 (27%)	23,23,23	0.72	0
13	PO4	P	3013	-	4,4,4	0.70	0	6,6,6	0.29	0
14	HEM	P	501	3	30,50,50	2.87	10 (33%)	24,82,82	2.21	8 (33%)
14	HEM	P	502	3	30,50,50	2.95	10 (33%)	24,82,82	2.42	8 (33%)
19	PEE	Q	3006	-	50,50,50	1.21	6 (12%)	51,55,55	0.83	4 (7%)
15	HEC	Q	501	4	24,50,50	2.00	4 (16%)	19,82,82	2.56	2 (10%)
21	GOL	R	4005	-	5,5,5	1.22	0	5,5,5	0.60	0
11	BHG	R	4007	-	18,18,18	1.78	4 (22%)	23,23,23	0.72	0
16	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	BHG	S	2011	-	18,18,18	1.72	3 (16%)	23,23,23	0.74	0
13	PO4	S	3012	-	4,4,4	0.69	0	6,6,6	0.30	0
18	CDL	T	3004	-	48,48,99	1.11	4 (8%)	50,60,111	1.19	4 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PO4	A	2013	-	-	0/0/0/0	0/0/0/0
11	BHG	A	4004	-	1/1/5/5	0/9/29/29	0/1/1/1
12	AZI	A	4011	-	-	0/0/0/0	0/0/0/0
21	GOL	B	2009	-	-	0/4/4/4	0/0/0/0
17	SMA	C	2001	-	-	0/33/34/34	0/2/2/2
20	ANY	C	2002	-	-	0/35/52/56	0/1/2/2
12	AZI	C	2005	-	-	0/0/0/0	0/0/0/0
19	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
21	GOL	C	2008	-	-	0/4/4/4	0/0/0/0
11	BHG	C	2010	-	1/1/5/5	0/9/29/29	0/1/1/1
11	BHG	C	4002	-	1/1/5/5	0/9/29/29	0/1/1/1
21	GOL	C	4006	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PO4	C	4008	-	-	0/0/0/0	0/0/0/0
14	HEM	C	501	3	-	0/10/54/54	0/0/8/8
14	HEM	C	502	3	-	0/10/54/54	0/0/8/8
18	CDL	D	2003	-	-	0/43/43/110	0/0/0/0
19	PEE	D	2006	-	-	0/29/29/54	0/0/0/0
11	BHG	D	4003	-	1/1/5/5	0/9/29/29	0/1/1/1
15	HEC	D	501	4	-	0/6/54/54	0/0/8/8
16	FES	E	501	5	-	0/0/4/4	0/1/1/1
13	PO4	F	2012	-	-	0/0/0/0	0/0/0/0
11	BHG	F	3011	-	1/1/5/5	0/9/29/29	0/1/1/1
11	BHG	F	4001	-	1/1/5/5	0/9/29/29	0/1/1/1
18	CDL	G	2004	-	-	0/52/52/110	0/0/0/0
12	AZI	G	4009	-	-	0/0/0/0	0/0/0/0
21	GOL	O	3009	-	-	0/4/4/4	0/0/0/0
12	AZI	O	4010	-	-	0/0/0/0	0/0/0/0
17	SMA	P	3001	-	-	0/33/34/34	0/2/2/2
20	ANY	P	3002	-	1/1/10/13	0/35/52/56	0/1/2/2
18	CDL	P	3003	-	-	0/43/43/110	0/0/0/0
12	AZI	P	3005	-	-	0/0/0/0	0/0/0/0
19	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
21	GOL	P	3008	-	-	0/4/4/4	0/0/0/0
11	BHG	P	3010	-	1/1/5/5	0/9/29/29	0/1/1/1
13	PO4	P	3013	-	-	0/0/0/0	0/0/0/0
14	HEM	P	501	3	-	0/10/54/54	0/0/8/8
14	HEM	P	502	3	-	0/10/54/54	0/0/8/8
19	PEE	Q	3006	-	-	0/54/54/54	0/0/0/0
15	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
21	GOL	R	4005	-	-	0/4/4/4	0/0/0/0
11	BHG	R	4007	-	1/1/5/5	0/9/29/29	0/1/1/1
16	FES	R	501	5	-	0/0/4/4	0/1/1/1
11	BHG	S	2011	-	1/1/5/5	0/9/29/29	0/1/1/1
13	PO4	S	3012	-	-	0/0/0/0	0/0/0/0
18	CDL	T	3004	-	-	0/57/57/110	0/0/0/0

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	502	HEM	C3B-CAB	-7.00	1.38	1.51
14	P	501	HEM	C2D-C3D	-6.81	1.34	1.54
15	Q	501	HEC	C3C-C2C	-6.52	1.33	1.40
14	P	502	HEM	C3C-CAC	-6.45	1.39	1.51
14	P	501	HEM	C3B-CAB	-6.32	1.39	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	501	HEM	C3B-CAB	-6.24	1.39	1.51
14	P	502	HEM	C2D-C3D	-6.23	1.35	1.54
14	C	501	HEM	C2D-C3D	-6.17	1.36	1.54
14	C	501	HEM	C3C-CAC	-6.15	1.39	1.51
14	P	501	HEM	C3C-CAC	-6.14	1.39	1.51
14	P	502	HEM	C3B-C4B	-6.10	1.46	1.51
14	C	502	HEM	C3B-CAB	-5.84	1.40	1.51
15	Q	501	HEC	C3B-C2B	-5.66	1.34	1.40
14	P	501	HEM	C3B-C4B	-5.65	1.46	1.51
14	C	502	HEM	C3C-CAC	-5.60	1.40	1.51
14	C	502	HEM	C2D-C3D	-5.34	1.38	1.54
15	D	501	HEC	C3C-C2C	-4.90	1.35	1.40
15	D	501	HEC	C3B-C2B	-4.84	1.35	1.40
14	P	501	HEM	C2C-C1C	-3.83	1.45	1.52
14	C	501	HEM	C3B-C4B	-3.74	1.48	1.51
14	C	502	HEM	C3D-C4D	-3.66	1.46	1.51
14	C	502	HEM	C2C-C1C	-3.39	1.46	1.52
14	P	502	HEM	C3D-C4D	-3.33	1.47	1.51
14	C	502	HEM	C3B-C4B	-3.30	1.48	1.51
14	C	501	HEM	C2C-C1C	-3.08	1.46	1.52
19	Q	3006	PEE	C19-C18	-2.97	1.34	1.51
19	P	3007	PEE	C19-C18	-2.92	1.34	1.51
14	P	502	HEM	C2C-C1C	-2.91	1.47	1.52
19	Q	3006	PEE	C22-C21	-2.89	1.34	1.51
14	P	501	HEM	C3D-C4D	-2.88	1.47	1.51
19	C	2007	PEE	C22-C21	-2.87	1.34	1.51
19	C	2007	PEE	C19-C18	-2.87	1.35	1.51
19	P	3007	PEE	C22-C21	-2.85	1.35	1.51
14	C	501	HEM	C3D-C4D	-2.75	1.48	1.51
18	T	3004	CDL	OB8-CB6	-2.38	1.39	1.45
18	T	3004	CDL	OA8-CA6	-2.22	1.40	1.45
18	G	2004	CDL	OA8-CA6	-2.12	1.40	1.45
18	G	2004	CDL	OB8-CB6	-2.09	1.40	1.45
14	C	501	HEM	C2D-C1D	-2.07	1.45	1.51
17	P	3001	SMA	C6-C5	2.00	1.44	1.37
11	P	3010	BHG	C1-C2	2.02	1.58	1.52
11	P	3010	BHG	O5-C5	2.03	1.49	1.44
19	D	2006	PEE	C31-C30	2.04	1.56	1.50
19	Q	3006	PEE	C3-C2	2.05	1.56	1.50
11	C	2010	BHG	O5-C5	2.07	1.49	1.44
15	Q	501	HEC	C4B-NB	2.07	1.39	1.36
11	F	3011	BHG	O5-C5	2.08	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	P	3003	CDL	O1-C1	2.09	1.49	1.43
20	P	3002	ANY	C6-C1	2.10	1.45	1.41
11	F	4001	BHG	O5-C5	2.14	1.49	1.44
11	C	2010	BHG	C4-C5	2.14	1.57	1.53
17	C	2001	SMA	O1-C8A	2.16	1.40	1.36
20	C	2002	ANY	C7-N2	2.18	1.39	1.34
18	T	3004	CDL	CB3-CB4	2.19	1.56	1.50
18	D	2003	CDL	O1-C1	2.19	1.50	1.43
20	P	3002	ANY	C5-C6	2.19	1.43	1.39
11	D	4003	BHG	O5-C5	2.21	1.49	1.44
14	C	501	HEM	C4C-NC	2.22	1.38	1.36
14	C	501	HEM	C1C-NC	2.23	1.38	1.36
11	R	4007	BHG	O5-C5	2.23	1.49	1.44
11	S	2011	BHG	O5-C5	2.25	1.50	1.44
11	C	4002	BHG	O5-C5	2.25	1.50	1.44
20	C	2002	ANY	C5-C6	2.25	1.43	1.39
19	D	2006	PEE	C1-C2	2.27	1.57	1.50
18	G	2004	CDL	O1-C1	2.30	1.50	1.43
20	P	3002	ANY	O8-C21	2.30	1.39	1.34
20	P	3002	ANY	O5-C14	2.31	1.39	1.34
18	T	3004	CDL	O1-C1	2.33	1.50	1.43
19	C	2007	PEE	P-O1P	2.33	1.59	1.51
14	P	501	HEM	C4C-NC	2.34	1.38	1.36
11	D	4003	BHG	C4-C5	2.36	1.58	1.53
11	F	3011	BHG	C4-C5	2.37	1.58	1.53
17	P	3001	SMA	O1-C8A	2.42	1.40	1.36
11	F	4001	BHG	C4-C5	2.43	1.58	1.53
19	D	2006	PEE	C3-C2	2.51	1.57	1.50
11	R	4007	BHG	C4-C5	2.53	1.58	1.53
20	C	2002	ANY	C13-C12	2.55	1.58	1.53
11	P	3010	BHG	C4-C5	2.56	1.58	1.53
19	C	2007	PEE	O2-C10	2.57	1.42	1.34
15	Q	501	HEC	C3C-C4C	2.57	1.48	1.42
20	C	2002	ANY	O5-C14	2.58	1.40	1.34
20	C	2002	ANY	O8-C21	2.58	1.40	1.34
11	C	4002	BHG	C4-C5	2.59	1.58	1.53
19	D	2006	PEE	O3-C30	2.60	1.41	1.33
20	P	3002	ANY	C7-N2	2.63	1.40	1.34
19	Q	3006	PEE	O2-C10	2.67	1.42	1.34
20	P	3002	ANY	C10-C9	2.69	1.58	1.53
11	A	4004	BHG	C4-C5	2.69	1.58	1.53
19	D	2006	PEE	O2-C10	2.74	1.42	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	3007	PEE	O2-C10	2.75	1.42	1.34
19	P	3007	PEE	P-O1P	2.78	1.61	1.51
19	Q	3006	PEE	P-O1P	2.79	1.61	1.51
17	P	3001	SMA	C4A-C8A	2.80	1.44	1.41
19	D	2006	PEE	P-O1P	2.81	1.61	1.51
20	P	3002	ANY	C13-C12	2.88	1.59	1.53
19	P	3007	PEE	O3-C30	2.90	1.42	1.33
15	D	501	HEC	C1A-NA	2.91	1.40	1.36
15	D	501	HEC	C3C-C4C	2.92	1.49	1.42
19	Q	3006	PEE	O3-C30	2.95	1.42	1.33
17	C	2001	SMA	C6-C7	2.99	1.44	1.38
17	P	3001	SMA	C6-C7	3.00	1.44	1.38
17	C	2001	SMA	C4-C3	3.07	1.50	1.41
11	P	3010	BHG	O5-C1	3.07	1.49	1.41
11	A	4004	BHG	O5-C1	3.08	1.49	1.41
19	C	2007	PEE	O3-C30	3.08	1.42	1.33
14	P	502	HEM	C1C-NC	3.09	1.39	1.36
11	A	4004	BHG	O1-C1	3.16	1.45	1.40
11	C	2010	BHG	O5-C1	3.20	1.50	1.41
14	P	501	HEM	C1C-NC	3.21	1.40	1.36
17	P	3001	SMA	C7-C8	3.24	1.44	1.40
11	F	4001	BHG	O5-C1	3.25	1.50	1.41
11	C	4002	BHG	O5-C1	3.25	1.50	1.41
11	D	4003	BHG	O5-C1	3.30	1.50	1.41
11	R	4007	BHG	O5-C1	3.32	1.50	1.41
17	C	2001	SMA	C7-C8	3.33	1.44	1.40
20	P	3002	ANY	C3-C2	3.38	1.45	1.39
11	F	3011	BHG	O5-C1	3.39	1.50	1.41
11	S	2011	BHG	O5-C1	3.39	1.50	1.41
17	P	3001	SMA	C4-C3	3.40	1.51	1.41
20	C	2002	ANY	C3-C2	3.45	1.45	1.39
14	P	502	HEM	C4C-NC	3.47	1.40	1.36
20	C	2002	ANY	C10-C9	3.53	1.60	1.53
17	C	2001	SMA	C4A-C8A	3.75	1.46	1.41
20	P	3002	ANY	C2-C1	3.75	1.46	1.40
20	C	2002	ANY	C12-C11	3.81	1.60	1.52
20	P	3002	ANY	C12-C11	3.82	1.60	1.52
14	C	501	HEM	CBB-CAB	3.97	1.52	1.29
20	C	2002	ANY	C2-C1	4.01	1.47	1.40
14	C	502	HEM	CBB-CAB	4.09	1.52	1.29
20	C	2002	ANY	C8-N1	4.14	1.40	1.34
11	F	3011	BHG	O1-C1	4.29	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	502	HEM	CBC-CAC	4.31	1.54	1.29
11	P	3010	BHG	O1-C1	4.32	1.47	1.40
14	C	502	HEM	CBC-CAC	4.35	1.54	1.29
14	P	501	HEM	CBC-CAC	4.35	1.54	1.29
11	R	4007	BHG	O1-C1	4.44	1.48	1.40
11	C	2010	BHG	O1-C1	4.44	1.48	1.40
11	F	4001	BHG	O1-C1	4.48	1.48	1.40
11	D	4003	BHG	O1-C1	4.53	1.48	1.40
11	S	2011	BHG	O1-C1	4.58	1.48	1.40
11	C	4002	BHG	O1-C1	4.58	1.48	1.40
14	C	502	HEM	C1C-NC	4.60	1.41	1.36
14	C	501	HEM	CBC-CAC	4.62	1.56	1.29
14	P	501	HEM	CBB-CAB	4.70	1.56	1.29
14	P	502	HEM	CBB-CAB	4.75	1.56	1.29
17	C	2001	SMA	O1-C2	4.77	1.40	1.35
20	P	3002	ANY	C8-N1	4.78	1.40	1.34
17	P	3001	SMA	O1-C2	4.85	1.41	1.35
17	C	2001	SMA	C4-C4A	6.50	1.50	1.41
17	P	3001	SMA	C4-C4A	6.70	1.50	1.41

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	501	HEC	CBB-CAB-C3B	-8.59	108.25	127.35
15	D	501	HEC	CBC-CAC-C3C	-7.34	111.05	127.35
15	D	501	HEC	CBB-CAB-C3B	-7.16	111.45	127.35
15	Q	501	HEC	CBC-CAC-C3C	-5.89	114.27	127.35
17	P	3001	SMA	C9-C10-C11	-5.17	108.65	114.75
17	C	2001	SMA	C3-C4-C4A	-4.73	114.79	121.35
17	C	2001	SMA	C9-C10-C11	-4.68	109.23	114.75
17	P	3001	SMA	C3-C4-C4A	-4.40	115.25	121.35
18	T	3004	CDL	CB4-OB6-CB5	-4.29	109.82	117.92
18	G	2004	CDL	CB4-OB6-CB5	-3.79	110.77	117.92
20	C	2002	ANY	O5-C14-O6	-3.42	119.58	124.19
20	P	3002	ANY	O5-C14-O6	-3.34	119.69	124.19
20	C	2002	ANY	O2-C8-N1	-3.26	121.82	125.84
20	P	3002	ANY	O2-C8-N1	-3.12	121.99	125.84
18	T	3004	CDL	CA4-OA6-CA5	-3.11	110.42	117.89
18	G	2004	CDL	CA4-OA6-CA5	-2.85	111.06	117.89
18	G	2004	CDL	CA6-CA4-CA3	-2.81	105.50	112.07
18	P	3003	CDL	CB6-CB4-CB3	-2.73	105.68	112.07
18	D	2003	CDL	CB4-OB6-CB5	-2.69	111.44	117.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	2003	CDL	CB6-CB4-CB3	-2.64	105.89	112.07
18	P	3003	CDL	CB4-OB6-CB5	-2.50	111.90	117.89
18	G	2004	CDL	CB6-CB4-CB3	-2.40	106.47	112.07
14	P	501	HEM	CAA-C2A-C1A	-2.38	124.42	127.01
20	P	3002	ANY	O4-C20-O7	-2.30	121.09	124.19
18	T	3004	CDL	CB6-OB8-CB7	-2.20	111.57	117.14
18	G	2004	CDL	CB6-OB8-CB7	-2.13	111.76	117.14
18	T	3004	CDL	CA6-CA4-CA3	-2.10	107.15	112.07
20	C	2002	ANY	O8-C21-O9	-2.05	119.67	123.89
20	P	3002	ANY	O8-C21-O9	-2.02	119.72	123.89
11	F	4001	BHG	O1-C1-C2	2.01	110.58	108.04
17	P	3001	SMA	C4-C3-C2	2.05	120.71	117.73
19	D	2006	PEE	O3-C3-C2	2.06	114.22	108.69
11	C	4002	BHG	C1'-O1-C1	2.08	117.58	113.94
14	C	502	HEM	C2C-C1C-CHC	2.16	126.96	123.68
19	Q	3006	PEE	C23-C22-C21	2.17	125.74	114.53
14	C	502	HEM	C3C-CAC-CBC	2.25	127.90	124.46
14	P	502	HEM	C2C-C1C-CHC	2.26	127.12	123.68
19	C	2007	PEE	C22-C21-C20	2.28	126.32	114.53
19	P	3007	PEE	C22-C21-C20	2.31	126.44	114.53
17	C	2001	SMA	C4-C3-C2	2.38	121.19	117.73
20	C	2002	ANY	C25-C22-C21	2.42	119.39	111.03
19	Q	3006	PEE	C19-C18-C17	2.43	127.07	114.53
19	Q	3006	PEE	C22-C21-C20	2.48	127.32	114.53
20	P	3002	ANY	C25-C22-C23	2.48	123.05	111.90
14	C	501	HEM	CMD-C2D-C3D	2.51	125.46	114.35
14	P	501	HEM	CMD-C2D-C3D	2.51	125.47	114.35
19	P	3007	PEE	C23-C22-C21	2.55	127.67	114.53
19	P	3007	PEE	C20-C19-C18	2.55	127.72	114.53
19	C	2007	PEE	C23-C22-C21	2.56	127.74	114.53
19	C	2007	PEE	C20-C19-C18	2.57	127.78	114.53
19	C	2007	PEE	C19-C18-C17	2.58	127.86	114.53
19	P	3007	PEE	C19-C18-C17	2.60	127.97	114.53
14	P	501	HEM	C3C-CAC-CBC	2.67	128.55	124.46
19	Q	3006	PEE	C20-C19-C18	2.70	128.49	114.53
14	C	501	HEM	C2D-C3D-C4D	2.86	106.34	101.50
14	C	502	HEM	C2D-C3D-C4D	2.91	106.43	101.50
20	C	2002	ANY	O7-C20-C9	2.92	130.19	125.20
20	P	3002	ANY	O7-C20-C9	3.02	130.37	125.20
14	P	502	HEM	C3C-CAC-CBC	3.04	129.12	124.46
14	P	501	HEM	C2D-C3D-C4D	3.07	106.70	101.50
14	P	502	HEM	CMD-C2D-C3D	3.07	127.91	114.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	502	HEM	CMD-C2D-C3D	3.18	128.40	114.35
20	P	3002	ANY	C23-C22-C21	3.48	123.05	111.03
14	P	502	HEM	C3B-CAB-CBB	3.59	129.96	124.46
14	P	502	HEM	CAD-C3D-C4D	3.69	125.48	112.47
14	C	502	HEM	C3B-CAB-CBB	3.80	130.28	124.46
14	C	502	HEM	CAD-C3D-C4D	3.85	126.05	112.47
14	P	501	HEM	CAD-C3D-C4D	4.14	127.06	112.47
14	C	502	HEM	CMC-C2C-C3C	4.25	127.14	116.53
14	C	501	HEM	CMC-C2C-C3C	4.28	127.21	116.53
14	P	502	HEM	CMC-C2C-C3C	4.29	127.25	116.53
14	P	501	HEM	CMC-C2C-C3C	4.30	127.27	116.53
14	C	501	HEM	CAD-C3D-C2D	4.36	125.75	113.22
14	C	501	HEM	CAD-C3D-C4D	4.38	127.91	112.47
14	C	501	HEM	CMB-C2B-C3B	4.40	127.50	116.53
14	P	501	HEM	CAD-C3D-C2D	4.53	126.25	113.22
20	C	2002	ANY	C25-C22-C23	4.71	133.03	111.90
14	C	502	HEM	CMB-C2B-C3B	4.78	128.46	116.53
14	P	502	HEM	CMB-C2B-C3B	4.86	128.65	116.53
14	P	501	HEM	CMB-C2B-C3B	4.89	128.73	116.53
14	C	502	HEM	CAD-C3D-C2D	4.91	127.34	113.22
17	C	2001	SMA	C9-C2-C3	5.29	127.53	120.56
14	P	502	HEM	CAD-C3D-C2D	5.74	129.72	113.22
17	P	3001	SMA	C9-C2-C3	5.85	128.27	120.56

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	D	4003	BHG	C4
11	P	3010	BHG	C4
11	S	2011	BHG	C4
20	P	3002	ANY	C22
11	A	4004	BHG	C4
11	F	3011	BHG	C4
11	F	4001	BHG	C4
11	C	4002	BHG	C4
11	C	2010	BHG	C4
11	R	4007	BHG	C4

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	C	2001	SMA	2	0
20	C	2002	ANY	1	0
21	C	2008	GOL	1	0
11	C	4002	BHG	2	0
14	C	501	HEM	1	0
14	C	502	HEM	2	0
19	D	2006	PEE	3	0
11	D	4003	BHG	3	0
15	D	501	HEC	3	0
11	F	3011	BHG	2	0
11	F	4001	BHG	1	0
17	P	3001	SMA	2	0
20	P	3002	ANY	2	0
18	P	3003	CDL	2	0
19	P	3007	PEE	1	0
14	P	501	HEM	1	0
14	P	502	HEM	1	0
19	Q	3006	PEE	3	0
15	Q	501	HEC	1	0
21	R	4005	GOL	1	0
11	R	4007	BHG	1	0
11	S	2011	BHG	3	0
18	T	3004	CDL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/446 (99%)	0.34	10 (2%) 64 70	25, 39, 60, 115	0
1	N	441/446 (98%)	0.47	25 (5%) 27 35	33, 52, 76, 139	1 (0%)
2	B	424/439 (96%)	0.27	9 (2%) 67 72	29, 42, 66, 94	0
2	O	424/439 (96%)	0.32	15 (3%) 48 57	30, 47, 70, 124	0
3	C	365/379 (96%)	0.06	3 (0%) 87 90	23, 36, 53, 108	0
3	P	365/379 (96%)	0.08	4 (1%) 82 86	29, 39, 53, 106	0
4	D	241/241 (100%)	0.08	1 (0%) 93 94	31, 44, 64, 82	0
4	Q	241/241 (100%)	0.16	3 (1%) 81 85	35, 48, 67, 89	0
5	E	196/196 (100%)	1.13	43 (21%) 1 1	35, 62, 106, 111	0
5	R	196/196 (100%)	0.44	9 (4%) 36 45	34, 51, 77, 95	0
6	F	99/110 (90%)	0.09	1 (1%) 84 87	27, 40, 69, 79	0
6	S	99/110 (90%)	0.29	4 (4%) 42 51	33, 42, 80, 102	0
7	G	75/81 (92%)	0.61	8 (10%) 8 11	29, 53, 76, 89	0
7	T	76/81 (93%)	0.88	14 (18%) 2 2	37, 63, 93, 95	0
8	H	66/78 (84%)	0.39	2 (3%) 54 62	43, 59, 77, 81	0
8	U	66/78 (84%)	1.04	11 (16%) 2 3	50, 66, 89, 104	0
9	I	43/78 (55%)	1.72	15 (34%) 0 0	34, 65, 84, 89	0
9	V	43/78 (55%)	2.35	21 (48%) 0 0	38, 72, 86, 91	0
10	J	33/62 (53%)	1.13	5 (15%) 3 4	37, 54, 115, 130	0
10	W	62/62 (100%)	1.83	22 (35%) 0 0	44, 74, 129, 144	0
All	All	3997/4220 (94%)	0.40	225 (5%) 28 36	23, 45, 81, 144	1 (0%)

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	227	ALA	19.3
7	G	75	ALA	12.3
10	J	62	LYS	10.5
10	W	2	ALA	10.3
10	W	1	VAL	9.9
1	N	226	ASP	8.1
2	O	12	GLU	8.0
10	J	31	PHE	8.0
2	B	232	LEU	7.8
10	W	12	LEU	7.6
10	J	32	GLU	7.6
2	O	17	VAL	7.0
9	V	41	PRO	7.0
1	N	229	PRO	6.8
2	B	233	SER	6.4
10	J	30	PHE	6.1
5	E	187	PHE	6.1
1	N	2	ALA	6.0
7	T	76	ALA	6.0
9	V	36	ALA	5.9
10	W	25	VAL	5.8
10	W	5	LEU	5.8
9	V	33	ALA	5.7
5	E	104	LYS	5.7
5	E	83	GLU	5.7
1	A	2	ALA	5.6
2	B	12	GLU	5.6
7	T	1	GLY	5.5
9	V	78	TYR	5.5
1	N	222	THR	5.5
9	I	78	TYR	5.4
2	O	21	PRO	5.4
2	O	19	PRO	5.3
5	E	112	VAL	5.3
2	B	230	LEU	5.3
4	Q	241	LYS	5.2
3	C	16	ASN	5.2
10	W	62	LYS	5.1
10	W	3	PRO	5.1
5	E	76	ILE	5.0
5	E	78	LEU	5.0
1	N	225	GLU	5.0
1	N	228	VAL	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	132	TRP	4.9
5	R	27	GLU	4.8
1	A	225	GLU	4.8
9	V	38	SER	4.8
10	W	19	THR	4.7
7	T	30	PHE	4.7
5	E	107	ASP	4.6
5	E	194	ILE	4.6
10	W	21	ALA	4.6
1	N	365	LEU	4.6
5	E	192	MET	4.6
9	V	50	LEU	4.6
2	B	231	GLY	4.5
5	E	167	ALA	4.5
1	A	227	ALA	4.4
3	C	17	ALA	4.4
7	T	29	TYR	4.4
5	E	195	VAL	4.3
7	T	31	SER	4.3
5	E	80	ASP	4.3
5	E	84	GLY	4.2
10	W	13	LEU	4.2
8	U	51	GLU	4.2
9	I	63	PRO	4.1
5	E	127	VAL	4.1
9	V	63	PRO	4.1
1	A	223	TYR	4.0
10	W	9	LEU	4.0
1	A	226	ASP	4.0
4	Q	1	SER	4.0
5	E	103	LYS	4.0
10	W	14	PHE	4.0
1	A	222	THR	4.0
9	V	42	VAL	3.9
1	N	20	ASP	3.9
6	S	12	TRP	3.9
8	U	49	GLN	3.9
5	E	108	GLN	3.8
5	R	70	ALA	3.8
2	O	20	HIS	3.8
5	E	71	MET	3.8
8	U	47	ARG	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	101	ARG	3.7
9	I	50	LEU	3.7
9	V	48	SER	3.7
10	W	16	ARG	3.7
5	E	81	ILE	3.6
5	E	111	ALA	3.6
10	W	17	THR	3.6
9	I	37	THR	3.5
9	I	49	VAL	3.5
5	E	114	VAL	3.5
5	E	79	SER	3.5
10	W	20	PHE	3.4
2	O	233	SER	3.4
7	G	30	PHE	3.4
10	J	61	ASN	3.4
8	U	48	SER	3.3
9	V	54	SER	3.3
1	A	443	TRP	3.3
8	U	34	ARG	3.3
9	I	42	VAL	3.3
2	B	20	HIS	3.3
5	E	77	LYS	3.3
9	I	70	LEU	3.3
5	R	16	PRO	3.3
7	G	29	TYR	3.2
2	B	18	PRO	3.2
8	U	44	VAL	3.2
6	S	16	ILE	3.1
2	O	230	LEU	3.1
5	E	188	THR	3.1
9	I	62	ARG	3.1
5	E	110	ALA	3.1
5	E	186	GLU	3.1
5	R	29	SER	3.1
9	V	32	ALA	3.0
9	V	72	VAL	3.0
5	R	25	SER	3.0
8	U	71	HIS	3.0
9	V	37	THR	3.0
7	T	43	ALA	3.0
3	C	155	TYR	3.0
5	E	193	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	P	168	PHE	2.9
2	O	18	PRO	2.9
9	V	43	LEU	2.9
9	V	35	PRO	2.9
9	I	32	ALA	2.8
2	O	215	VAL	2.8
1	N	192	ALA	2.8
9	I	60	ALA	2.8
10	W	28	ALA	2.8
5	E	131	GLU	2.8
4	Q	144	ARG	2.7
3	P	16	ASN	2.7
10	W	6	THR	2.7
9	V	61	GLY	2.7
1	N	206	ARG	2.7
7	T	32	LYS	2.7
3	P	17	ALA	2.7
1	N	230	THR	2.7
5	E	100	HIS	2.7
1	N	224	ASP	2.6
5	E	133	VAL	2.6
10	W	7	ALA	2.6
10	W	8	ARG	2.6
2	B	17	VAL	2.6
5	E	49	TYR	2.6
5	E	106	ILE	2.6
4	D	3	LEU	2.6
7	G	43	ALA	2.6
9	V	57	GLY	2.6
7	T	33	GLY	2.6
5	E	116	GLN	2.6
6	S	14	GLU	2.5
3	P	330	ALA	2.5
1	N	219	LEU	2.5
7	G	1	GLY	2.5
1	N	213	GLN	2.5
9	V	62	ARG	2.4
7	T	73	ASN	2.4
1	N	66	GLY	2.4
1	A	262	TRP	2.4
5	E	191	ASP	2.4
7	T	28	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	U	67	HIS	2.4
5	R	75	GLU	2.4
9	V	51	CYS	2.3
5	R	33	LYS	2.3
9	I	48	SER	2.3
2	O	232	LEU	2.3
5	E	38	LEU	2.3
5	E	124	LEU	2.3
6	F	13	LEU	2.3
6	S	13	LEU	2.3
5	R	23	LYS	2.3
1	N	209	LEU	2.3
1	N	231	LEU	2.3
2	O	267	ALA	2.3
8	H	51	GLU	2.3
10	W	10	TYR	2.3
1	N	193	PRO	2.3
9	I	71	ASN	2.3
9	V	34	VAL	2.2
10	W	26	VAL	2.2
9	I	34	VAL	2.2
2	O	347	ILE	2.2
7	T	38	LEU	2.2
10	W	15	ARG	2.2
1	N	81	SER	2.2
1	N	187	SER	2.2
1	A	229	PRO	2.2
1	N	102	LEU	2.2
8	U	13	LEU	2.2
2	B	391	SER	2.2
2	O	249	GLY	2.2
9	I	61	GLY	2.2
5	E	134	ILE	2.2
5	E	154	GLY	2.1
5	E	155	GLY	2.1
5	R	35	PHE	2.1
5	E	68	VAL	2.1
9	V	49	VAL	2.1
7	T	74	PRO	2.1
7	G	34	ILE	2.1
9	I	73	PRO	2.1
2	O	362	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	T	34	ILE	2.1
8	H	34	ARG	2.1
1	N	15	GLN	2.1
1	N	16	VAL	2.1
5	E	113	GLU	2.1
2	O	388	ALA	2.1
7	G	68	LYS	2.1
1	N	216	PHE	2.1
7	G	64	GLN	2.0
8	U	26	GLN	2.0
1	A	286	GLY	2.0
8	U	62	LEU	2.0
5	E	130	PRO	2.0
7	T	44	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	BHG	C	2010	18/18	0.63	0.38	28.70	94,103,108,108	0
11	BHG	F	3011	18/18	0.57	0.43	21.70	108,113,116,116	0
11	BHG	S	2011	18/18	0.42	0.46	19.57	61,89,94,98	0
11	BHG	F	4001	18/18	0.14	0.72	18.45	146,154,157,158	0
21	GOL	C	2008	6/6	0.89	0.31	18.37	61,65,68,75	0
11	BHG	C	4002	18/18	0.55	0.51	11.09	114,122,125,125	0
11	BHG	P	3010	18/18	0.63	0.37	10.64	103,107,112,112	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	BHG	D	4003	18/18	0.28	0.70	7.86	160,169,171,171	0
12	AZI	A	4011	3/3	0.20	0.46	7.03	61,61,66,69	0
21	GOL	O	3009	6/6	0.56	0.65	6.64	82,84,85,85	0
21	GOL	B	2009	6/6	0.36	0.59	6.17	84,85,86,86	0
11	BHG	R	4007	18/18	0.65	0.34	5.87	85,95,98,99	0
19	PEE	D	2006	26/51	0.67	0.30	5.27	85,98,108,109	0
12	AZI	C	2005	3/3	0.67	0.19	5.26	54,54,56,58	0
12	AZI	G	4009	3/3	0.69	0.22	4.92	66,66,67,68	0
19	PEE	Q	3006	51/51	0.86	0.29	4.66	65,75,98,100	0
18	CDL	T	3004	49/100	0.91	0.23	4.26	74,89,107,107	0
18	CDL	G	2004	44/100	0.88	0.21	4.25	73,87,99,102	0
21	GOL	P	3008	6/6	0.82	0.15	3.11	67,69,71,71	0
19	PEE	P	3007	49/51	0.94	0.20	2.41	41,57,81,81	0
19	PEE	C	2007	49/51	0.95	0.18	2.34	35,55,81,83	0
16	FES	R	501	4/4	0.98	0.14	2.06	35,35,37,37	0
18	CDL	D	2003	39/100	0.79	0.18	1.61	53,78,93,94	0
21	GOL	R	4005	6/6	0.81	0.20	1.37	81,83,84,85	0
13	PO4	F	2012	5/5	0.95	0.12	1.27	81,82,83,84	0
20	ANY	P	3002	37/40	0.95	0.16	0.82	33,39,67,71	0
18	CDL	P	3003	39/100	0.84	0.19	0.80	61,89,111,111	0
17	SMA	P	3001	37/37	0.95	0.13	0.66	27,40,44,46	0
14	HEM	C	502	43/43	0.98	0.13	0.58	22,28,34,37	0
17	SMA	C	2001	37/37	0.96	0.13	0.46	31,39,44,48	0
16	FES	E	501	4/4	0.97	0.10	0.34	41,41,43,43	0
14	HEM	P	502	43/43	0.97	0.13	0.30	27,31,36,40	0
15	HEC	Q	501	43/43	0.97	0.12	0.20	38,45,48,51	0
11	BHG	A	4004	18/18	0.96	0.13	0.17	28,34,40,42	0
20	ANY	C	2002	37/40	0.95	0.14	0.09	31,39,65,70	0
12	AZI	P	3005	3/3	0.78	0.12	-0.04	51,51,54,56	0
14	HEM	C	501	43/43	0.97	0.12	-0.04	20,31,38,47	0
15	HEC	D	501	43/43	0.98	0.12	-0.09	35,41,44,45	0
14	HEM	P	501	43/43	0.98	0.12	-0.19	30,34,42,46	0
21	GOL	C	4006	6/6	0.62	0.52	-	96,98,99,100	0
13	PO4	A	2013	5/5	0.71	0.16	-	119,120,121,122	0
13	PO4	C	4008	5/5	0.76	0.17	-	153,153,153,153	0
12	AZI	O	4010	3/3	0.60	0.66	-	102,102,104,104	0
13	PO4	S	3012	5/5	0.93	0.15	-	97,97,99,100	0
13	PO4	P	3013	5/5	0.91	0.10	-	104,105,106,106	0

6.5 Other polymers ⓘ

There are no such residues in this entry.