



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:37 PM GMT

PDB ID : 1GGF  
Title : CRYSTAL STRUCTURE OF CATALASE HP11 FROM ESCHERICHIA COLI, VARIANT HIS128ASN, COMPLEX WITH HYDROGEN PEROXIDE.  
Authors : Melik-Adamyany, W.R.; Bravo, J.; Carpena, X.; Switala, J.; Mate, M.J.; Fita, I.; Loewen, P.C.  
Deposited on : 2000-08-21  
Resolution : 2.28 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](mailto: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

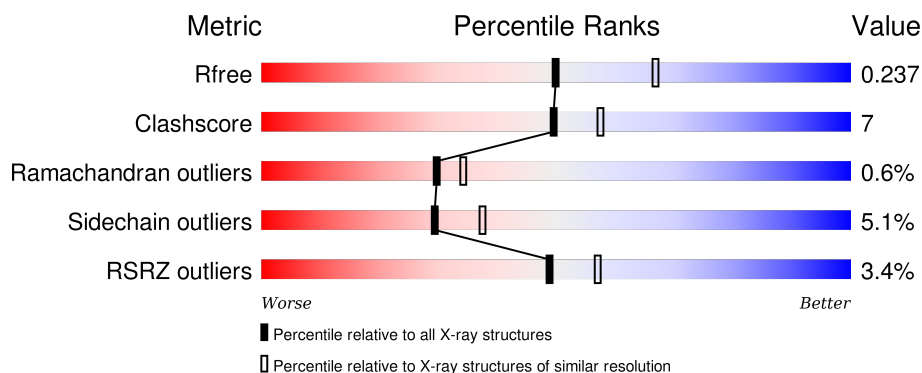
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

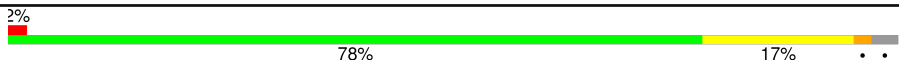



The reported resolution of this entry is 2.28 Å.

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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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  $\geq 3$ , 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	753	
1	B	753	
1	C	753	
1	D	753	

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
3	PEO	A	3001	-	-	-	X
3	PEO	A	3002	-	-	X	-
3	PEO	A	3003	-	-	X	-
3	PEO	B	4002	-	-	-	X
3	PEO	B	4003	-	-	-	X
3	PEO	D	3004	-	-	-	X
3	PEO	D	6001	-	-	-	X
3	PEO	D	6002	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25199 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 CATALASE HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5744	3645	1004	1083	12			
1	B	727	Total	C	N	O	S	0	0	0
			5744	3645	1004	1083	12			
1	C	727	Total	C	N	O	S	0	0	0
			5744	3645	1004	1083	12			
1	D	727	Total	C	N	O	S	0	0	0
			5744	3645	1004	1083	12			

There are 4 discrepancies between the modelled and reference sequences:

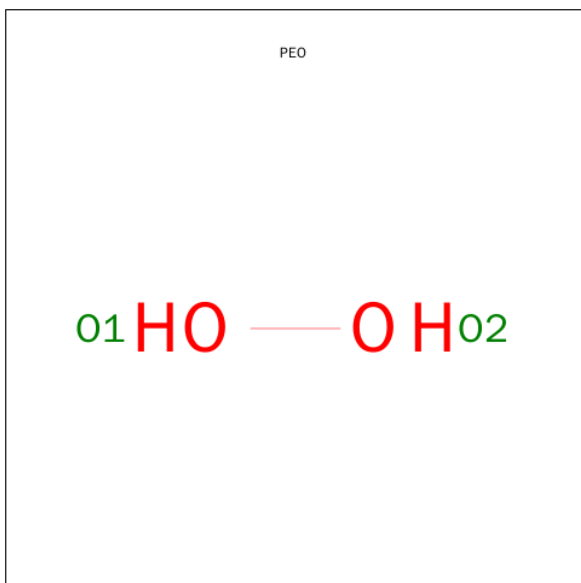
Chain	Residue	Modelled	Actual	Comment	Reference
A	128	ASN	HIS	ENGINEERED	UNP P21179
B	128	ASN	HIS	ENGINEERED	UNP P21179
C	128	ASN	HIS	ENGINEERED	UNP P21179
D	128	ASN	HIS	ENGINEERED	UNP P21179

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula:  $\text{H}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 2 2	0	0
3	A	1	Total O 2 2	0	0
3	A	1	Total O 2 2	0	0
3	D	1	Total O 2 2	0	0
3	B	1	Total O 2 2	0	0
3	B	1	Total O 2 2	0	0
3	B	1	Total O 2 2	0	0
3	C	1	Total O 2 2	0	0
3	C	1	Total O 2 2	0	0
3	C	1	Total O 2 2	0	0
3	D	1	Total O 2 2	0	0
3	D	1	Total O 2 2	0	0
3	D	1	Total O 2 2	0	0

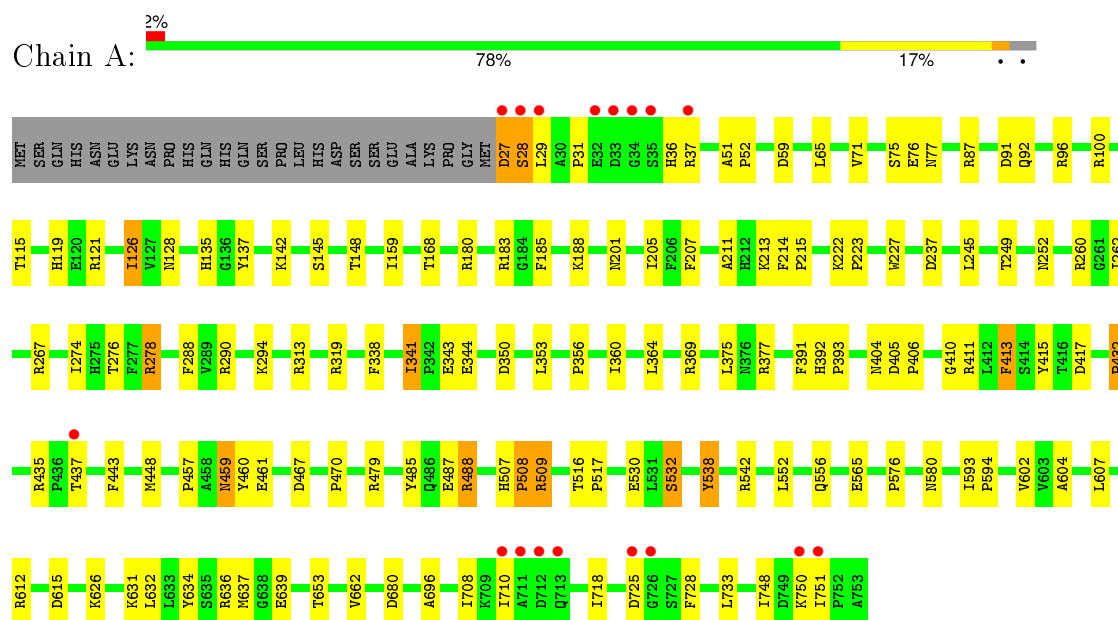
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	581	Total O 581 581	0	0
4	B	440	Total O 440 440	0	0
4	C	474	Total O 474 474	0	0
4	D	530	Total O 530 530	0	0

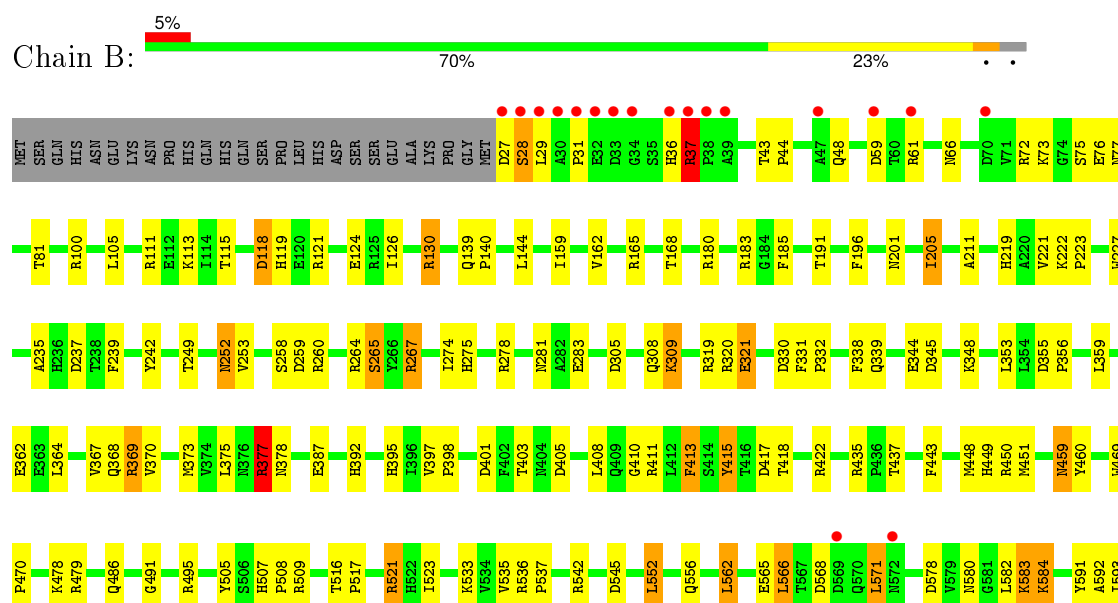
### 3 Residue-property plots

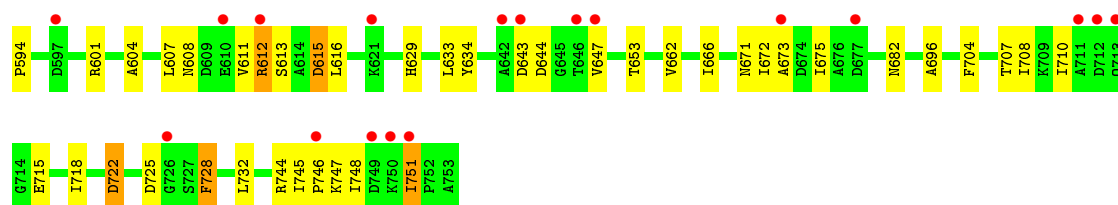
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: CATALASE HPII

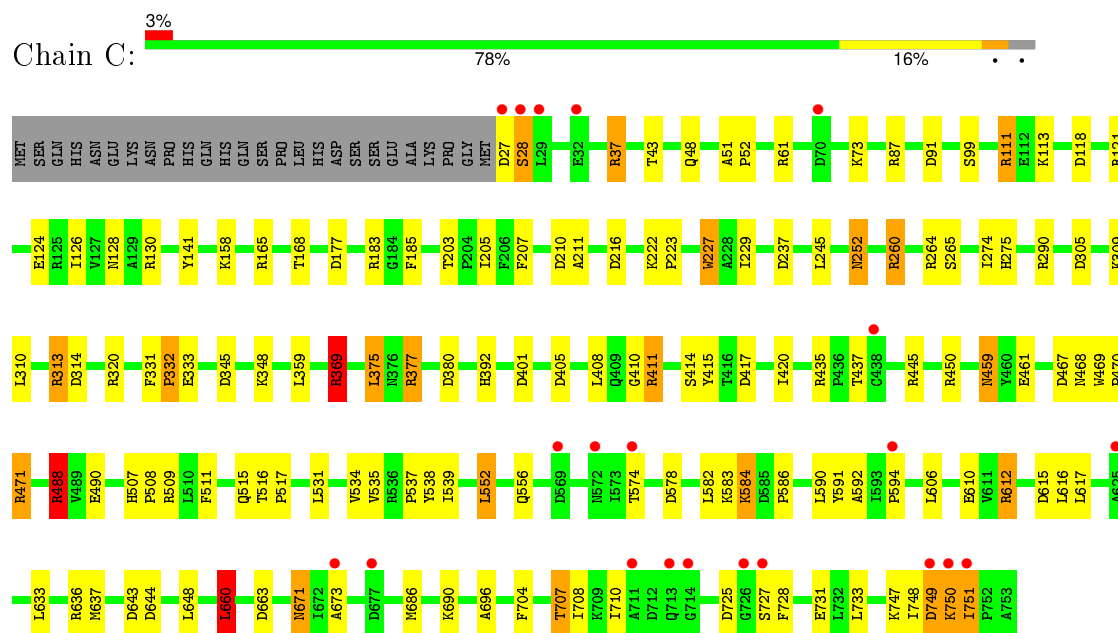


#### • Molecule 1: CATALASE HPII

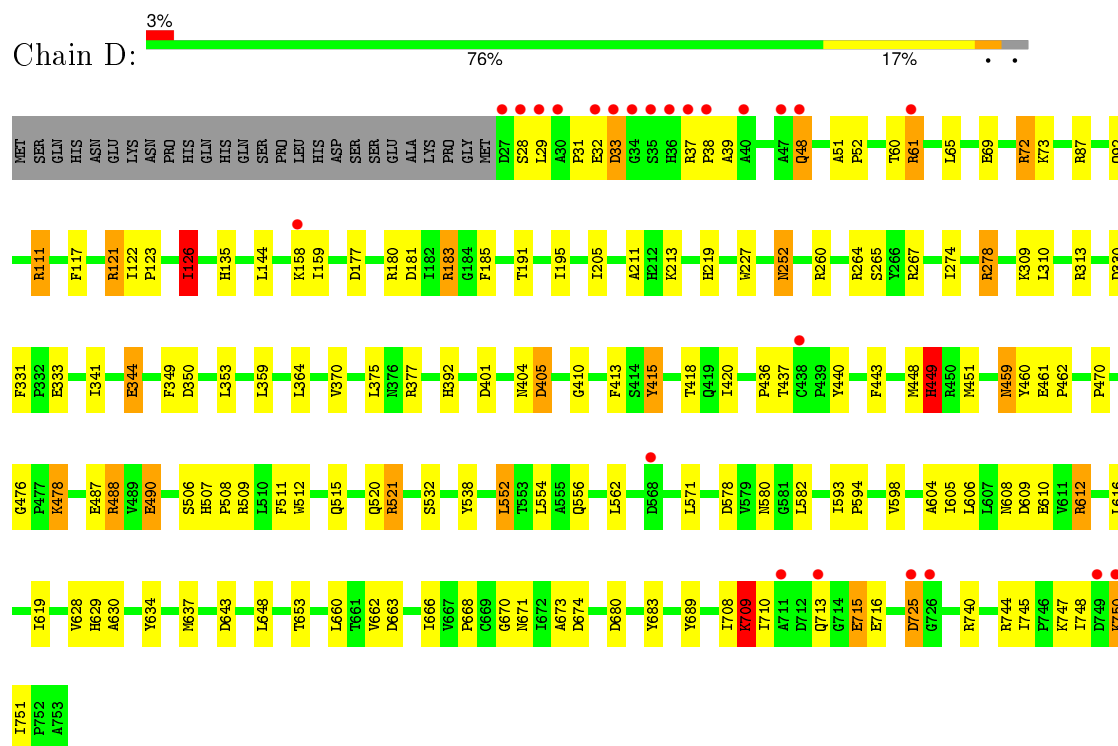




- Molecule 1: CATALASE HPII



- Molecule 1: CATALASE HP11





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.37Å 133.41Å 121.92Å 90.00° 109.63° 90.00°	Depositor
Resolution (Å)	87.95 – 2.28 19.84 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.3 (87.95-2.28) 98.5 (19.84-2.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.28Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.174 , 0.254 0.171 , 0.237	Depositor DCC
$R_{free}$ test set	6348 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.4	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 125885 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	25199	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: HEM, PEO

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	0.54	0/5899	1.31	33/8020 (0.4%)
1	B	0.52	0/5899	1.37	58/8020 (0.7%)
1	C	0.51	0/5899	1.32	42/8020 (0.5%)
1	D	0.53	0/5899	1.36	46/8020 (0.6%)
All	All	0.53	0/23596	1.34	179/32080 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ARG	NE-CZ-NH2	-15.91	112.34	120.30
1	D	488	ARG	NE-CZ-NH1	14.75	127.68	120.30
1	D	488	ARG	CD-NE-CZ	14.53	143.95	123.60
1	C	320	ARG	NE-CZ-NH2	-13.71	113.44	120.30
1	D	121	ARG	NE-CZ-NH1	12.75	126.67	120.30
1	B	377	ARG	NE-CZ-NH2	-12.61	113.99	120.30
1	D	87	ARG	NE-CZ-NH1	12.55	126.57	120.30
1	B	165	ARG	NE-CZ-NH2	12.40	126.50	120.30
1	B	377	ARG	NE-CZ-NH1	12.07	126.34	120.30
1	C	130	ARG	NE-CZ-NH2	-12.04	114.28	120.30
1	B	121	ARG	NE-CZ-NH1	11.94	126.27	120.30
1	B	37	ARG	CD-NE-CZ	11.75	140.05	123.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	260	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	D	377	ARG	NE-CZ-NH1	-11.28	114.66	120.30
1	C	435	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	B	495	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	D	61	ARG	NE-CZ-NH1	-10.80	114.90	120.30
1	D	740	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	A	260	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	B	130	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	B	165	ARG	NE-CZ-NH1	-10.09	115.26	120.30
1	C	121	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	C	445	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	D	449	HIS	CA-CB-CG	9.76	130.20	113.60
1	B	744	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	B	267	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	B	495	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	C	118	ASP	CB-CG-OD1	9.41	126.77	118.30
1	D	278	ARG	CD-NE-CZ	9.26	136.57	123.60
1	B	521	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	C	405	ASP	CB-CG-OD2	9.17	126.56	118.30
1	B	130	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	D	61	ARG	NE-CZ-NH2	8.90	124.75	120.30
1	B	521	ARG	CD-NE-CZ	8.87	136.01	123.60
1	A	479	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	C	320	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	B	320	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	C	121	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	D	121	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	C	165	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	C	435	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	B	401	ASP	CB-CG-OD1	-8.35	110.78	118.30
1	C	264	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	C	450	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	A	542	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	D	405	ASP	CB-CG-OD1	8.00	125.50	118.30
1	C	401	ASP	CB-CG-OD2	8.00	125.50	118.30
1	C	313	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	A	377	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	D	267	ARG	NE-CZ-NH1	-7.89	116.36	120.30
1	A	180	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	313	ARG	NE-CZ-NH2	7.86	124.23	120.30
1	C	509	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	C	509	ARG	NE-CZ-NH1	-7.80	116.40	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	ASP	CB-CG-OD1	7.74	125.26	118.30
1	C	369	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	B	369	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	D	260	ARG	NH1-CZ-NH2	7.62	127.78	119.40
1	D	488	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	A	37	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	B	509	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	A	479	ARG	CD-NE-CZ	7.56	134.18	123.60
1	D	183	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	A	488	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	C	177	ASP	CB-CG-OD1	-7.53	111.53	118.30
1	D	264	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	B	180	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	D	401	ASP	CB-CG-OD2	7.34	124.91	118.30
1	D	183	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	A	87	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	D	177	ASP	CB-CG-OD2	7.27	124.84	118.30
1	D	521	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	C	488	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	C	87	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	242	TYR	CB-CG-CD2	-7.06	116.76	121.00
1	D	111	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	509	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	B	744	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	417	ASP	N-CA-CB	-6.73	98.48	110.60
1	D	680	ASP	CB-CG-OD2	6.73	124.36	118.30
1	B	72	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	A	290	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	C	471	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	D	72	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	C	467	ASP	CB-CG-OD1	6.59	124.24	118.30
1	D	278	ARG	NE-CZ-NH1	-6.53	117.04	120.30
1	A	485	TYR	CB-CG-CD1	-6.52	117.09	121.00
1	B	259	ASP	CB-CG-OD2	6.47	124.13	118.30
1	D	709	LYS	CA-CB-CG	6.47	127.64	113.40
1	B	111	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	A	319	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	615	ASP	CB-CG-OD2	6.44	124.09	118.30
1	B	542	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	D	61	ARG	CD-NE-CZ	6.39	132.54	123.60
1	D	264	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	121	ARG	CD-NE-CZ	6.32	132.45	123.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	A	631	LYS	CA-CB-CG	6.14	126.90	113.40
1	A	278	ARG	NE-CZ-NH1	-6.11	117.24	120.30
1	A	350	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	A	538	TYR	CB-CG-CD2	6.07	124.64	121.00
1	B	479	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	601	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	D	725	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	B	545	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	278	ARG	CD-NE-CZ	5.98	131.97	123.60
1	B	417	ASP	N-CA-CB	-5.98	99.84	110.60
1	D	725	ASP	CB-CG-OD1	5.95	123.66	118.30
1	D	740	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	D	521	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	D	663	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	183	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	377	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	C	615	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	405	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	121	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	264	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	422	ARG	CA-CB-CG	5.59	125.71	113.40
1	B	435	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	636	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	D	506	SER	CB-CA-C	5.59	120.72	110.10
1	C	210	ASP	CB-CG-OD1	5.58	123.32	118.30
1	D	73	LYS	CA-CB-CG	5.55	125.61	113.40
1	A	680	ASP	CB-CG-OD2	5.53	123.27	118.30
1	B	37	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	D	260	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	615	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	422	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	C	111	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	C	660	LEU	CA-CB-CG	5.50	127.94	115.30
1	B	505	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	C	749	ASP	CB-CG-OD1	5.45	123.21	118.30
1	C	216	ASP	CB-CG-OD1	5.45	123.20	118.30
1	D	344	GLU	CB-CA-C	-5.42	99.55	110.40
1	A	100	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	319	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	578	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	411	ARG	NE-CZ-NH2	-5.41	117.60	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	267	ARG	NH1-CZ-NH2	5.40	125.34	119.40
1	C	177	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	242	TYR	CB-CG-CD1	5.35	124.21	121.00
1	B	387	GLU	OE1-CD-OE2	-5.35	116.88	123.30
1	A	377	ARG	CD-NE-CZ	5.33	131.07	123.60
1	A	485	TYR	CB-CG-CD2	5.33	124.20	121.00
1	B	495	ARG	CD-NE-CZ	5.33	131.07	123.60
1	B	479	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	542	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	126	ILE	CB-CG1-CD1	-5.30	99.06	113.90
1	A	37	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	403	THR	N-CA-CB	5.28	120.34	110.30
1	A	435	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	411	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	100	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	C	260	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	C	467	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	C	663	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	121	ARG	CD-NE-CZ	5.24	130.93	123.60
1	D	313	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	D	350	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	338	PHE	CB-CG-CD2	5.19	124.43	120.80
1	C	314	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	267	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	450	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	C	290	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	509	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	C	320	ARG	CD-NE-CZ	5.13	130.79	123.60
1	D	111	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	509	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	338	PHE	CB-CG-CD2	5.12	124.38	120.80
1	B	722	ASP	CA-CB-CG	-5.09	102.19	113.40
1	C	118	ASP	OD1-CG-OD2	-5.09	113.62	123.30
1	B	118	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	478	LYS	N-CA-CB	-5.05	101.50	110.60
1	C	203	THR	N-CA-CB	5.05	119.90	110.30
1	B	81	THR	CA-CB-CG2	5.05	119.47	112.40
1	B	267	ARG	NH1-CZ-NH2	5.05	124.95	119.40
1	B	260	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	D	715	GLU	CA-CB-CG	5.04	124.48	113.40
1	B	265	SER	N-CA-CB	-5.03	102.95	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	207	PHE	Mainchain

## 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	5744	0	5577	73	1
1	B	5744	0	5577	108	1
1	C	5744	0	5577	77	0
1	D	5744	0	5577	92	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
2	C	43	0	30	5	0
2	D	43	0	30	4	0
3	A	6	0	0	5	0
3	B	6	0	0	3	0
3	C	6	0	0	2	0
3	D	8	0	0	4	0
4	A	581	0	0	5	0
4	B	440	0	0	11	0
4	C	474	0	0	8	0
4	D	530	0	0	6	0
All	All	25199	0	22428	325	1

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 7.

All (325) 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)
3:C:5003:PEO:O2	3:C:5003:PEO:O1	1.53	1.27
3:A:3002:PEO:O1	3:A:3002:PEO:O2	1.53	1.26
3:C:5001:PEO:O1	3:C:5001:PEO:O2	1.52	1.26
3:A:3003:PEO:O2	3:A:3003:PEO:O1	1.53	1.25
3:D:6002:PEO:O1	3:D:6002:PEO:O2	1.52	1.25

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3004:PEO:O1	3:D:3004:PEO:O2	1.54	1.25
3:D:6003:PEO:O2	3:D:6003:PEO:O1	1.54	1.25
3:B:4003:PEO:O1	3:B:4003:PEO:O2	1.54	1.24
3:B:4002:PEO:O2	3:B:4002:PEO:O1	1.54	1.22
3:B:4001:PEO:O1	3:B:4001:PEO:O2	1.54	1.20
1:D:709:LYS:HG2	1:D:751:ILE:HD11	1.52	0.91
1:C:126:ILE:HD12	2:C:760:HEM:HMD1	1.51	0.90
1:D:39:ALA:H	1:D:48:GLN:HE21	1.20	0.89
1:D:39:ALA:H	1:D:48:GLN:NE2	1.74	0.85
1:A:710:ILE:HD13	1:A:718:ILE:HG13	1.63	0.80
1:D:126:ILE:HD11	2:D:760:HEM:HMD1	1.63	0.80
1:C:345:ASP:HA	1:C:348:LYS:HD3	1.64	0.78
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.66	0.77
1:B:345:ASP:HA	1:B:348:LYS:HD2	1.67	0.76
1:D:126:ILE:CD1	2:D:760:HEM:HMD1	2.17	0.75
1:C:584:LYS:HE3	1:C:586:PRO:HG3	1.68	0.75
1:A:457:PRO:HG2	1:C:37:ARG:NH2	2.01	0.74
1:D:126:ILE:HD12	1:D:126:ILE:H	1.54	0.73
1:B:451:MET:HG3	1:D:451:MET:HE1	1.71	0.71
1:B:29:LEU:HD13	1:C:245:LEU:HD13	1.73	0.71
1:C:490:GLU:HG3	1:D:490:GLU:HG3	1.71	0.70
1:B:583:LYS:O	1:B:584:LYS:HB3	1.92	0.69
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.73	0.69
1:D:710:ILE:HG23	1:D:715:GLU:HG2	1.74	0.69
1:A:639:GLU:HG3	4:A:3553:HOH:O	1.93	0.69
1:B:666:ILE:HG12	1:B:696:ALA:HB3	1.75	0.68
1:D:671:ASN:HD21	1:D:673:ALA:HB3	1.58	0.67
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.75	0.67
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.09	0.67
1:A:532:SER:HB2	1:D:637:MET:HG3	1.75	0.66
4:A:3560:HOH:O	1:C:28:SER:HA	1.94	0.66
1:A:96:ARG:HD3	4:A:3378:HOH:O	1.97	0.64
1:B:183:ARG:HG2	4:B:4287:HOH:O	1.97	0.64
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.80	0.64
1:B:222:LYS:HB3	1:B:223:PRO:HD2	1.80	0.64
1:D:32:GLU:O	1:D:33:ASP:HB3	1.98	0.63
1:B:281:ASN:OD1	1:B:283:GLU:HG2	1.98	0.62
1:B:413:PHE:CZ	1:C:111:ARG:HB2	2.34	0.62
1:B:583:LYS:HE2	1:B:583:LYS:H	1.63	0.62
1:D:180:ARG:O	1:D:181:ASP:HB2	1.98	0.62
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.83	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:GLN:HG3	1:B:159:ILE:HG12	1.83	0.61
1:B:556:GLN:HG2	1:B:566:LEU:CD2	2.31	0.61
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.85	0.60
1:D:126:ILE:HD12	1:D:126:ILE:N	2.14	0.60
1:D:689:TYR:HA	1:D:744:ARG:NH1	2.16	0.59
1:A:92:GLN:HA	1:D:213:LYS:HD3	1.83	0.59
1:C:696:ALA:HB1	1:C:728:PHE:CZ	2.39	0.57
1:B:275:HIS:CD2	1:B:408:LEU:HB2	2.39	0.57
1:B:604:ALA:HB2	1:B:662:VAL:HG11	1.85	0.57
1:B:36:HIS:NE2	1:B:37:ARG:NE	2.52	0.56
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.05	0.56
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.87	0.56
1:D:612:ARG:HA	1:D:643:ASP:OD2	2.05	0.56
1:A:341:ILE:HD11	1:A:360:ILE:HD13	1.86	0.56
1:C:43:THR:HG21	1:C:48:GLN:HG3	1.87	0.56
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.41	0.56
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.88	0.56
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.88	0.56
1:B:415:TYR:O	1:B:418:THR:HG22	2.06	0.56
1:B:634:TYR:O	1:B:653:THR:HA	2.06	0.55
1:A:637:MET:HG3	1:D:532:SER:HB2	1.89	0.55
1:A:748:ILE:O	1:A:751:ILE:HG13	2.07	0.55
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.89	0.55
1:D:183:ARG:HG2	4:D:6381:HOH:O	2.06	0.55
1:D:629:HIS:HD2	4:D:6324:HOH:O	1.90	0.54
1:D:745:ILE:O	1:D:748:ILE:HG12	2.07	0.54
1:A:294:LYS:NZ	4:A:3246:HOH:O	2.40	0.54
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.89	0.54
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.38	0.54
1:D:341:ILE:HD13	1:D:349:PHE:CZ	2.43	0.53
1:D:359:LEU:H	1:D:507:HIS:HD2	1.57	0.53
1:C:37:ARG:NH1	4:C:5406:HOH:O	2.41	0.52
1:D:488:ARG:NH2	4:D:6503:HOH:O	2.36	0.52
1:C:552:LEU:HD13	1:C:556:GLN:NE2	2.25	0.52
1:B:196:PHE:HA	1:B:395:HIS:O	2.09	0.52
1:C:124:GLU:HG2	4:C:5100:HOH:O	2.09	0.52
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.44	0.52
1:A:245:LEU:HD13	1:D:29:LEU:HD13	1.91	0.52
1:D:608:ASN:HD21	1:D:670:GLY:HA3	1.75	0.52
1:C:552:LEU:HD22	1:C:552:LEU:O	2.10	0.51
1:C:141:TYR:CD1	1:C:369:ARG:HG3	2.45	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LYS:HB3	1:C:223:PRO:CD	2.41	0.51
1:C:113:LYS:HD2	4:C:5215:HOH:O	2.10	0.51
1:D:619:ILE:HD13	1:D:666:ILE:HG21	1.92	0.51
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.91	0.51
1:D:61:ARG:HH12	1:D:72:ARG:HH12	1.57	0.51
1:B:359:LEU:H	1:B:507:HIS:HD2	1.58	0.51
1:A:457:PRO:HG2	1:C:37:ARG:HH21	1.72	0.50
1:C:310:LEU:HD13	1:C:660:LEU:HB3	1.93	0.50
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.93	0.50
1:C:345:ASP:O	1:C:348:LYS:HB2	2.11	0.50
1:D:69:GLU:OE2	1:D:72:ARG:NH1	2.43	0.50
1:C:671:ASN:HD21	1:C:673:ALA:HB3	1.75	0.50
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.91	0.50
1:A:65:LEU:HD21	1:A:135:HIS:CG	2.47	0.50
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.14	0.50
1:D:605:ILE:HD12	1:D:630:ALA:HB1	1.94	0.50
1:C:158:LYS:HD2	4:C:5466:HOH:O	2.12	0.49
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.47	0.49
1:D:476:GLY:HA3	4:D:6087:HOH:O	2.12	0.49
1:B:552:LEU:O	1:B:556:GLN:HG3	2.12	0.49
1:C:222:LYS:HB3	1:C:223:PRO:HD2	1.94	0.49
1:C:411:ARG:HG3	2:C:760:HEM:HMC3	1.95	0.49
1:D:604:ALA:HB2	1:D:662:VAL:HG11	1.93	0.49
2:C:760:HEM:HBC2	2:C:760:HEM:CMC	2.43	0.49
1:C:211:ALA:HB3	1:C:410:GLY:HA3	1.94	0.49
1:A:725:ASP:H	1:A:728:PHE:HB3	1.77	0.49
1:B:562:LEU:HA	1:C:637:MET:HB2	1.95	0.49
1:A:532:SER:HB2	1:D:637:MET:CG	2.43	0.49
1:B:222:LYS:HB3	1:B:223:PRO:CD	2.42	0.48
1:C:690:LYS:HE2	4:C:5271:HOH:O	2.12	0.48
1:B:73:LYS:HE3	1:D:440:TYR:O	2.13	0.48
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.94	0.48
1:D:364:LEU:HD11	1:D:580:ASN:HB2	1.93	0.48
1:D:126:ILE:CD1	1:D:126:ILE:H	2.21	0.48
1:B:718:ILE:HG12	4:B:4021:HOH:O	2.13	0.48
1:B:59:ASP:HA	1:B:61:ARG:CZ	2.44	0.48
4:A:3295:HOH:O	1:D:126:ILE:HG13	2.12	0.48
1:B:666:ILE:HD11	1:B:732:LEU:CD1	2.44	0.48
4:B:4182:HOH:O	1:D:52:PRO:HG3	2.13	0.48
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.61	0.48
1:C:158:LYS:HB3	4:C:5466:HOH:O	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:HIS:CG	1:B:408:LEU:HB2	2.49	0.48
1:B:43:THR:HG21	1:B:48:GLN:HG3	1.96	0.47
1:D:750:LYS:HD2	1:D:751:ILE:HG13	1.96	0.47
1:A:509:ARG:HD2	1:A:576:PRO:HD2	1.96	0.47
1:C:749:ASP:HB3	1:C:750:LYS:HE2	1.96	0.47
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.28	0.47
1:A:604:ALA:HB2	1:A:662:VAL:HG11	1.96	0.47
1:B:267:ARG:HG2	1:B:332:PRO:HB3	1.96	0.47
1:D:511:PHE:O	1:D:515:GLN:HG2	2.15	0.47
1:B:76:GLU:O	1:B:77:ASN:HB2	2.14	0.47
3:A:3001:PEO:O2	3:A:3002:PEO:O2	2.31	0.47
1:D:122:ILE:HB	1:D:123:PRO:HD2	1.97	0.47
1:C:612:ARG:HB2	1:C:612:ARG:CZ	2.45	0.47
1:B:535:VAL:O	1:B:537:PRO:HD3	2.15	0.47
1:D:598:VAL:HG22	1:D:628:VAL:HG22	1.97	0.47
1:A:516:THR:HB	1:A:517:PRO:HD2	1.97	0.47
1:D:60:THR:O	1:D:61:ARG:HD2	2.15	0.47
1:B:211:ALA:HB3	1:B:410:GLY:HA3	1.96	0.47
1:B:305:ASP:O	1:B:309:LYS:HB2	2.15	0.47
1:B:249:THR:O	1:B:253:VAL:HG23	2.15	0.47
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.96	0.47
1:C:275:HIS:CD2	1:C:408:LEU:HD13	2.49	0.47
1:C:260:ARG:HD3	1:C:590:LEU:HD21	1.95	0.47
1:B:748:ILE:O	1:B:751:ILE:HG22	2.15	0.47
1:A:36:HIS:H	1:A:36:HIS:CD2	2.33	0.46
1:B:344:GLU:H	1:B:344:GLU:CD	2.18	0.46
1:D:359:LEU:H	1:D:507:HIS:CD2	2.33	0.46
1:B:449:HIS:CD2	1:D:449:HIS:CD2	3.03	0.46
1:C:727:SER:O	1:C:731:GLU:HG3	2.14	0.46
1:B:258:SER:HA	1:B:523:ILE:HG12	1.97	0.46
1:B:191:THR:HB	4:B:4063:HOH:O	2.15	0.46
1:A:626:LYS:HG3	1:A:733:LEU:HD13	1.96	0.46
1:B:459:ASN:HD22	1:B:460:TYR:HD2	1.63	0.46
1:B:162:VAL:HG21	1:B:373:MET:SD	2.55	0.46
1:C:52:PRO:HB3	1:C:380:ASP:HA	1.97	0.46
1:C:583:LYS:O	1:C:584:LYS:HB3	2.15	0.46
1:B:309:LYS:HE2	4:B:4213:HOH:O	2.15	0.46
1:C:535:VAL:O	1:C:537:PRO:HD3	2.16	0.46
1:C:591:TYR:O	1:C:592:ALA:C	2.54	0.46
1:B:205:ILE:HB	1:B:356:PRO:O	2.16	0.46
1:B:44:PRO:HB3	1:B:629:HIS:CD2	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:HIS:CE1	1:C:420:ILE:HG21	2.52	0.46
1:B:118:ASP:OD1	1:C:417:ASP:OD2	2.34	0.45
1:C:332:PRO:HB2	1:C:375:LEU:HB2	1.97	0.45
1:B:364:LEU:HD11	1:B:580:ASN:HB2	1.98	0.45
1:D:65:LEU:HD21	1:D:135:HIS:CG	2.51	0.45
1:A:459:ASN:HD22	1:A:460:TYR:HD2	1.65	0.45
1:C:331:PHE:O	1:C:333:GLU:HG3	2.16	0.45
1:C:488:ARG:HB2	1:C:488:ARG:HE	1.54	0.45
1:C:643:ASP:OD1	1:C:644:ASP:N	2.50	0.45
1:B:448:MET:HG3	1:D:122:ILE:HG22	1.98	0.45
2:C:760:HEM:HBC2	2:C:760:HEM:HMC1	1.99	0.45
1:A:413:PHE:CZ	1:D:111:ARG:HB2	2.52	0.45
1:D:331:PHE:O	1:D:333:GLU:HG3	2.17	0.45
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.47	0.45
1:C:617:LEU:HD12	4:C:5419:HOH:O	2.16	0.45
1:D:606:LEU:O	1:D:668:PRO:HD2	2.17	0.45
1:C:748:ILE:O	1:C:751:ILE:HG23	2.17	0.45
1:D:126:ILE:HD13	2:D:760:HEM:HMD1	1.98	0.44
1:B:583:LYS:H	1:B:583:LYS:CE	2.30	0.44
1:B:486:GLN:OE1	4:B:4416:HOH:O	2.21	0.44
1:B:355:ASP:HA	1:B:356:PRO:HD2	1.92	0.44
2:B:760:HEM:CMC	2:B:760:HEM:HBC2	2.47	0.44
1:B:331:PHE:HA	1:B:332:PRO:HD3	1.85	0.44
1:B:309:LYS:HD2	1:C:313:ARG:NH2	2.32	0.44
1:D:415:TYR:O	1:D:418:THR:HG22	2.16	0.44
1:A:530:GLU:OE2	3:A:3003:PEO:O1	2.36	0.44
1:B:339:GLN:HG3	1:B:367:VAL:HG22	1.99	0.44
1:B:362:GLU:HG2	1:B:367:VAL:HG23	1.98	0.44
1:B:615:ASP:O	1:B:616:LEU:C	2.56	0.44
1:B:469:TRP:HA	1:B:470:PRO:C	2.38	0.44
1:B:449:HIS:HB2	1:D:449:HIS:CE1	2.53	0.44
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.47	0.44
1:A:29:LEU:HD12	1:C:468:ASN:HB2	2.00	0.44
1:A:27:ASP:HA	1:C:471:ARG:CZ	2.48	0.44
1:D:634:TYR:O	1:D:653:THR:HA	2.17	0.44
1:D:309:LYS:NZ	1:D:683:TYR:OH	2.50	0.44
1:A:364:LEU:HD11	1:A:580:ASN:HB2	1.98	0.44
1:D:512:TRP:CH2	1:D:520:GLN:HB3	2.53	0.44
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.21	0.44
1:D:404:ASN:O	1:D:405:ASP:C	2.56	0.43
1:C:490:GLU:HG3	1:D:490:GLU:CG	2.45	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:HIS:HD2	4:B:4242:HOH:O	2.00	0.43
1:C:751:ILE:O	1:C:751:ILE:HG12	2.17	0.43
1:D:195:ILE:HD11	1:D:436:PRO:HA	2.01	0.43
1:A:404:ASN:O	1:A:405:ASP:C	2.55	0.43
1:D:310:LEU:HD13	1:D:660:LEU:HB3	1.98	0.43
1:A:276:THR:CG2	1:A:288:PHE:HB3	2.49	0.43
1:A:207:PHE:O	1:A:249:THR:HA	2.19	0.43
1:B:115:THR:O	1:B:119:HIS:HD2	2.01	0.43
1:C:578:ASP:HB2	1:C:582:LEU:O	2.18	0.43
1:A:392:HIS:ND1	1:A:393:PRO:HD2	2.33	0.43
1:B:507:HIS:N	1:B:508:PRO:CD	2.81	0.43
1:D:158:LYS:HB2	1:D:158:LYS:HE3	1.92	0.43
1:B:397:VAL:HB	1:B:398:PRO:HD2	2.01	0.43
1:A:459:ASN:CG	1:B:219:HIS:HB3	2.39	0.43
1:A:71:VAL:HG21	1:A:432:PRO:HG2	2.01	0.43
1:C:305:ASP:O	1:C:309:LYS:HG3	2.18	0.43
1:A:115:THR:O	1:A:119:HIS:HD2	2.01	0.43
1:A:211:ALA:HB3	1:A:410:GLY:HA3	2.00	0.43
1:A:213:LYS:HD3	1:D:92:GLN:HA	2.00	0.43
1:B:593:ILE:HA	1:B:594:PRO:HD2	1.76	0.43
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.54	0.43
1:C:359:LEU:H	1:C:507:HIS:HD2	1.66	0.43
1:A:76:GLU:O	1:A:77:ASN:HB2	2.19	0.43
1:B:451:MET:SD	4:B:4438:HOH:O	2.62	0.43
1:C:686:MET:O	1:C:751:ILE:HD11	2.19	0.43
1:B:126:ILE:CG2	2:B:760:HEM:HMD1	2.49	0.43
1:C:227:TRP:CE3	1:C:229:ILE:HD12	2.54	0.43
1:B:31:PRO:HG3	1:C:538:TYR:CE2	2.53	0.43
1:A:145:SER:HA	1:A:148:THR:O	2.19	0.43
1:D:478:LYS:HE2	4:D:6481:HOH:O	2.19	0.43
3:D:6001:PEO:O2	3:D:6002:PEO:O2	2.37	0.42
1:A:126:ILE:HG12	1:D:117:PHE:CZ	2.54	0.42
1:A:356:PRO:HG3	1:A:405:ASP:OD1	2.19	0.42
1:B:578:ASP:HB3	1:B:582:LEU:O	2.20	0.42
1:D:671:ASN:ND2	1:D:673:ALA:HB3	2.29	0.42
1:A:27:ASP:O	1:A:28:SER:HB2	2.19	0.42
1:B:521:ARG:HE	1:B:745:ILE:HG21	1.84	0.42
1:A:593:ILE:HA	1:A:594:PRO:HD2	1.88	0.42
1:A:31:PRO:HD2	1:A:36:HIS:CD2	2.55	0.42
1:D:211:ALA:HB3	1:D:410:GLY:HA3	2.01	0.42
1:A:288:PHE:CE2	1:A:343:GLU:HA	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:TYR:CE2	1:D:31:PRO:HG3	2.54	0.42
1:D:593:ILE:HA	1:D:594:PRO:HD2	1.86	0.42
1:C:704:PHE:O	1:C:707:THR:HG22	2.20	0.42
1:B:61:ARG:HG2	1:B:66:ASN:OD1	2.20	0.42
1:B:377:ARG:HD2	1:B:378:ASN:O	2.20	0.42
1:D:459:ASN:HD22	1:D:460:TYR:HD2	1.67	0.42
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.54	0.42
1:B:130:ARG:HB3	1:B:168:THR:OG1	2.20	0.42
1:B:118:ASP:HA	1:C:126:ILE:CD1	2.49	0.42
1:A:31:PRO:HG3	1:D:538:TYR:CE2	2.55	0.42
1:C:51:ALA:HB1	1:C:52:PRO:CD	2.49	0.42
1:B:607:LEU:HD22	1:B:611:VAL:HG21	2.01	0.42
1:D:609:ASP:N	1:D:674:ASP:OD1	2.53	0.42
1:B:612:ARG:HD2	1:B:643:ASP:OD2	2.20	0.42
1:B:643:ASP:OD1	1:B:644:ASP:N	2.53	0.42
1:B:708:ILE:HG13	1:B:710:ILE:HD12	2.02	0.42
1:D:708:ILE:HD12	1:D:710:ILE:HD11	2.01	0.42
1:D:552:LEU:HD13	1:D:556:GLN:HG3	2.02	0.42
1:A:634:TYR:O	1:A:653:THR:HA	2.20	0.42
1:B:604:ALA:HB1	1:B:633:LEU:HD22	2.00	0.42
1:B:675:ILE:HG13	1:B:704:PHE:HZ	1.84	0.42
1:A:91:ASP:HB3	1:C:461:GLU:OE1	2.20	0.42
1:B:235:ALA:HB1	1:B:533:LYS:HD3	2.01	0.42
1:A:708:ILE:HG13	1:A:710:ILE:HD12	2.02	0.41
1:B:330:ASP:OD1	1:B:629:HIS:HE1	2.02	0.41
1:B:201:ASN:OD1	2:B:760:HEM:HMB2	2.20	0.41
1:B:368:GLN:HB2	4:B:4375:HOH:O	2.19	0.41
1:A:137:TYR:HB2	1:A:159:ILE:HG23	2.01	0.41
1:B:591:TYR:O	1:B:592:ALA:C	2.59	0.41
1:A:201:ASN:OD1	3:A:3002:PEO:O1	2.38	0.41
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.62	0.41
1:D:37:ARG:HA	1:D:38:PRO:HD2	1.92	0.41
1:B:221:VAL:HG23	1:B:239:PHE:CD1	2.55	0.41
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.55	0.41
1:C:592:ALA:O	1:C:594:PRO:HD3	2.20	0.41
1:A:126:ILE:HD12	1:D:121:ARG:CZ	2.51	0.41
1:C:511:PHE:O	1:C:515:GLN:HG2	2.20	0.41
1:B:745:ILE:HB	1:B:746:PRO:HD3	2.01	0.41
1:B:124:GLU:HG2	4:C:5045:HOH:O	2.20	0.41
1:A:516:THR:HB	1:A:517:PRO:CD	2.51	0.41
1:C:51:ALA:HB1	1:C:52:PRO:HD2	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ILE:HD12	2:B:760:HEM:HMB1	2.02	0.41
1:B:516:THR:HB	1:B:517:PRO:CD	2.51	0.41
1:A:262:ILE:O	1:A:262:ILE:HG13	2.21	0.41
1:B:264:ARG:HH12	1:B:321:GLU:CD	2.24	0.41
1:B:237:ASP:OD2	1:B:536:ARG:HG3	2.20	0.41
1:C:469:TRP:HA	1:C:470:PRO:C	2.40	0.41
1:B:113:LYS:HD2	4:B:4183:HOH:O	2.19	0.41
1:D:488:ARG:NH1	1:D:490:GLU:OE1	2.49	0.41
1:A:637:MET:HB2	1:D:562:LEU:HA	2.03	0.41
1:A:602:VAL:HG13	1:A:662:VAL:HA	2.03	0.41
1:B:616:LEU:HA	1:B:616:LEU:HD23	1.81	0.41
1:B:252:ASN:HA	1:B:252:ASN:HD22	1.75	0.41
1:A:222:LYS:HB3	1:A:223:PRO:HD2	2.03	0.41
1:A:488:ARG:NH1	1:B:491:GLY:HA2	2.36	0.41
1:C:128:ASN:HA	1:C:168:THR:O	2.20	0.41
1:C:507:HIS:N	1:C:508:PRO:HD2	2.35	0.41
1:A:128:ASN:HA	1:A:168:THR:O	2.22	0.41
1:A:461:GLU:OE1	1:C:91:ASP:HB3	2.20	0.41
1:D:461:GLU:HB2	1:D:462:PRO:HA	2.02	0.41
1:B:535:VAL:HG22	4:B:4320:HOH:O	2.21	0.40
1:A:405:ASP:HA	1:A:406:PRO:HD2	1.97	0.40
1:B:671:ASN:OD1	1:B:673:ALA:HB3	2.21	0.40
1:B:715:GLU:CG	1:B:747:LYS:HE2	2.51	0.40
1:D:507:HIS:N	1:D:508:PRO:CD	2.84	0.40
1:C:516:THR:HB	1:C:517:PRO:CD	2.51	0.40
1:C:534:VAL:HG11	1:C:539:ILE:HB	2.04	0.40
1:A:507:HIS:N	1:A:508:PRO:CD	2.84	0.40
1:B:105:LEU:HD11	1:D:413:PHE:HB2	2.03	0.40
1:D:158:LYS:HD2	4:D:6525:HOH:O	2.20	0.40
1:B:608:ASN:HD22	1:B:672:ILE:HD13	1.86	0.40
1:A:411:ARG:HG2	2:A:760:HEM:C2C	2.57	0.40
1:B:308:GLN:OE1	1:C:313:ARG:NH1	2.51	0.40
1:A:188:LYS:HB2	1:A:391:PHE:CE1	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:OD1	1:B:369:ARG:NH2[2_545]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	725/753 (96%)	701 (97%)	21 (3%)	3 (0%)	39	47
1	B	725/753 (96%)	686 (95%)	34 (5%)	5 (1%)	26	30
1	C	725/753 (96%)	698 (96%)	23 (3%)	4 (1%)	30	34
1	D	725/753 (96%)	699 (96%)	22 (3%)	4 (1%)	30	34
All	All	2900/3012 (96%)	2784 (96%)	100 (3%)	16 (1%)	30	34

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	B	28	SER
1	C	28	SER
1	C	725	ASP
1	D	33	ASP
1	B	584	LYS
1	D	725	ASP
1	A	75	SER
1	A	415	TYR
1	B	75	SER
1	B	613	SER
1	C	414	SER
1	D	28	SER
1	D	415	TYR
1	B	415	TYR
1	C	415	TYR

### 5.3.2 Protein sidechains [i](#)

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	612/636 (96%)	587 (96%)	25 (4%)	37	49
1	B	612/636 (96%)	581 (95%)	31 (5%)	29	37
1	C	612/636 (96%)	576 (94%)	36 (6%)	24	30
1	D	612/636 (96%)	580 (95%)	32 (5%)	29	36
All	All	2448/2544 (96%)	2324 (95%)	124 (5%)	29	37

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	126	ILE
1	A	142	LYS
1	A	185	PHE
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	252	ASN
1	A	341	ILE
1	A	344	GLU
1	A	353	LEU
1	A	369	ARG
1	A	375	LEU
1	A	413	PHE
1	A	432	PRO
1	A	437	THR
1	A	448	MET
1	A	459	ASN
1	A	508	PRO
1	A	532	SER
1	A	552	LEU
1	A	556	GLN
1	A	565	GLU
1	A	612	ARG
1	A	750	LYS
1	B	27	ASP
1	B	28	SER
1	B	37	ARG
1	B	140	PRO
1	B	185	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	205	ILE
1	B	227	TRP
1	B	252	ASN
1	B	265	SER
1	B	309	LYS
1	B	321	GLU
1	B	353	LEU
1	B	375	LEU
1	B	377	ARG
1	B	392	HIS
1	B	413	PHE
1	B	437	THR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	612	ARG
1	B	647	VAL
1	B	722	ASP
1	B	725	ASP
1	B	728	PHE
1	B	751	ILE
1	C	27	ASP
1	C	37	ARG
1	C	61	ARG
1	C	73	LYS
1	C	99	SER
1	C	185	PHE
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	265	SER
1	C	332	PRO
1	C	369	ARG
1	C	375	LEU
1	C	377	ARG
1	C	392	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	437	THR
1	C	459	ASN
1	C	488	ARG
1	C	531	LEU
1	C	552	LEU
1	C	574	THR
1	C	584	LYS
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	660	LEU
1	C	671	ASN
1	C	707	THR
1	C	733	LEU
1	C	747	LYS
1	C	750	LYS
1	C	751	ILE
1	D	48	GLN
1	D	126	ILE
1	D	159	ILE
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	252	ASN
1	D	265	SER
1	D	344	GLU
1	D	353	LEU
1	D	375	LEU
1	D	392	HIS
1	D	437	THR
1	D	448	MET
1	D	449	HIS
1	D	459	ASN
1	D	478	LYS
1	D	490	GLU
1	D	521	ARG
1	D	552	LEU
1	D	554	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	582	LEU
1	D	610	GLU
1	D	612	ARG
1	D	616	LEU
1	D	648	LEU
1	D	709	LYS
1	D	713	GLN
1	D	716	GLU
1	D	747	LYS
1	D	750	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	119	HIS
1	A	212	HIS
1	A	449	HIS
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	119	HIS
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	486	GLN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN
1	D	629	HIS
1	D	671	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	713	GLN

### 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 ⓘ

17 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	$\# Z  > 2$
3	PEO	A	3001	2	1,1,1	1.02	0	0,0,0	0.00	-
3	PEO	A	3002	-	1,1,1	1.27	0	0,0,0	0.00	-
3	PEO	A	3003	-	1,1,1	1.33	0	0,0,0	0.00	-
2	HEM	A	760	1,3	30,50,50	2.38	7 (23%)	24,82,82	2.74	10 (41%)
3	PEO	B	4001	-	1,1,1	1.39	0	0,0,0	0.00	-
3	PEO	B	4002	2	1,1,1	1.40	0	0,0,0	0.00	-
3	PEO	B	4003	-	1,1,1	1.37	0	0,0,0	0.00	-
2	HEM	B	760	1,3	30,50,50	2.45	7 (23%)	24,82,82	2.88	11 (45%)
3	PEO	C	5001	-	1,1,1	1.17	0	0,0,0	0.00	-
3	PEO	C	5002	2	1,1,1	1.13	0	0,0,0	0.00	-
3	PEO	C	5003	-	1,1,1	1.24	0	0,0,0	0.00	-
2	HEM	C	760	1,3	30,50,50	2.51	8 (26%)	24,82,82	2.57	10 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEO	D	3004	-	1,1,1	1.50	0	0,0,0	0.00	-
3	PEO	D	6001	-	1,1,1	1.14	0	0,0,0	0.00	-
3	PEO	D	6002	-	1,1,1	1.23	0	0,0,0	0.00	-
3	PEO	D	6003	-	1,1,1	1.44	0	0,0,0	0.00	-
2	HEM	D	760	1	30,50,50	2.56	8 (26%)	24,82,82	2.42	9 (37%)

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
3	PEO	A	3001	2	-	0/0/0/0	0/0/0/0
3	PEO	A	3002	-	-	0/0/0/0	0/0/0/0
3	PEO	A	3003	-	-	0/0/0/0	0/0/0/0
2	HEM	A	760	1,3	-	0/10/54/54	0/0/8/8
3	PEO	B	4001	-	-	0/0/0/0	0/0/0/0
3	PEO	B	4002	2	-	0/0/0/0	0/0/0/0
3	PEO	B	4003	-	-	0/0/0/0	0/0/0/0
2	HEM	B	760	1,3	-	0/10/54/54	0/0/8/8
3	PEO	C	5001	-	-	0/0/0/0	0/0/0/0
3	PEO	C	5002	2	-	0/0/0/0	0/0/0/0
3	PEO	C	5003	-	-	0/0/0/0	0/0/0/0
2	HEM	C	760	1,3	-	0/10/54/54	0/0/8/8
3	PEO	D	3004	-	-	0/0/0/0	0/0/0/0
3	PEO	D	6001	-	-	0/0/0/0	0/0/0/0
3	PEO	D	6002	-	-	0/0/0/0	0/0/0/0
3	PEO	D	6003	-	-	0/0/0/0	0/0/0/0
2	HEM	D	760	1	-	0/10/54/54	0/0/8/8

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760	HEM	C2D-C3D	-7.44	1.32	1.54
2	B	760	HEM	C2D-C3D	-7.27	1.32	1.54
2	A	760	HEM	C2D-C3D	-7.18	1.33	1.54
2	D	760	HEM	C2D-C3D	-7.11	1.33	1.54
2	C	760	HEM	C3B-C4B	-6.72	1.45	1.51
2	B	760	HEM	C3B-C4B	-6.46	1.46	1.51
2	D	760	HEM	C3B-C4B	-6.39	1.46	1.51
2	D	760	HEM	C3D-C4D	-5.82	1.44	1.51
2	A	760	HEM	C3D-C4D	-5.57	1.44	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	C3B-C4B	-5.18	1.47	1.51
2	B	760	HEM	C3D-C4D	-5.16	1.44	1.51
2	C	760	HEM	C3D-C4D	-4.38	1.46	1.51
2	D	760	HEM	C2C-C1C	-4.18	1.44	1.52
2	C	760	HEM	C2C-C1C	-4.11	1.44	1.52
2	B	760	HEM	C2C-C1C	-4.09	1.44	1.52
2	A	760	HEM	C2C-C1C	-3.51	1.45	1.52
2	A	760	HEM	C2D-C1D	-2.47	1.43	1.51
2	B	760	HEM	C2D-C1D	-2.17	1.44	1.51
2	C	760	HEM	CAA-C2A	2.10	1.55	1.52
2	B	760	HEM	C1C-NC	2.12	1.38	1.36
2	D	760	HEM	FE-NC	2.12	2.04	1.95
2	D	760	HEM	C3B-CAB	2.15	1.55	1.51
2	D	760	HEM	C1C-NC	2.22	1.38	1.36
2	B	760	HEM	C4C-NC	2.29	1.38	1.36
2	C	760	HEM	C4C-NC	2.46	1.39	1.36
2	A	760	HEM	C4C-NC	2.51	1.39	1.36
2	C	760	HEM	C3C-CAC	2.60	1.56	1.51
2	C	760	HEM	C1C-NC	2.71	1.39	1.36
2	A	760	HEM	C3C-CAC	2.76	1.56	1.51
2	D	760	HEM	C4C-NC	3.82	1.40	1.36

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HEM	C3C-CAC-CBC	-6.34	114.73	124.46
2	B	760	HEM	C3C-CAC-CBC	-4.57	117.45	124.46
2	B	760	HEM	CMA-C3A-C4A	-4.55	120.83	128.36
2	C	760	HEM	C3C-CAC-CBC	-3.69	118.79	124.46
2	C	760	HEM	CMA-C3A-C4A	-3.15	123.15	128.36
2	A	760	HEM	C4B-CHC-C1C	-3.13	120.58	125.82
2	C	760	HEM	CAA-C2A-C1A	-2.65	124.13	127.01
2	B	760	HEM	CAA-C2A-C1A	-2.45	124.35	127.01
2	A	760	HEM	CAA-C2A-C1A	-2.36	124.45	127.01
2	D	760	HEM	CMA-C3A-C4A	-2.09	124.91	128.36
2	D	760	HEM	CAA-C2A-C1A	-2.08	124.75	127.01
2	A	760	HEM	CMA-C3A-C4A	-2.07	124.94	128.36
2	D	760	HEM	C2C-C1C-CHC	2.21	127.05	123.68
2	C	760	HEM	CMA-C3A-C2A	2.22	129.88	125.24
2	B	760	HEM	CMA-C3A-C2A	2.87	131.24	125.24
2	C	760	HEM	CAD-C3D-C4D	2.97	122.94	112.47
2	A	760	HEM	CMD-C2D-C3D	3.03	127.73	114.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HEM	CAD-C3D-C4D	3.18	123.69	112.47
2	D	760	HEM	CAD-C3D-C4D	3.21	123.78	112.47
2	B	760	HEM	CAD-C3D-C4D	3.26	123.97	112.47
2	B	760	HEM	CMD-C2D-C3D	3.45	129.63	114.35
2	D	760	HEM	CMD-C2D-C3D	3.64	130.44	114.35
2	C	760	HEM	CMD-C2D-C3D	3.66	130.53	114.35
2	C	760	HEM	C2D-C3D-C4D	3.67	107.72	101.50
2	A	760	HEM	C2D-C3D-C4D	3.77	107.89	101.50
2	D	760	HEM	C2D-C3D-C4D	3.84	108.01	101.50
2	B	760	HEM	C2D-C3D-C4D	4.00	108.29	101.50
2	B	760	HEM	CBA-CAA-C2A	4.30	120.24	112.53
2	C	760	HEM	CMC-C2C-C3C	4.56	127.92	116.53
2	A	760	HEM	CMB-C2B-C3B	4.65	128.13	116.53
2	D	760	HEM	CMC-C2C-C3C	4.81	128.54	116.53
2	A	760	HEM	CMC-C2C-C3C	4.84	128.61	116.53
2	B	760	HEM	CMC-C2C-C3C	5.02	129.05	116.53
2	B	760	HEM	CAD-C3D-C2D	5.03	127.69	113.22
2	C	760	HEM	CMB-C2B-C3B	5.07	129.19	116.53
2	B	760	HEM	CMB-C2B-C3B	5.08	129.21	116.53
2	D	760	HEM	CMB-C2B-C3B	5.09	129.23	116.53
2	D	760	HEM	CAD-C3D-C2D	5.21	128.21	113.22
2	A	760	HEM	CAD-C3D-C2D	5.29	128.42	113.22
2	C	760	HEM	CAD-C3D-C2D	5.60	129.32	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	PEO	1	0
3	A	3002	PEO	3	0
3	A	3003	PEO	2	0
2	A	760	HEM	2	0
3	B	4001	PEO	1	0
3	B	4002	PEO	1	0
3	B	4003	PEO	1	0
2	B	760	HEM	4	0
3	C	5001	PEO	1	0
3	C	5003	PEO	1	0
2	C	760	HEM	5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3004	PEO	1	0
3	D	6001	PEO	1	0
3	D	6002	PEO	2	0
3	D	6003	PEO	1	0
2	D	760	HEM	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	727/753 (96%)	-0.31	17 (2%) 64 71	10, 20, 43, 91	1 (0%)
1	B	727/753 (96%)	-0.12	36 (4%) 32 40	13, 22, 46, 91	1 (0%)
1	C	727/753 (96%)	-0.18	21 (2%) 55 63	12, 22, 45, 90	1 (0%)
1	D	727/753 (96%)	-0.25	24 (3%) 50 58	11, 20, 44, 92	1 (0%)
All	All	2908/3012 (96%)	-0.21	98 (3%) 49 57	10, 21, 45, 92	4 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	726	GLY	9.2
1	B	27	ASP	7.7
1	D	27	ASP	7.7
1	B	726	GLY	6.1
1	B	28	SER	5.9
1	C	28	SER	5.8
1	A	32	GLU	5.6
1	C	726	GLY	5.5
1	A	28	SER	5.5
1	D	28	SER	5.5
1	C	27	ASP	4.9
1	A	751	ILE	4.7
1	B	29	LEU	4.7
1	A	27	ASP	4.3
1	D	32	GLU	4.2
1	B	32	GLU	3.9
1	A	29	LEU	3.6
1	B	47	ALA	3.6
1	D	750	LYS	3.5
1	B	61	ARG	3.5
1	D	33	ASP	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	34	GLY	3.4
1	D	30	ALA	3.4
1	B	39	ALA	3.4
1	D	749	ASP	3.3
1	D	29	LEU	3.3
1	B	712	ASP	3.3
1	D	438	CYS	3.2
1	D	35	SER	3.2
1	B	612	ARG	3.1
1	A	750	LYS	3.1
1	A	35	SER	3.1
1	B	37	ARG	3.1
1	B	677	ASP	3.0
1	C	749	ASP	3.0
1	B	33	ASP	3.0
1	B	750	LYS	2.9
1	B	572	ASN	2.9
1	C	574	THR	2.8
1	C	572	ASN	2.8
1	C	677	ASP	2.8
1	B	34	GLY	2.8
1	D	725	ASP	2.8
1	D	711	ALA	2.7
1	C	711	ALA	2.7
1	C	569	ASP	2.7
1	C	714	GLY	2.7
1	A	710	ILE	2.7
1	C	438	CYS	2.6
1	B	597	ASP	2.6
1	B	749	ASP	2.6
1	B	713	GLN	2.6
1	A	37	ARG	2.6
1	B	70	ASP	2.5
1	B	31	PRO	2.5
1	B	642	ALA	2.5
1	C	751	ILE	2.5
1	A	711	ALA	2.5
1	B	647	VAL	2.5
1	A	712	ASP	2.5
1	B	38	PRO	2.5
1	B	30	ALA	2.4
1	D	38	PRO	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	750	LYS	2.4
1	D	47	ALA	2.4
1	C	29	LEU	2.3
1	D	40	ALA	2.3
1	B	569	ASP	2.3
1	C	727	SER	2.3
1	A	437	THR	2.3
1	D	37	ARG	2.3
1	D	158	LYS	2.2
1	B	621	LYS	2.2
1	B	746	PRO	2.2
1	A	33	ASP	2.2
1	C	70	ASP	2.2
1	C	673	ALA	2.2
1	C	594	PRO	2.2
1	B	646	THR	2.2
1	C	32	GLU	2.2
1	B	59	ASP	2.2
1	D	713	GLN	2.2
1	B	610	GLU	2.1
1	D	61	ARG	2.1
1	B	673	ALA	2.1
1	A	34	GLY	2.1
1	D	36	HIS	2.1
1	A	713	GLN	2.1
1	B	751	ILE	2.1
1	B	643	ASP	2.1
1	C	625	ALA	2.0
1	A	726	GLY	2.0
1	A	725	ASP	2.0
1	D	568	ASP	2.0
1	B	36	HIS	2.0
1	C	713	GLN	2.0
1	D	48	GLN	2.0
1	B	711	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	PEO	B	4002	2/2	0.92	0.20	8.93	25,25,25,28	0
3	PEO	D	3004	2/2	0.89	0.25	7.26	33,33,33,34	0
3	PEO	A	3001	2/2	0.96	0.16	3.47	29,29,29,29	0
3	PEO	D	6001	2/2	0.98	0.14	2.72	21,21,21,22	0
3	PEO	B	4003	2/2	0.94	0.15	2.61	31,31,31,32	0
3	PEO	D	6002	2/2	0.93	0.13	2.37	18,18,18,18	0
3	PEO	C	5003	2/2	0.98	0.10	0.62	18,18,18,18	0
3	PEO	C	5002	2/2	0.98	0.12	0.61	34,34,34,35	0
3	PEO	C	5001	2/2	0.99	0.08	0.12	20,20,20,21	0
2	HEM	D	760	43/43	0.97	0.10	-0.09	10,15,16,18	0
3	PEO	A	3003	2/2	0.98	0.08	-0.21	22,22,22,25	0
3	PEO	D	6003	2/2	0.96	0.09	-0.27	21,21,21,23	0
2	HEM	C	760	43/43	0.98	0.09	-0.31	16,18,19,21	0
2	HEM	A	760	43/43	0.98	0.09	-0.45	9,14,16,18	0
2	HEM	B	760	43/43	0.98	0.09	-0.66	12,16,18,18	0
3	PEO	A	3002	2/2	0.98	0.06	-1.82	13,13,13,16	0
3	PEO	B	4001	2/2	0.98	0.07	-1.90	17,17,17,19	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.