



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:16 AM GMT

PDB ID : 2C7F
Title : THE STRUCTURE OF A FAMILY 51 ARABINOFURANOSIDASE, ARAF51, FROM CLOSTRIDIUM THERMOCELLUM IN COMPLEX WITH 1,5-ALPHA-L-ARABINOTRIOSE.
Authors : Taylor, E.J.; Smith, N.L.; Turkenburg, J.P.; D'Souza, S.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2005-11-23
Resolution : 2.70 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

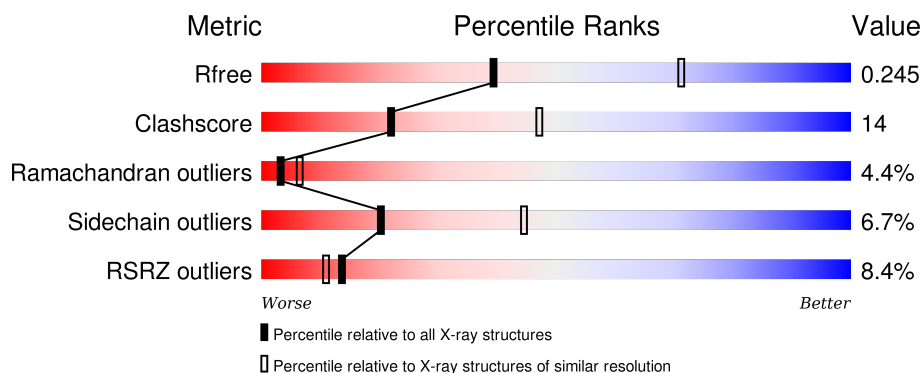
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	513	<div> <div>9%</div> <div>76%</div> <div>14%</div> <div>• • •</div> </div>
1	B	513	<div> <div>5%</div> <div>75%</div> <div>16%</div> <div>5%</div> <div>• • •</div> </div>
1	C	513	<div> <div>10%</div> <div>72%</div> <div>18%</div> <div>5%</div> <div>• • •</div> </div>
1	D	513	<div> <div>7%</div> <div>75%</div> <div>17%</div> <div>• • •</div> </div>
1	E	513	<div> <div>8%</div> <div>75%</div> <div>16%</div> <div>• • •</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	513	

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
2	AHR	A	1504	-	-	-	X
2	AHR	E	1504	-	-	-	X
3	EDO	B	1505	-	-	-	X
3	EDO	D	1506	-	-	-	X
3	EDO	D	1507	-	-	-	X
3	EDO	E	1506	-	-	-	X
4	AHR	B	1504	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24046 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 ALPHA-L-ARABINOFURANOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3971	2523	676	750	22			
1	B	497	Total	C	N	O	S	0	0	0
			3972	2518	680	753	21			
1	C	496	Total	C	N	O	S	0	1	0
			3977	2523	679	753	22			
1	D	499	Total	C	N	O	S	0	0	0
			3978	2522	680	754	22			
1	E	492	Total	C	N	O	S	0	0	1
			3886	2465	663	738	20			
1	F	496	Total	C	N	O	S	0	0	0
			3959	2513	674	751	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
B	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
C	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
D	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
E	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
F	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			28	15	13		
2	C	3	Total	C	O	0	0
			28	15	13		
2	D	3	Total	C	O	0	0
			28	15	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	3	Total	C	O	0	0
			28	15	13		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	2	Total	C	O	0	0
			19	10	9		
4	F	2	Total	C	O	0	0
			19	10	9		

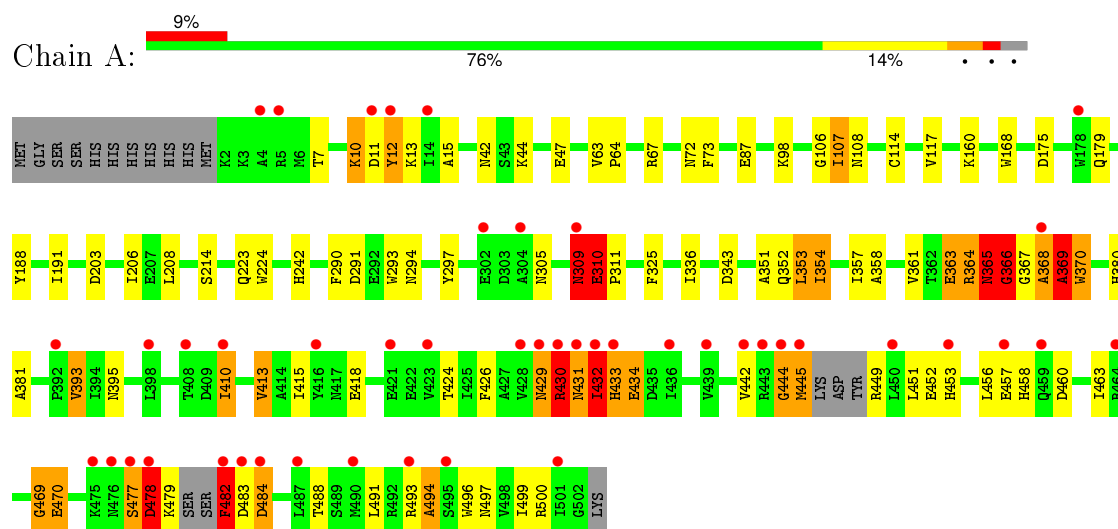
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	17	Total	O	0	0
			17	17		
5	C	19	Total	O	0	0
			19	19		
5	D	21	Total	O	0	0
			21	21		
5	E	15	Total	O	0	0
			15	15		
5	F	19	Total	O	0	0
			19	19		

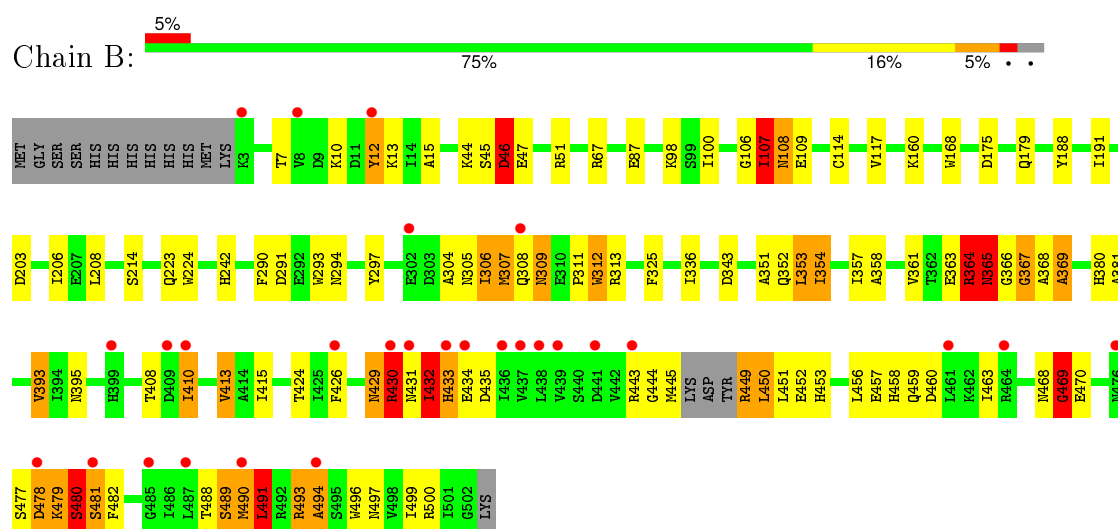
3 Residue-property plots

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: ALPHA-L-ARABINOFURANOSIDASE

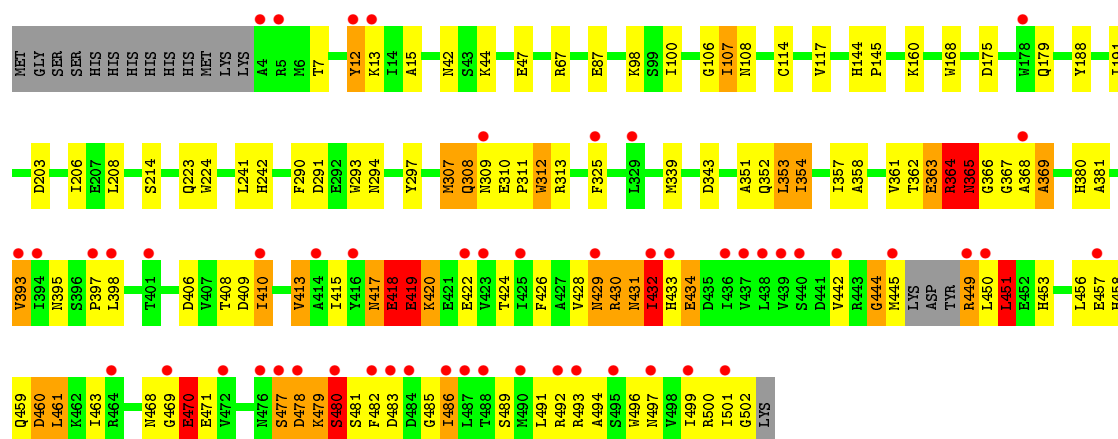


• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE

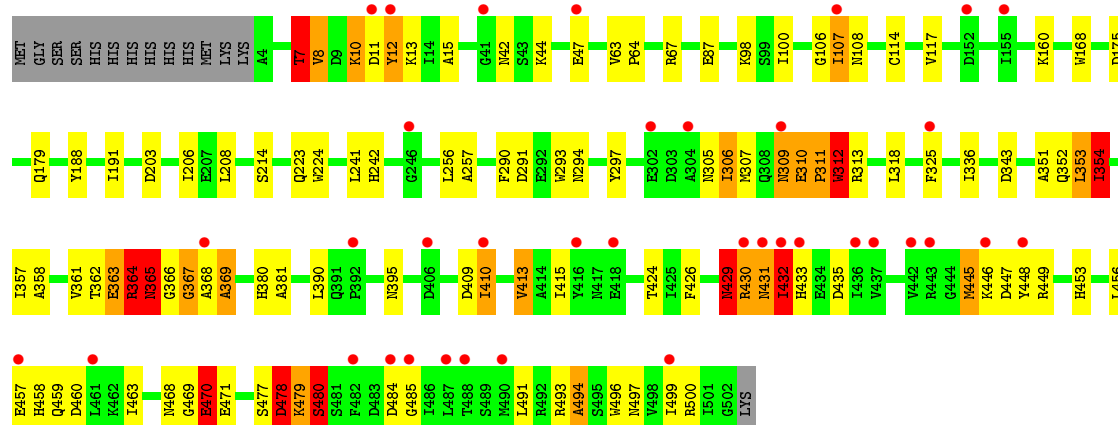
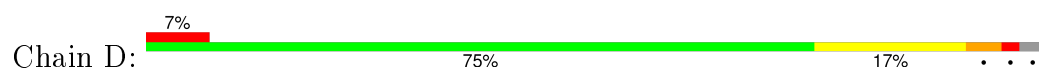


• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE

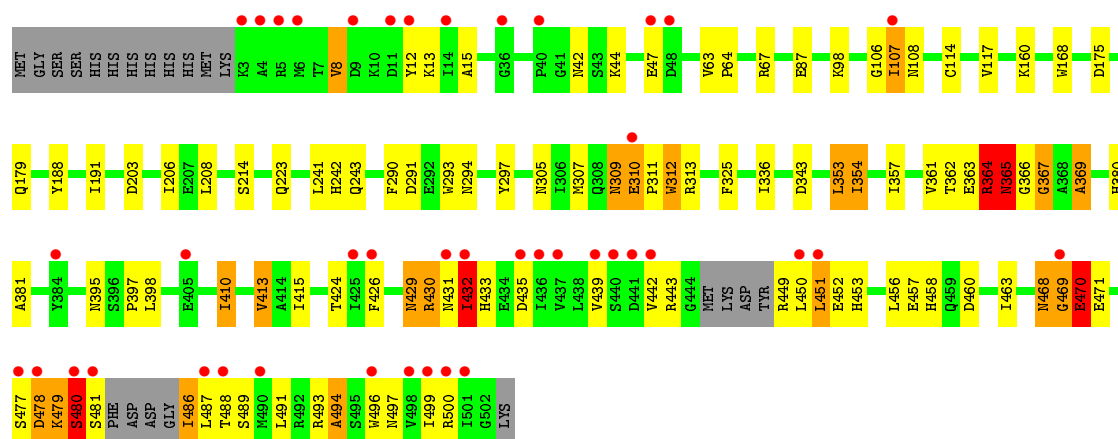
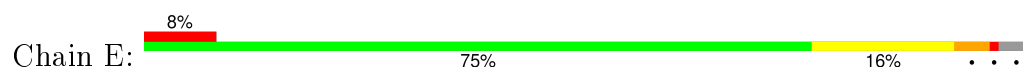




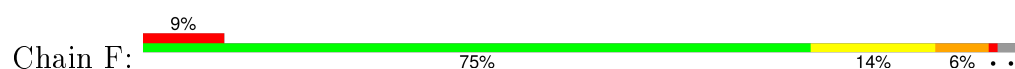
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE

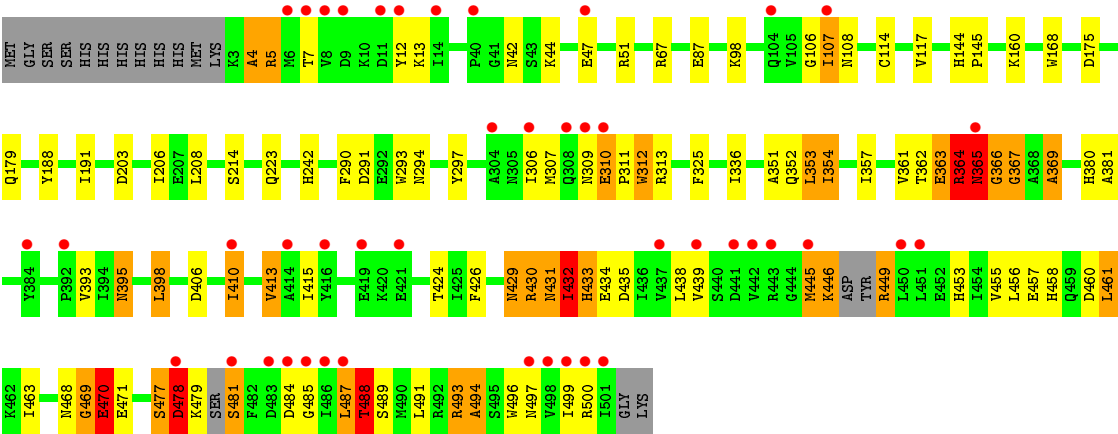


• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE



• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.34Å 173.34Å 272.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.86 – 2.70 59.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (145.86-2.70) 99.7 (59.58-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.255 0.231 , 0.245	Depositor DCC
R_{free} test set	5684 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 113743 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24046	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AHR, EDO

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	0.35	0/4061	0.57	1/5499 (0.0%)
1	B	0.36	0/4063	0.59	2/5503 (0.0%)
1	C	0.36	0/4068	0.58	0/5514
1	D	0.34	0/4071	0.57	1/5516 (0.0%)
1	E	0.33	0/3973	0.55	0/5382
1	F	0.32	0/4049	0.55	1/5485 (0.0%)
All	All	0.34	0/24285	0.57	5/32899 (0.0%)

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	A	0	18
1	B	0	20
1	C	0	17
1	D	0	15
1	E	0	11
1	F	1	17
All	All	1	98

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	ASP	N-CA-C	6.22	127.80	111.00
1	F	461	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	310	GLU	N-CA-C	5.37	125.50	111.00
1	B	491	LEU	CA-CB-CG	5.25	127.36	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	390	LEU	CB-CG-CD2	5.05	119.59	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	479	LYS	CA

All (98) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	GLN	Peptide
1	A	309	ASN	Peptide
1	A	353	LEU	Peptide
1	A	365	ASN	Peptide
1	A	366	GLY	Peptide
1	A	367	GLY	Peptide
1	A	368	ALA	Peptide
1	A	369	ALA	Peptide
1	A	393	VAL	Peptide
1	A	429	ASN	Peptide
1	A	430	ARG	Peptide
1	A	431	ASN	Peptide
1	A	433	HIS	Peptide
1	A	444	GLY	Peptide
1	A	469	GLY	Peptide
1	A	478	ASP	Peptide
1	A	482	PHE	Peptide
1	A	72	ASN	Peptide
1	B	107	ILE	Peptide
1	B	109	GLU	Peptide
1	B	223	GLN	Peptide
1	B	304	ALA	Peptide
1	B	306	ILE	Peptide
1	B	307	MET	Peptide
1	B	309	ASN	Peptide
1	B	312	TRP	Peptide
1	B	353	LEU	Peptide
1	B	365	ASN	Peptide
1	B	366	GLY	Peptide
1	B	367	GLY	Peptide
1	B	429	ASN	Peptide
1	B	430	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	432	ILE	Peptide
1	B	444	GLY	Peptide
1	B	45	SER	Peptide
1	B	469	GLY	Peptide
1	B	489	SER	Peptide
1	B	491	LEU	Peptide
1	C	223	GLN	Peptide
1	C	307	MET	Peptide
1	C	312	TRP	Peptide
1	C	353	LEU	Peptide
1	C	364	ARG	Peptide
1	C	365	ASN	Peptide
1	C	367	GLY	Peptide
1	C	417	ASN	Peptide
1	C	418	GLU	Peptide
1	C	419	GLU	Peptide
1	C	429	ASN	Peptide
1	C	431	ASN	Peptide
1	C	444	GLY	Peptide
1	C	450	LEU	Peptide
1	C	460	ASP	Peptide
1	C	470	GLU	Peptide
1	C	471	GLU	Peptide
1	D	223	GLN	Peptide
1	D	307	MET	Peptide
1	D	309	ASN	Peptide
1	D	311	PRO	Peptide
1	D	312	TRP	Peptide
1	D	353	LEU	Peptide
1	D	364	ARG	Peptide
1	D	365	ASN	Peptide
1	D	367	GLY	Peptide
1	D	429	ASN	Peptide
1	D	431	ASN	Peptide
1	D	471	GLU	Peptide
1	D	478	ASP	Peptide
1	D	480	SER	Peptide
1	D	7	THR	Peptide
1	E	223	GLN	Peptide
1	E	307	MET	Peptide
1	E	312	TRP	Peptide
1	E	353	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	E	364	ARG	Peptide
1	E	367	GLY	Peptide
1	E	429	ASN	Peptide
1	E	430	ARG	Peptide
1	E	443	ARG	Peptide
1	E	471	GLU	Peptide
1	E	480	SER	Peptide
1	F	223	GLN	Peptide
1	F	307	MET	Peptide
1	F	312	TRP	Peptide
1	F	353	LEU	Peptide
1	F	364	ARG	Peptide
1	F	365	ASN	Peptide
1	F	366	GLY	Peptide
1	F	367	GLY	Peptide
1	F	4	ALA	Peptide
1	F	429	ASN	Peptide
1	F	431	ASN	Peptide
1	F	445	MET	Peptide
1	F	471	GLU	Peptide
1	F	477	SER	Peptide
1	F	478	ASP	Peptide
1	F	487	LEU	Peptide
1	F	488	THR	Peptide

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	3971	0	3869	112	0
1	B	3972	0	3852	113	0
1	C	3977	0	3857	123	0
1	D	3978	0	3854	111	0
1	E	3886	0	3756	98	0
1	F	3959	0	3834	106	0
2	A	28	0	21	0	0
2	C	28	0	21	0	0
2	D	28	0	21	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	28	0	21	0	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	C	4	0	6	0	0
3	D	8	0	12	0	0
3	E	8	0	12	0	0
3	F	4	0	6	0	0
4	B	19	0	15	0	0
4	F	19	0	15	0	0
5	A	26	0	0	0	0
5	B	17	0	0	0	0
5	C	19	0	0	0	0
5	D	21	0	0	0	0
5	E	15	0	0	1	0
5	F	19	0	0	0	0
All	All	24046	0	23190	654	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 14.

All (654) 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)
1:C:478:ASP:CB	1:C:479:LYS:HB2	1.30	1.62
1:A:431:ASN:HA	1:A:432:ILE:CG2	1.39	1.53
1:E:431:ASN:CB	1:E:432:ILE:HG22	1.35	1.52
1:C:478:ASP:HB3	1:C:479:LYS:CB	1.46	1.45
1:A:431:ASN:CA	1:A:432:ILE:HG22	1.43	1.43
1:C:478:ASP:CA	1:C:479:LYS:HB2	1.50	1.35
1:B:450:LEU:HD12	1:B:451:LEU:N	1.48	1.26
1:F:445:MET:CA	1:F:446:LYS:HB2	1.61	1.25
1:E:431:ASN:HA	1:E:432:ILE:CB	1.62	1.23
1:A:478:ASP:CB	1:A:479:LYS:HB3	1.70	1.22
1:D:429:ASN:HA	1:D:430:ARG:CB	1.70	1.22
1:F:477:SER:HB2	1:F:478:ASP:OD1	1.42	1.19
1:F:4:ALA:HB1	1:F:5:ARG:CB	1.72	1.18
1:B:450:LEU:C	1:B:450:LEU:HD12	1.52	1.18
1:C:478:ASP:CB	1:C:479:LYS:CB	2.10	1.18
1:E:431:ASN:CA	1:E:432:ILE:HB	1.72	1.18
1:E:431:ASN:CB	1:E:432:ILE:CG2	2.23	1.17
1:E:432:ILE:H	1:E:493:ARG:HB2	1.09	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:ASP:HB3	1:A:479:LYS:HB3	1.15	1.13
1:E:431:ASN:HB2	1:E:432:ILE:HG22	1.27	1.12
1:F:445:MET:HA	1:F:446:LYS:HB2	1.12	1.12
1:B:469:GLY:HA2	1:B:470:GLU:HB2	1.21	1.11
1:B:449:ARG:HH11	1:B:449:ARG:HG2	1.07	1.10
1:E:429:ASN:O	1:E:431:ASN:O	1.67	1.10
1:B:469:GLY:HA2	1:B:470:GLU:CB	1.81	1.09
1:F:4:ALA:CB	1:F:5:ARG:CB	2.30	1.09
1:B:107:ILE:HG13	1:B:108:ASN:H	1.10	1.08
1:D:429:ASN:HA	1:D:430:ARG:HB3	1.27	1.08
1:C:418:GLU:HG3	1:C:419:GLU:CB	1.83	1.07
1:D:409:ASP:O	1:D:429:ASN:HB2	1.54	1.07
1:F:478:ASP:HB3	1:F:479:LYS:HA	1.26	1.07
1:B:449:ARG:HH11	1:B:449:ARG:CG	1.67	1.07
1:F:477:SER:CB	1:F:478:ASP:OD1	2.02	1.07
1:C:418:GLU:CG	1:C:419:GLU:HB3	1.85	1.06
1:E:431:ASN:HB3	1:E:432:ILE:CG2	1.82	1.05
1:A:478:ASP:HA	1:A:479:LYS:HB2	1.36	1.05
1:A:444:GLY:CA	1:A:445:MET:HB2	1.88	1.04
1:B:490:MET:O	1:B:491:LEU:HD23	1.56	1.03
1:F:4:ALA:CA	1:F:5:ARG:CB	2.37	1.03
1:D:431:ASN:HA	1:D:432:ILE:HG22	1.37	1.02
1:C:444:GLY:HA3	1:C:445:MET:HB2	1.40	1.02
1:E:431:ASN:HB3	1:E:432:ILE:HG22	1.07	1.02
1:A:444:GLY:HA3	1:A:445:MET:HB2	1.40	1.00
1:C:485:GLY:HA2	1:C:486:ILE:O	1.59	1.00
1:F:445:MET:CB	1:F:446:LYS:HB2	1.91	1.00
1:B:450:LEU:CD1	1:B:450:LEU:C	2.30	0.99
1:A:478:ASP:HB3	1:A:479:LYS:CB	1.92	0.99
1:C:478:ASP:HB3	1:C:479:LYS:HB3	1.38	0.99
1:C:478:ASP:HA	1:C:479:LYS:HB2	1.40	0.98
1:A:442:VAL:HG22	1:A:445:MET:HB3	1.45	0.97
1:B:107:ILE:HG13	1:B:108:ASN:N	1.73	0.97
1:E:429:ASN:O	1:E:431:ASN:N	1.99	0.96
1:D:429:ASN:CA	1:D:430:ARG:HB3	1.94	0.96
1:C:478:ASP:CA	1:C:479:LYS:CB	2.40	0.95
1:A:353:LEU:C	1:A:354:ILE:HG12	1.86	0.95
1:E:431:ASN:CA	1:E:432:ILE:CB	2.34	0.94
1:B:450:LEU:CD1	1:B:451:LEU:N	2.30	0.94
1:E:432:ILE:H	1:E:493:ARG:CB	1.80	0.93
1:F:4:ALA:HA	1:F:5:ARG:CB	1.96	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:GLY:HA3	1:C:445:MET:CB	1.98	0.93
1:F:398:LEU:HD12	1:F:406:ASP:CA	1.99	0.92
1:A:478:ASP:CB	1:A:479:LYS:CB	2.46	0.92
1:B:431:ASN:C	1:B:432:ILE:HG22	1.89	0.92
1:B:449:ARG:N	1:B:482:PHE:CE2	2.38	0.91
1:C:418:GLU:HG3	1:C:419:GLU:HB3	0.95	0.91
1:A:478:ASP:CA	1:A:479:LYS:CB	2.48	0.90
1:F:478:ASP:HB3	1:F:479:LYS:CA	2.02	0.89
1:D:305:ASN:O	1:D:309:ASN:HB2	1.71	0.89
1:F:478:ASP:CB	1:F:479:LYS:HA	2.02	0.89
1:A:431:ASN:HA	1:A:432:ILE:CB	2.03	0.88
1:B:449:ARG:N	1:B:482:PHE:HE2	1.72	0.88
1:B:449:ARG:HG2	1:B:449:ARG:NH1	1.83	0.88
1:D:7:THR:C	1:D:8:VAL:CG2	2.43	0.87
1:A:478:ASP:HA	1:A:479:LYS:CB	2.05	0.87
1:D:429:ASN:HA	1:D:430:ARG:HB2	1.55	0.87
1:B:432:ILE:HG12	1:B:432:ILE:O	1.75	0.87
1:F:445:MET:HA	1:F:446:LYS:CB	2.03	0.86
1:A:478:ASP:CA	1:A:479:LYS:HB2	2.05	0.86
1:B:469:GLY:CA	1:B:470:GLU:CB	2.53	0.85
1:F:432:ILE:O	1:F:433:HIS:CD2	2.30	0.85
1:D:309:ASN:HB3	1:D:310:GLU:HB2	1.57	0.85
1:A:310:GLU:H	1:A:311:PRO:HD3	1.41	0.85
1:E:431:ASN:HA	1:E:432:ILE:HB	0.86	0.84
1:B:480:SER:HA	1:B:481:SER:CB	2.07	0.84
1:F:398:LEU:CD1	1:F:406:ASP:HB3	2.07	0.84
1:F:398:LEU:HD12	1:F:406:ASP:CB	2.08	0.84
1:A:305:ASN:O	1:A:309:ASN:HB2	1.78	0.83
1:F:398:LEU:HD12	1:F:406:ASP:HA	1.57	0.83
1:F:445:MET:HB3	1:F:446:LYS:CB	2.08	0.83
1:B:431:ASN:C	1:B:432:ILE:CG2	2.46	0.83
1:D:7:THR:C	1:D:8:VAL:HG23	1.98	0.82
1:B:368:ALA:O	1:B:369:ALA:HB3	1.77	0.82
1:E:431:ASN:CA	1:E:432:ILE:CG2	2.57	0.82
1:B:353:LEU:HB3	1:B:354:ILE:HG13	1.61	0.82
1:A:431:ASN:OD1	1:A:433:HIS:HB2	1.78	0.82
1:F:445:MET:CB	1:F:446:LYS:CB	2.58	0.81
1:A:432:ILE:O	1:A:432:ILE:HD13	1.81	0.80
1:B:431:ASN:O	1:B:432:ILE:CG2	2.30	0.80
1:B:7:THR:CG2	1:B:393:VAL:HB	2.11	0.80
1:D:309:ASN:ND2	1:D:310:GLU:HG3	1.96	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LEU:C	1:B:354:ILE:HG12	2.01	0.80
1:E:431:ASN:HA	1:E:432:ILE:CG2	2.11	0.80
1:B:432:ILE:CG1	1:B:432:ILE:O	2.30	0.80
1:C:7:THR:CG2	1:C:393:VAL:HB	2.12	0.79
1:B:368:ALA:O	1:B:369:ALA:CB	2.30	0.79
1:B:306:ILE:O	1:B:306:ILE:CG2	2.30	0.79
1:F:445:MET:CA	1:F:446:LYS:CB	2.50	0.79
1:B:431:ASN:O	1:B:432:ILE:HG23	1.83	0.79
1:E:432:ILE:N	1:E:493:ARG:HB2	1.93	0.78
1:E:431:ASN:O	1:E:494:ALA:N	2.13	0.78
1:A:393:VAL:HG21	1:D:12:TYR:CE1	2.19	0.78
1:E:397:PRO:C	1:E:398:LEU:HD23	2.04	0.78
1:D:7:THR:CA	1:D:8:VAL:HG23	2.13	0.78
1:D:7:THR:HA	1:D:8:VAL:HG23	1.66	0.77
1:C:417:ASN:HA	1:C:418:GLU:HB3	1.65	0.77
1:F:431:ASN:HD21	1:F:434:GLU:CG	1.98	0.77
1:A:7:THR:CG2	1:A:393:VAL:HG12	2.14	0.77
1:C:417:ASN:HA	1:C:418:GLU:CB	2.15	0.76
1:D:431:ASN:CA	1:D:432:ILE:HG22	2.16	0.76
1:A:431:ASN:CB	1:A:432:ILE:HG22	2.15	0.76
1:B:469:GLY:CA	1:B:470:GLU:HB2	2.10	0.76
1:F:398:LEU:HD13	1:F:406:ASP:C	2.06	0.76
1:F:398:LEU:CD1	1:F:406:ASP:CA	2.64	0.75
1:E:486:ILE:CG2	1:E:487:LEU:N	2.49	0.75
1:F:7:THR:CG2	1:F:393:VAL:HB	2.16	0.75
1:B:449:ARG:CG	1:B:449:ARG:NH1	2.40	0.75
1:A:7:THR:HG22	1:A:393:VAL:HG12	1.66	0.75
1:F:398:LEU:HD12	1:F:406:ASP:HB3	1.66	0.74
1:E:353:LEU:HB3	1:E:354:ILE:HG12	1.69	0.74
1:D:353:LEU:C	1:D:354:ILE:HG12	2.08	0.74
1:B:429:ASN:O	1:B:494:ALA:HA	1.88	0.74
1:D:310:GLU:H	1:D:311:PRO:HD3	1.50	0.74
1:F:363:GLU:O	1:F:364:ARG:HB2	1.87	0.74
1:A:431:ASN:OD1	1:A:434:GLU:HB2	1.88	0.74
1:B:306:ILE:HG22	1:B:306:ILE:O	1.86	0.74
1:F:353:LEU:HB3	1:F:354:ILE:HG12	1.70	0.74
1:C:363:GLU:O	1:C:364:ARG:HB2	1.87	0.73
1:A:444:GLY:N	1:A:445:MET:HB2	2.03	0.73
1:B:480:SER:HA	1:B:481:SER:HB2	1.69	0.73
1:A:12:TYR:CE2	1:D:12:TYR:CE2	2.77	0.73
1:F:435:ASP:OD1	1:F:493:ARG:HG2	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:HIS:H	1:B:493:ARG:HB2	1.54	0.73
1:A:336:ILE:HG23	1:A:413:VAL:HG22	1.71	0.73
1:F:336:ILE:HG23	1:F:413:VAL:HG22	1.71	0.72
1:F:4:ALA:O	1:F:438:LEU:HA	1.89	0.72
1:E:243:GLN:NE2	5:E:2011:HOH:O	2.21	0.72
1:E:336:ILE:HG23	1:E:413:VAL:HG22	1.71	0.72
1:C:469:GLY:HA2	1:C:470:GLU:HB3	1.72	0.72
1:F:469:GLY:HA2	1:F:470:GLU:CB	2.20	0.71
1:F:431:ASN:HA	1:F:432:ILE:HG22	1.72	0.71
1:A:353:LEU:O	1:A:354:ILE:HG12	1.91	0.71
1:F:469:GLY:HA2	1:F:470:GLU:HB3	1.71	0.71
1:E:469:GLY:HA2	1:E:470:GLU:CB	2.20	0.71
1:D:336:ILE:HG23	1:D:413:VAL:HG22	1.71	0.71
1:C:469:GLY:HA2	1:C:470:GLU:CB	2.20	0.71
1:B:336:ILE:HG23	1:B:413:VAL:HG22	1.71	0.71
1:D:409:ASP:O	1:D:429:ASN:CB	2.37	0.70
1:D:309:ASN:C	1:D:310:GLU:CG	2.60	0.70
1:C:478:ASP:HA	1:C:479:LYS:CB	2.13	0.70
1:F:431:ASN:C	1:F:432:ILE:HG22	2.12	0.70
1:E:469:GLY:HA2	1:E:470:GLU:HB3	1.72	0.70
1:D:469:GLY:HA2	1:D:470:GLU:CB	2.20	0.70
1:B:12:TYR:CE2	1:C:12:TYR:CE2	2.80	0.70
1:D:469:GLY:HA2	1:D:470:GLU:HB3	1.73	0.69
1:E:450:LEU:HD22	1:E:481:SER:HA	1.74	0.69
1:D:100:ILE:HG12	1:D:312:TRP:O	1.92	0.69
1:B:431:ASN:OD1	1:B:434:GLU:N	2.22	0.69
1:F:431:ASN:ND2	1:F:434:GLU:CG	2.55	0.69
1:A:310:GLU:N	1:A:311:PRO:HD3	2.08	0.69
1:E:486:ILE:HG22	1:E:487:LEU:N	2.07	0.69
1:C:431:ASN:HD21	1:C:434:GLU:HG3	1.58	0.69
1:C:353:LEU:C	1:C:354:ILE:HG12	2.13	0.69
1:F:477:SER:CA	1:F:478:ASP:OD1	2.41	0.69
1:C:485:GLY:CA	1:C:486:ILE:O	2.38	0.69
1:F:477:SER:C	1:F:478:ASP:OD1	2.31	0.68
1:F:398:LEU:CD1	1:F:406:ASP:C	2.61	0.68
1:F:431:ASN:ND2	1:F:434:GLU:HG3	2.08	0.68
1:D:479:LYS:O	1:D:480:SER:HB2	1.94	0.68
1:B:106:GLY:C	1:B:107:ILE:CG2	2.62	0.67
1:A:431:ASN:HA	1:A:432:ILE:HG22	0.70	0.67
1:D:311:PRO:HB2	1:D:312:TRP:CD1	2.28	0.67
1:C:417:ASN:HA	1:C:418:GLU:HG2	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:361:VAL:O	1:F:369:ALA:HA	1.94	0.67
1:D:309:ASN:CG	1:D:310:GLU:HG3	2.16	0.67
1:C:100:ILE:HG12	1:C:312:TRP:O	1.95	0.67
1:C:419:GLU:HG3	1:C:420:LYS:HB2	1.75	0.66
1:D:309:ASN:O	1:D:310:GLU:CG	2.43	0.66
1:D:361:VAL:O	1:D:369:ALA:HA	1.94	0.66
1:C:444:GLY:CA	1:C:445:MET:CB	2.73	0.66
1:F:431:ASN:O	1:F:433:HIS:N	2.28	0.66
1:A:393:VAL:HG21	1:D:12:TYR:CZ	2.31	0.66
1:C:361:VAL:O	1:C:369:ALA:HA	1.95	0.66
1:C:417:ASN:OD1	1:C:418:GLU:N	2.30	0.65
1:F:398:LEU:HD11	1:F:406:ASP:HB3	1.78	0.65
1:A:442:VAL:CG2	1:A:445:MET:HB3	2.22	0.65
1:C:429:ASN:O	1:C:429:ASN:CG	2.33	0.65
1:A:42:ASN:ND2	1:A:366:GLY:O	2.22	0.65
1:E:361:VAL:O	1:E:369:ALA:HA	1.95	0.65
1:B:361:VAL:O	1:B:369:ALA:HA	1.96	0.65
1:F:5:ARG:CB	1:F:395:ASN:O	2.45	0.65
1:C:431:ASN:ND2	1:C:431:ASN:O	2.30	0.65
1:F:445:MET:HB3	1:F:446:LYS:HB3	1.79	0.65
1:A:444:GLY:H	1:A:445:MET:HB2	1.62	0.65
1:D:363:GLU:O	1:D:364:ARG:HB2	1.97	0.65
1:D:353:LEU:O	1:D:354:ILE:HG12	1.96	0.65
1:E:410:ILE:HD11	1:E:491:LEU:HD12	1.79	0.65
1:D:380:HIS:HD2	1:D:496:TRP:HE1	1.45	0.65
1:F:365:ASN:N	1:F:365:ASN:OD1	2.30	0.64
1:E:431:ASN:HB2	1:E:433:HIS:H	1.63	0.64
1:A:444:GLY:HA3	1:A:445:MET:CB	2.21	0.64
1:D:7:THR:OG1	1:D:8:VAL:N	2.30	0.64
1:C:429:ASN:C	1:C:431:ASN:H	2.00	0.64
1:C:451:LEU:HD12	1:C:501:ILE:C	2.17	0.64
1:F:410:ILE:HD11	1:F:491:LEU:HD12	1.80	0.64
1:D:410:ILE:HD11	1:D:491:LEU:HD12	1.80	0.64
1:B:380:HIS:HD2	1:B:496:TRP:HE1	1.45	0.64
1:E:380:HIS:HD2	1:E:496:TRP:HE1	1.46	0.64
1:E:431:ASN:O	1:E:493:ARG:HA	1.97	0.63
1:C:410:ILE:HD11	1:C:491:LEU:HD12	1.79	0.63
1:C:417:ASN:O	1:C:422:GLU:N	2.26	0.63
1:C:417:ASN:CG	1:C:418:GLU:HG2	2.18	0.63
1:E:439:VAL:HG12	1:E:488:THR:HG22	1.80	0.63
1:B:429:ASN:OD1	1:B:431:ASN:N	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ILE:HD11	1:A:491:LEU:HD12	1.80	0.63
1:A:429:ASN:O	1:A:494:ALA:HA	1.97	0.63
1:C:478:ASP:HB3	1:C:479:LYS:CA	2.25	0.63
1:E:429:ASN:O	1:E:431:ASN:C	2.36	0.63
1:A:380:HIS:HD2	1:A:496:TRP:HE1	1.46	0.63
1:C:380:HIS:HD2	1:C:496:TRP:HE1	1.46	0.63
1:E:305:ASN:O	1:E:309:ASN:HB2	1.98	0.63
1:A:431:ASN:C	1:A:432:ILE:HG22	2.19	0.62
1:B:410:ILE:HD11	1:B:491:LEU:HD12	1.80	0.62
1:D:100:ILE:CG1	1:D:312:TRP:O	2.46	0.62
1:D:410:ILE:HD12	1:D:429:ASN:HB3	1.81	0.62
1:A:469:GLY:HA2	1:A:470:GLU:HB2	1.81	0.62
1:B:106:GLY:C	1:B:107:ILE:HG23	2.19	0.62
1:B:7:THR:HG22	1:B:393:VAL:HB	1.79	0.62
1:D:309:ASN:ND2	1:D:310:GLU:OE2	2.32	0.62
1:A:453:HIS:ND1	1:A:499:ILE:HG12	2.14	0.62
1:D:453:HIS:ND1	1:D:499:ILE:HG12	2.15	0.62
1:C:453:HIS:ND1	1:C:499:ILE:HG12	2.14	0.62
1:C:408:THR:O	1:C:430:ARG:HD3	2.00	0.62
1:B:353:LEU:O	1:B:354:ILE:HG12	1.99	0.62
1:D:380:HIS:CD2	1:D:496:TRP:HE1	2.18	0.62
1:B:380:HIS:CD2	1:B:496:TRP:HE1	2.18	0.62
1:E:380:HIS:CD2	1:E:496:TRP:HE1	2.18	0.62
1:A:432:ILE:H	1:A:494:ALA:N	1.98	0.62
1:E:429:ASN:C	1:E:431:ASN:N	2.50	0.62
1:D:309:ASN:CB	1:D:310:GLU:HG3	2.29	0.62
1:D:353:LEU:HB3	1:D:354:ILE:HG13	1.80	0.62
1:B:410:ILE:HD12	1:B:429:ASN:HB2	1.81	0.62
1:B:453:HIS:ND1	1:B:499:ILE:HG12	2.15	0.62
1:E:453:HIS:ND1	1:E:499:ILE:HG12	2.15	0.61
1:C:478:ASP:CG	1:C:479:LYS:HB2	2.17	0.61
1:A:380:HIS:CD2	1:A:496:TRP:HE1	2.18	0.61
1:E:429:ASN:O	1:E:429:ASN:CG	2.39	0.61
1:F:453:HIS:ND1	1:F:499:ILE:HG12	2.16	0.61
1:C:7:THR:HG22	1:C:393:VAL:HB	1.81	0.61
1:A:478:ASP:HB3	1:A:479:LYS:CA	2.31	0.61
1:A:442:VAL:HG22	1:A:445:MET:CB	2.26	0.61
1:A:449:ARG:HG2	1:A:449:ARG:O	1.98	0.61
1:E:431:ASN:HB2	1:E:432:ILE:CG2	2.15	0.61
1:F:398:LEU:CD1	1:F:406:ASP:CB	2.72	0.61
1:B:480:SER:HA	1:B:481:SER:HB3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:431:ASN:CG	1:F:431:ASN:O	2.38	0.61
1:C:431:ASN:HA	1:C:432:ILE:HB	1.83	0.61
1:C:380:HIS:CD2	1:C:496:TRP:HE1	2.18	0.60
1:C:419:GLU:HG3	1:C:419:GLU:O	2.01	0.60
1:B:408:THR:O	1:B:430:ARG:HD2	2.01	0.60
1:C:479:LYS:O	1:C:480:SER:CB	2.49	0.60
1:C:417:ASN:HA	1:C:418:GLU:CG	2.31	0.60
1:B:480:SER:CA	1:B:481:SER:HB2	2.31	0.59
1:C:100:ILE:CG1	1:C:312:TRP:O	2.50	0.59
1:E:365:ASN:N	1:E:365:ASN:OD1	2.35	0.59
1:C:479:LYS:O	1:C:480:SER:HB3	2.03	0.59
1:F:429:ASN:O	1:F:494:ALA:N	2.35	0.59
1:F:432:ILE:O	1:F:433:HIS:HD2	1.85	0.59
1:B:51:ARG:HH22	1:B:367:GLY:HA3	1.68	0.59
1:D:309:ASN:O	1:D:310:GLU:HG3	2.03	0.59
1:A:353:LEU:HB3	1:A:354:ILE:HG13	1.83	0.59
1:A:368:ALA:O	1:A:369:ALA:HB3	2.01	0.59
1:E:8:VAL:HG22	1:E:442:VAL:HG23	1.85	0.59
1:F:431:ASN:CA	1:F:432:ILE:HG22	2.32	0.58
1:A:310:GLU:H	1:A:311:PRO:CD	2.16	0.58
1:B:353:LEU:HB3	1:B:354:ILE:CG1	2.32	0.58
1:E:431:ASN:C	1:E:494:ALA:N	2.57	0.58
1:D:309:ASN:HB3	1:D:310:GLU:CB	2.31	0.58
1:E:362:THR:HG22	1:E:369:ALA:HB2	1.84	0.58
1:A:410:ILE:HD12	1:A:429:ASN:HB2	1.86	0.58
1:F:353:LEU:CB	1:F:354:ILE:HG12	2.34	0.58
1:C:362:THR:HG22	1:C:369:ALA:HB2	1.85	0.58
1:F:410:ILE:HD12	1:F:429:ASN:HB2	1.86	0.58
1:E:432:ILE:N	1:E:493:ARG:C	2.57	0.58
1:B:469:GLY:HA2	1:B:470:GLU:HB3	1.80	0.58
1:A:469:GLY:HA2	1:A:470:GLU:CB	2.34	0.58
1:D:445:MET:HB2	1:D:447:ASP:H	1.68	0.58
1:D:429:ASN:CB	1:D:430:ARG:HB3	2.34	0.58
1:E:398:LEU:HD23	1:E:398:LEU:N	2.16	0.58
1:A:434:GLU:H	1:A:493:ARG:HB3	1.68	0.57
1:E:431:ASN:C	1:E:494:ALA:H	2.07	0.57
1:F:455:VAL:HG23	1:F:497:ASN:OD1	2.03	0.57
1:F:362:THR:HG22	1:F:369:ALA:HB2	1.85	0.57
1:F:453:HIS:CE1	1:F:497:ASN:ND2	2.72	0.57
1:E:353:LEU:CB	1:E:354:ILE:HG12	2.33	0.57
1:D:362:THR:HG22	1:D:369:ALA:HB2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:ILE:H	1:E:493:ARG:CA	2.17	0.57
1:A:442:VAL:HG13	1:A:445:MET:C	2.25	0.57
1:C:431:ASN:HA	1:C:432:ILE:HG22	1.85	0.57
1:C:417:ASN:O	1:C:422:GLU:O	2.23	0.57
1:C:417:ASN:OD1	1:C:420:LYS:HB3	2.04	0.57
1:C:417:ASN:OD1	1:C:418:GLU:CG	2.53	0.56
1:D:309:ASN:C	1:D:310:GLU:HG3	2.24	0.56
1:F:458:HIS:HD2	1:F:460:ASP:H	1.53	0.56
1:B:481:SER:HB3	1:B:488:THR:O	2.06	0.56
1:B:51:ARG:HH12	1:B:367:GLY:CA	2.18	0.56
1:C:491:LEU:HD22	1:C:497:ASN:ND2	2.21	0.56
1:A:431:ASN:CA	1:A:432:ILE:CB	2.78	0.56
1:A:478:ASP:CG	1:A:479:LYS:HB3	2.25	0.56
1:F:380:HIS:CD2	1:F:496:TRP:HE1	2.24	0.56
1:C:419:GLU:O	1:C:419:GLU:CG	2.53	0.56
1:C:339:MET:HE1	1:C:413:VAL:CG1	2.36	0.56
1:B:100:ILE:HG12	1:B:312:TRP:O	2.05	0.56
1:B:477:SER:HB2	1:B:478:ASP:OD1	2.06	0.56
1:E:458:HIS:HD2	1:E:460:ASP:H	1.54	0.56
1:B:469:GLY:CA	1:B:470:GLU:HB3	2.35	0.56
1:C:431:ASN:HA	1:C:432:ILE:CB	2.36	0.56
1:B:429:ASN:O	1:B:494:ALA:CA	2.54	0.55
1:B:458:HIS:HD2	1:B:460:ASP:H	1.54	0.55
1:B:480:SER:CA	1:B:481:SER:CB	2.81	0.55
1:E:431:ASN:HB2	1:E:433:HIS:N	2.21	0.55
1:D:458:HIS:HD2	1:D:460:ASP:H	1.54	0.55
1:B:491:LEU:HD22	1:B:497:ASN:ND2	2.21	0.55
1:B:354:ILE:H	1:B:358:ALA:CB	2.20	0.55
1:D:257:ALA:HA	1:D:430:ARG:NH1	2.21	0.55
1:A:458:HIS:HD2	1:A:460:ASP:H	1.54	0.55
1:F:398:LEU:CD1	1:F:406:ASP:HA	2.32	0.55
1:D:305:ASN:O	1:D:309:ASN:CB	2.48	0.55
1:B:353:LEU:C	1:B:354:ILE:CG1	2.73	0.55
1:D:310:GLU:N	1:D:311:PRO:HD3	2.22	0.55
1:E:491:LEU:HD22	1:E:497:ASN:ND2	2.21	0.55
1:F:449:ARG:O	1:F:449:ARG:HG2	2.05	0.55
1:D:491:LEU:HD22	1:D:497:ASN:ND2	2.22	0.54
1:E:8:VAL:HG22	1:E:8:VAL:O	2.06	0.54
1:B:431:ASN:OD1	1:B:434:GLU:HB2	2.07	0.54
1:D:309:ASN:O	1:D:310:GLU:HG2	2.06	0.54
1:B:393:VAL:HG22	1:C:12:TYR:OH	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LEU:HD22	1:A:497:ASN:ND2	2.22	0.54
1:A:429:ASN:C	1:A:431:ASN:H	2.11	0.54
1:A:432:ILE:H	1:A:493:ARG:C	2.11	0.54
1:D:42:ASN:ND2	1:D:366:GLY:O	2.41	0.54
1:D:445:MET:HG3	1:D:448:TYR:CG	2.42	0.54
1:A:393:VAL:CG2	1:D:12:TYR:CE1	2.90	0.54
1:B:100:ILE:CG1	1:B:312:TRP:O	2.56	0.53
1:B:12:TYR:OH	1:C:393:VAL:HG22	2.08	0.53
1:F:7:THR:HG23	1:F:393:VAL:HB	1.91	0.53
1:C:431:ASN:HA	1:C:432:ILE:CG2	2.38	0.53
1:C:398:LEU:N	1:C:398:LEU:HD23	2.22	0.53
1:D:7:THR:C	1:D:8:VAL:HG22	2.27	0.53
1:E:311:PRO:HB2	1:E:312:TRP:CD1	2.44	0.53
1:F:311:PRO:HB2	1:F:312:TRP:CD1	2.43	0.53
1:C:417:ASN:CA	1:C:418:GLU:HG2	2.38	0.53
1:D:354:ILE:H	1:D:358:ALA:CB	2.22	0.53
1:E:397:PRO:O	1:E:398:LEU:HD23	2.09	0.53
1:D:309:ASN:ND2	1:D:310:GLU:CG	2.69	0.52
1:B:432:ILE:O	1:B:433:HIS:CD2	2.63	0.52
1:C:397:PRO:C	1:C:398:LEU:HD23	2.30	0.52
1:F:51:ARG:HH12	1:F:367:GLY:HA3	1.74	0.52
1:E:468:ASN:O	1:E:469:GLY:O	2.27	0.52
1:C:42:ASN:ND2	1:C:366:GLY:O	2.39	0.52
1:E:435:ASP:OD1	1:E:493:ARG:HG2	2.10	0.52
1:C:477:SER:HB2	1:C:478:ASP:OD1	2.09	0.52
1:A:433:HIS:N	1:A:493:ARG:HB2	2.25	0.52
1:C:449:ARG:HA	1:C:482:PHE:CD2	2.45	0.52
1:D:429:ASN:O	1:D:429:ASN:CG	2.48	0.51
1:B:431:ASN:O	1:B:433:HIS:HB2	2.10	0.51
1:F:491:LEU:HD22	1:F:497:ASN:ND2	2.24	0.51
1:F:7:THR:HG22	1:F:393:VAL:HB	1.91	0.51
1:D:431:ASN:O	1:D:431:ASN:CG	2.48	0.51
1:A:477:SER:HB2	1:A:478:ASP:OD1	2.10	0.51
1:D:364:ARG:O	1:D:365:ASN:C	2.49	0.51
1:B:364:ARG:O	1:B:365:ASN:C	2.49	0.51
1:C:354:ILE:H	1:C:358:ALA:CB	2.23	0.51
1:A:432:ILE:H	1:A:493:ARG:CA	2.24	0.51
1:D:67:ARG:HD2	1:D:291:ASP:HB2	1.93	0.51
1:F:398:LEU:CD1	1:F:406:ASP:O	2.59	0.51
1:D:353:LEU:C	1:D:354:ILE:CG1	2.75	0.51
1:D:429:ASN:HB2	1:D:430:ARG:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:LEU:CD1	1:C:501:ILE:C	2.80	0.50
1:C:175:ASP:OD1	1:C:214:SER:OG	2.28	0.50
1:B:175:ASP:OD1	1:B:214:SER:OG	2.29	0.50
1:E:8:VAL:CG2	1:E:8:VAL:O	2.59	0.50
1:A:188:TYR:HA	1:A:191:ILE:HG22	1.93	0.50
1:B:67:ARG:HD2	1:B:291:ASP:HB2	1.93	0.50
1:C:417:ASN:OD1	1:C:418:GLU:HG2	2.11	0.50
1:B:188:TYR:HA	1:B:191:ILE:HG22	1.93	0.50
1:B:429:ASN:O	1:B:494:ALA:N	2.43	0.50
1:B:478:ASP:HB3	1:B:479:LYS:CB	2.42	0.50
1:A:393:VAL:CG2	1:D:12:TYR:CZ	2.94	0.50
1:C:188:TYR:HA	1:C:191:ILE:HG22	1.93	0.50
1:E:67:ARG:HD2	1:E:291:ASP:HB2	1.93	0.50
1:F:4:ALA:CB	1:F:395:ASN:O	2.60	0.50
1:B:480:SER:HB2	1:B:489:SER:HA	1.93	0.50
1:D:188:TYR:HA	1:D:191:ILE:HG22	1.93	0.50
1:E:429:ASN:O	1:E:429:ASN:OD1	2.30	0.50
1:E:429:ASN:O	1:E:431:ASN:CA	2.60	0.50
1:C:307:MET:O	1:C:308:GLN:HB2	2.12	0.50
1:F:432:ILE:HD13	1:F:433:HIS:CD2	2.47	0.50
1:F:431:ASN:OD1	1:F:431:ASN:O	2.30	0.50
1:C:429:ASN:C	1:C:431:ASN:N	2.65	0.50
1:F:67:ARG:HD2	1:F:291:ASP:HB2	1.94	0.50
1:C:429:ASN:O	1:C:429:ASN:OD1	2.30	0.49
1:E:8:VAL:CG2	1:E:442:VAL:HG23	2.42	0.49
1:D:445:MET:SD	1:D:445:MET:N	2.85	0.49
1:F:398:LEU:HD13	1:F:406:ASP:O	2.10	0.49
1:B:51:ARG:HH12	1:B:367:GLY:HA2	1.76	0.49
1:A:361:VAL:O	1:A:369:ALA:HA	2.12	0.49
1:A:451:LEU:HB2	1:A:500:ARG:O	2.12	0.49
1:F:188:TYR:HA	1:F:191:ILE:HG22	1.93	0.49
1:F:431:ASN:HD21	1:F:434:GLU:HG3	1.73	0.49
1:E:449:ARG:HG2	1:E:449:ARG:O	2.12	0.49
1:D:175:ASP:OD1	1:D:214:SER:OG	2.28	0.49
1:E:478:ASP:HB3	1:E:479:LYS:CB	2.43	0.49
1:B:432:ILE:CD1	1:B:432:ILE:O	2.59	0.49
1:C:458:HIS:HD2	1:C:460:ASP:H	1.61	0.49
1:F:453:HIS:CE1	1:F:497:ASN:HD22	2.31	0.49
1:C:339:MET:CE	1:C:413:VAL:CG1	2.90	0.49
1:A:10:LYS:HD2	1:A:11:ASP:OD1	2.12	0.49
1:A:67:ARG:HD2	1:A:291:ASP:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:SER:HB2	1:C:489:SER:HA	1.95	0.49
1:A:353:LEU:HB3	1:A:354:ILE:CG1	2.41	0.49
1:B:354:ILE:H	1:B:358:ALA:HB2	1.77	0.49
1:C:67:ARG:HD2	1:C:291:ASP:HB2	1.93	0.49
1:C:7:THR:HG23	1:C:393:VAL:HB	1.93	0.49
1:A:363:GLU:O	1:A:364:ARG:HB2	2.13	0.49
1:A:442:VAL:HG11	1:A:482:PHE:HZ	1.78	0.49
1:D:431:ASN:O	1:D:431:ASN:OD1	2.30	0.49
1:B:479:LYS:O	1:B:480:SER:HB3	2.12	0.49
1:C:431:ASN:CG	1:C:431:ASN:O	2.48	0.49
1:F:175:ASP:OD1	1:F:214:SER:OG	2.27	0.49
1:F:42:ASN:ND2	1:F:366:GLY:O	2.29	0.49
1:B:450:LEU:CD1	1:B:451:LEU:H	2.22	0.48
1:E:188:TYR:HA	1:E:191:ILE:HG22	1.93	0.48
1:F:4:ALA:HB1	1:F:395:ASN:O	2.13	0.48
1:A:310:GLU:N	1:A:311:PRO:CD	2.76	0.48
1:B:353:LEU:CB	1:B:354:ILE:HG13	2.38	0.48
1:A:175:ASP:OD1	1:A:214:SER:OG	2.28	0.48
1:F:429:ASN:OD1	1:F:431:ASN:HB3	2.13	0.48
1:E:480:SER:HB2	1:E:489:SER:HA	1.95	0.48
1:A:293:TRP:O	1:A:294:ASN:HB2	2.14	0.48
1:B:293:TRP:O	1:B:294:ASN:HB2	2.13	0.48
1:A:431:ASN:O	1:A:431:ASN:OD1	2.30	0.48
1:E:456:LEU:HB3	1:E:496:TRP:HB3	1.95	0.48
1:A:444:GLY:HA3	1:A:445:MET:SD	2.53	0.48
1:D:366:GLY:HA3	1:D:367:GLY:HA2	1.49	0.48
1:E:42:ASN:ND2	1:E:366:GLY:O	2.45	0.48
1:C:354:ILE:H	1:C:358:ALA:HB2	1.79	0.48
1:A:456:LEU:HB3	1:A:496:TRP:HB3	1.96	0.48
1:E:486:ILE:HG23	1:E:487:LEU:H	1.78	0.48
1:B:456:LEU:HB3	1:B:496:TRP:HB3	1.95	0.47
1:E:175:ASP:OD1	1:E:214:SER:OG	2.29	0.47
1:E:424:THR:HG23	1:E:500:ARG:HG2	1.96	0.47
1:B:435:ASP:OD1	1:B:493:ARG:HG2	2.14	0.47
1:B:354:ILE:N	1:B:358:ALA:HB1	2.29	0.47
1:F:435:ASP:OD1	1:F:493:ARG:CG	2.62	0.47
1:D:456:LEU:HB3	1:D:496:TRP:HB3	1.95	0.47
1:A:368:ALA:O	1:A:369:ALA:CB	2.62	0.47
1:C:456:LEU:HB3	1:C:496:TRP:HB3	1.95	0.47
1:C:417:ASN:OD1	1:C:418:GLU:HG3	2.14	0.47
1:A:451:LEU:HD23	1:A:451:LEU:HA	1.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:ILE:N	1:E:493:ARG:CA	2.77	0.47
1:F:453:HIS:HE1	1:F:497:ASN:HD22	1.63	0.47
1:B:424:THR:HG23	1:B:500:ARG:HG2	1.97	0.47
1:F:456:LEU:HB3	1:F:496:TRP:HB3	1.97	0.47
1:C:424:THR:HG23	1:C:500:ARG:HG2	1.96	0.47
1:D:354:ILE:H	1:D:358:ALA:HB2	1.79	0.47
1:F:424:THR:HG23	1:F:500:ARG:HG2	1.97	0.47
1:B:479:LYS:O	1:B:480:SER:CB	2.62	0.47
1:B:12:TYR:HE2	1:C:12:TYR:CE2	2.32	0.47
1:C:293:TRP:O	1:C:294:ASN:HB2	2.15	0.47
1:E:431:ASN:OD1	1:E:431:ASN:N	2.46	0.47
1:A:305:ASN:O	1:A:309:ASN:CB	2.57	0.47
1:B:51:ARG:NH2	1:B:367:GLY:HA3	2.29	0.47
1:D:256:LEU:O	1:D:430:ARG:NH1	2.48	0.46
1:A:351:ALA:HA	1:A:352:GLN:HA	1.69	0.46
1:F:293:TRP:O	1:F:294:ASN:HB2	2.14	0.46
1:D:293:TRP:O	1:D:294:ASN:HB2	2.15	0.46
1:A:429:ASN:O	1:A:494:ALA:N	2.48	0.46
1:D:309:ASN:HD22	1:D:310:GLU:CG	2.28	0.46
1:D:453:HIS:CE1	1:D:499:ILE:HG12	2.51	0.46
1:A:424:THR:HG23	1:A:500:ARG:HG2	1.97	0.46
1:D:429:ASN:O	1:D:494:ALA:HA	2.16	0.46
1:D:354:ILE:N	1:D:358:ALA:HB1	2.31	0.46
1:F:431:ASN:ND2	1:F:434:GLU:HG2	2.29	0.46
1:A:354:ILE:H	1:A:358:ALA:CB	2.28	0.46
1:C:353:LEU:HB3	1:C:354:ILE:HG13	1.98	0.46
1:C:449:ARG:O	1:C:501:ILE:HG23	2.14	0.46
1:A:453:HIS:CE1	1:A:499:ILE:HG12	2.51	0.46
1:F:351:ALA:HA	1:F:352:GLN:HA	1.68	0.46
1:C:431:ASN:C	1:C:433:HIS:H	2.16	0.46
1:D:306:ILE:HG21	1:D:318:LEU:CD2	2.45	0.46
1:E:203:ASP:O	1:E:206:ILE:HG12	2.16	0.46
1:D:424:THR:HG23	1:D:500:ARG:HG2	1.97	0.46
1:E:479:LYS:O	1:E:480:SER:HB3	2.14	0.46
1:F:481:SER:OG	1:F:481:SER:O	2.34	0.46
1:B:203:ASP:O	1:B:206:ILE:HG12	2.16	0.46
1:E:293:TRP:O	1:E:294:ASN:HB2	2.14	0.46
1:D:429:ASN:CA	1:D:430:ARG:CB	2.52	0.46
1:B:432:ILE:HD13	1:B:432:ILE:O	2.16	0.46
1:D:431:ASN:C	1:D:433:HIS:H	2.16	0.46
1:F:203:ASP:O	1:F:206:ILE:HG12	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:GLY:O	1:C:108:ASN:N	2.49	0.46
1:C:432:ILE:O	1:C:432:ILE:HD13	2.16	0.45
1:B:453:HIS:CE1	1:B:499:ILE:HG12	2.51	0.45
1:C:428:VAL:CG1	1:C:429:ASN:N	2.79	0.45
1:C:354:ILE:N	1:C:358:ALA:HB1	2.31	0.45
1:D:484:ASP:HA	1:D:485:GLY:HA2	1.53	0.45
1:E:479:LYS:O	1:E:480:SER:CB	2.64	0.45
1:A:106:GLY:O	1:A:108:ASN:N	2.49	0.45
1:A:203:ASP:O	1:A:206:ILE:HG12	2.16	0.45
1:D:363:GLU:HB2	1:D:367:GLY:C	2.37	0.45
1:E:453:HIS:CE1	1:E:499:ILE:HG12	2.52	0.45
1:D:447:ASP:CA	1:D:448:TYR:HB2	2.47	0.45
1:D:106:GLY:O	1:D:108:ASN:N	2.49	0.45
1:A:431:ASN:C	1:A:431:ASN:OD1	2.53	0.45
1:C:453:HIS:CE1	1:C:499:ILE:HG12	2.51	0.45
1:B:430:ARG:O	1:B:430:ARG:HG3	2.16	0.45
1:B:311:PRO:HB2	1:B:312:TRP:CD1	2.51	0.45
1:B:7:THR:HG23	1:B:393:VAL:HB	1.92	0.45
1:D:203:ASP:O	1:D:206:ILE:HG12	2.17	0.45
1:C:478:ASP:CG	1:C:479:LYS:CB	2.81	0.45
1:D:7:THR:O	1:D:8:VAL:HG22	2.17	0.45
1:F:453:HIS:CE1	1:F:499:ILE:HG12	2.52	0.45
1:A:429:ASN:O	1:A:494:ALA:CA	2.63	0.45
1:B:168:TRP:HB2	1:B:208:LEU:HD23	1.99	0.45
1:D:306:ILE:CG2	1:D:318:LEU:HD21	2.46	0.45
1:C:325:PHE:CZ	1:C:457:GLU:HA	2.52	0.45
1:C:203:ASP:O	1:C:206:ILE:HG12	2.17	0.45
1:B:381:ALA:HA	1:B:426:PHE:CE2	2.52	0.44
1:F:432:ILE:HD13	1:F:432:ILE:O	2.18	0.44
1:E:325:PHE:CZ	1:E:457:GLU:HA	2.53	0.44
1:E:106:GLY:O	1:E:108:ASN:N	2.50	0.44
1:F:106:GLY:O	1:F:108:ASN:N	2.50	0.44
1:A:429:ASN:C	1:A:431:ASN:N	2.70	0.44
1:E:429:ASN:C	1:E:431:ASN:H	2.17	0.44
1:F:487:LEU:HG	1:F:488:THR:CA	2.47	0.44
1:B:351:ALA:HA	1:B:352:GLN:HA	1.68	0.44
1:A:325:PHE:CZ	1:A:457:GLU:HA	2.53	0.44
1:C:444:GLY:HA3	1:C:445:MET:HB3	1.93	0.44
1:E:450:LEU:HD22	1:E:481:SER:CA	2.43	0.44
1:A:168:TRP:HB2	1:A:208:LEU:HD23	2.00	0.44
1:D:309:ASN:HD22	1:D:310:GLU:CD	2.20	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ILE:O	1:B:306:ILE:HG23	2.15	0.44
1:C:168:TRP:HB2	1:C:208:LEU:HD23	2.00	0.44
1:D:365:ASN:OD1	1:D:365:ASN:N	2.51	0.44
1:C:398:LEU:HD13	1:C:406:ASP:HB3	1.98	0.44
1:E:168:TRP:HB2	1:E:208:LEU:HD23	2.00	0.44
1:D:168:TRP:HB2	1:D:208:LEU:HD23	2.00	0.44
1:F:325:PHE:CZ	1:F:457:GLU:HA	2.53	0.44
1:C:478:ASP:HA	1:C:479:LYS:CG	2.48	0.44
1:A:431:ASN:O	1:A:431:ASN:CG	2.55	0.44
1:C:417:ASN:CA	1:C:418:GLU:CB	2.93	0.44
1:B:429:ASN:OD1	1:B:431:ASN:HB3	2.18	0.44
1:C:451:LEU:HD12	1:C:502:GLY:N	2.33	0.44
1:D:381:ALA:HA	1:D:426:PHE:CE2	2.53	0.44
1:B:12:TYR:CE2	1:C:12:TYR:HE2	2.33	0.43
1:C:339:MET:CE	1:C:413:VAL:HG11	2.48	0.43
1:D:325:PHE:CZ	1:D:457:GLU:HA	2.53	0.43
1:F:481:SER:O	1:F:488:THR:CA	2.66	0.43
1:F:381:ALA:HA	1:F:426:PHE:CE2	2.53	0.43
1:F:168:TRP:HB2	1:F:208:LEU:HD23	2.00	0.43
1:E:486:ILE:CG2	1:E:487:LEU:H	2.29	0.43
1:C:381:ALA:HA	1:C:426:PHE:CE2	2.54	0.43
1:A:381:ALA:HA	1:A:426:PHE:CE2	2.54	0.43
1:D:309:ASN:HB3	1:D:310:GLU:HG3	2.00	0.43
1:A:452:GLU:OE2	1:A:500:ARG:NH1	2.52	0.43
1:E:364:ARG:O	1:E:365:ASN:C	2.56	0.43
1:E:478:ASP:HA	1:E:479:LYS:CB	2.49	0.43
1:B:325:PHE:CZ	1:B:457:GLU:HA	2.53	0.43
1:F:4:ALA:O	1:F:439:VAL:N	2.45	0.43
1:B:478:ASP:HA	1:B:479:LYS:CB	2.49	0.43
1:B:450:LEU:CD1	1:B:452:GLU:N	2.81	0.42
1:A:354:ILE:H	1:A:358:ALA:HB2	1.83	0.42
1:B:478:ASP:CA	1:B:479:LYS:CB	2.97	0.42
1:E:478:ASP:CA	1:E:479:LYS:CB	2.97	0.42
1:C:417:ASN:C	1:C:417:ASN:OD1	2.57	0.42
1:A:354:ILE:N	1:A:358:ALA:HB1	2.34	0.42
1:D:100:ILE:HG13	1:D:312:TRP:O	2.18	0.42
1:F:380:HIS:HD2	1:F:496:TRP:NE1	2.17	0.42
1:C:451:LEU:HD12	1:C:501:ILE:CA	2.49	0.42
1:B:353:LEU:CB	1:B:354:ILE:CG1	2.97	0.42
2:D:1504:HR:H2'	2:D:1505:HR:H4'	2.00	0.42
1:F:144:HIS:HA	1:F:145:PRO:HD3	1.95	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:ASP:OD1	1:D:493:ARG:HG2	2.20	0.42
1:A:63:VAL:HA	1:A:64:PRO:HD3	1.92	0.42
1:F:429:ASN:O	1:F:494:ALA:HA	2.19	0.42
1:E:458:HIS:CD2	1:E:460:ASP:H	2.36	0.42
1:A:458:HIS:CD2	1:A:460:ASP:H	2.36	0.42
1:D:351:ALA:HA	1:D:352:GLN:HA	1.69	0.42
1:E:381:ALA:HA	1:E:426:PHE:CE2	2.54	0.42
1:E:309:ASN:O	1:E:310:GLU:HG2	2.20	0.42
1:C:417:ASN:CB	1:C:418:GLU:HG2	2.50	0.42
1:D:15:ALA:HB2	1:D:343:ASP:HB3	2.02	0.42
1:A:431:ASN:O	1:A:434:GLU:O	2.37	0.41
1:A:482:PHE:HD1	1:A:482:PHE:HA	1.68	0.41
1:D:114:CYS:HA	1:D:117:VAL:HG22	2.01	0.41
1:D:368:ALA:O	1:D:369:ALA:HB3	2.19	0.41
1:E:366:GLY:HA3	1:E:367:GLY:HA2	1.37	0.41
1:F:458:HIS:CD2	1:F:460:ASP:H	2.36	0.41
1:C:241:LEU:C	1:C:242:HIS:HD2	2.23	0.41
1:B:214:SER:O	1:B:242:HIS:HB2	2.20	0.41
1:B:434:GLU:C	1:B:493:ARG:HB3	2.41	0.41
1:D:431:ASN:O	1:D:433:HIS:N	2.38	0.41
1:A:380:HIS:HD2	1:A:496:TRP:NE1	2.16	0.41
1:A:10:LYS:H	1:A:10:LYS:HG3	1.62	0.41
1:A:214:SER:O	1:A:242:HIS:HB2	2.21	0.41
1:E:214:SER:O	1:E:242:HIS:HB2	2.20	0.41
1:F:114:CYS:HA	1:F:117:VAL:HG22	2.01	0.41
1:C:409:ASP:O	1:C:430:ARG:HB3	2.21	0.41
1:C:214:SER:O	1:C:242:HIS:HB2	2.20	0.41
1:F:214:SER:O	1:F:242:HIS:HB2	2.20	0.41
1:E:241:LEU:C	1:E:242:HIS:HD2	2.24	0.41
1:B:15:ALA:HB2	1:B:343:ASP:HB3	2.02	0.41
1:D:214:SER:O	1:D:242:HIS:HB2	2.21	0.41
1:A:114:CYS:HA	1:A:117:VAL:HG22	2.01	0.41
1:A:369:ALA:O	1:A:370:TRP:HB3	2.19	0.41
1:C:15:ALA:HB2	1:C:343:ASP:HB3	2.02	0.41
1:D:10:LYS:HD2	1:D:11:ASP:OD1	2.21	0.41
1:F:306:ILE:O	1:F:306:ILE:HG22	2.21	0.41
1:A:431:ASN:CA	1:A:432:ILE:CG2	2.30	0.41
1:E:432:ILE:N	1:E:493:ARG:CB	2.64	0.41
1:A:7:THR:HG21	1:A:393:VAL:HG12	2.01	0.41
1:C:461:LEU:HD12	1:C:461:LEU:HA	1.88	0.41
1:D:380:HIS:HD2	1:D:496:TRP:NE1	2.15	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:HIS:HA	1:C:145:PRO:HD3	1.96	0.40
1:C:368:ALA:O	1:C:369:ALA:HB3	2.21	0.40
1:E:63:VAL:HA	1:E:64:PRO:HD3	1.92	0.40
1:E:114:CYS:HA	1:E:117:VAL:HG22	2.02	0.40
1:E:15:ALA:HB2	1:E:343:ASP:HB3	2.02	0.40
1:B:114:CYS:HA	1:B:117:VAL:HG22	2.02	0.40
1:E:451:LEU:O	1:E:452:GLU:HB3	2.21	0.40
1:D:63:VAL:HA	1:D:64:PRO:HD3	1.92	0.40
1:A:15:ALA:HB2	1:A:343:ASP:HB3	2.02	0.40
1:A:353:LEU:HG	1:A:354:ILE:HG12	2.03	0.40
1:C:311:PRO:HB2	1:C:312:TRP:CD1	2.56	0.40
1:C:451:LEU:CD1	1:C:502:GLY:N	2.84	0.40
1:D:241:LEU:C	1:D:242:HIS:HD2	2.25	0.40
1:C:351:ALA:HA	1:C:352:GLN:HA	1.68	0.40
1:C:114:CYS:HA	1:C:117:VAL:HG22	2.02	0.40
1:D:477:SER:HB2	1:D:478:ASP:OD1	2.21	0.40
1:A:433:HIS:HB3	1:A:434:GLU:HG3	2.02	0.40
1:C:353:LEU:O	1:C:354:ILE:HG12	2.20	0.40
1:E:477:SER:HB2	1:E:478:ASP:OD1	2.22	0.40
1:D:431:ASN:C	1:D:432:ILE:HG22	2.42	0.40
1:F:431:ASN:HD21	1:F:434:GLU:HG2	1.81	0.40

There are no symmetry-related clashes.

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	490/513 (96%)	445 (91%)	26 (5%)	19 (4%)	4	8
1	B	493/513 (96%)	440 (89%)	28 (6%)	25 (5%)	2	4
1	C	493/513 (96%)	438 (89%)	30 (6%)	25 (5%)	2	4
1	D	497/513 (97%)	445 (90%)	31 (6%)	21 (4%)	3	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	484/513 (94%)	438 (90%)	27 (6%)	19 (4%)	4	8
1	F	490/513 (96%)	442 (90%)	27 (6%)	21 (4%)	3	7
All	All	2947/3078 (96%)	2648 (90%)	169 (6%)	130 (4%)	3	6

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	TRP
1	A	309	ASN
1	A	310	GLU
1	A	354	ILE
1	A	365	ASN
1	A	370	TRP
1	A	430	ARG
1	A	432	ILE
1	A	434	GLU
1	A	478	ASP
1	B	46	ASP
1	B	108	ASN
1	B	224	TRP
1	B	305	ASN
1	B	309	ASN
1	B	313	ARG
1	B	354	ILE
1	B	365	ASN
1	B	430	ARG
1	B	433	HIS
1	B	479	LYS
1	B	480	SER
1	B	481	SER
1	B	490	MET
1	C	224	TRP
1	C	313	ARG
1	C	354	ILE
1	C	419	GLU
1	C	430	ARG
1	C	432	ILE
1	C	451	LEU
1	C	478	ASP
1	C	479	LYS
1	C	480	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	481	SER
1	C	486	ILE
1	D	8	VAL
1	D	224	TRP
1	D	310	GLU
1	D	313	ARG
1	D	354	ILE
1	D	365	ASN
1	D	432	ILE
1	D	446	LYS
1	D	478	ASP
1	D	479	LYS
1	D	480	SER
1	E	365	ASN
1	E	430	ARG
1	E	432	ILE
1	E	479	LYS
1	E	480	SER
1	F	5	ARG
1	F	365	ASN
1	F	430	ARG
1	F	478	ASP
1	F	488	THR
1	A	107	ILE
1	A	363	GLU
1	B	107	ILE
1	B	363	GLU
1	B	369	ALA
1	B	478	ASP
1	C	107	ILE
1	C	309	ASN
1	C	364	ARG
1	C	365	ASN
1	C	420	LYS
1	C	470	GLU
1	D	363	GLU
1	D	470	GLU
1	E	309	ASN
1	E	310	GLU
1	E	313	ARG
1	E	469	GLY
1	E	470	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	478	ASP
1	F	309	ASN
1	F	310	GLU
1	F	313	ARG
1	F	364	ARG
1	F	470	GLU
1	A	364	ARG
1	A	484	ASP
1	B	307	MET
1	B	308	GLN
1	B	494	ALA
1	C	363	GLU
1	C	369	ALA
1	C	418	GLU
1	D	107	ILE
1	D	312	TRP
1	D	369	ALA
1	E	107	ILE
1	E	363	GLU
1	E	364	ARG
1	E	369	ALA
1	F	107	ILE
1	F	363	GLU
1	F	369	ALA
1	F	494	ALA
1	A	297	TYR
1	A	366	GLY
1	A	369	ALA
1	A	494	ALA
1	B	364	ARG
1	C	297	TYR
1	C	494	ALA
1	D	364	ARG
1	D	494	ALA
1	E	297	TYR
1	E	494	ALA
1	F	432	ILE
1	F	433	HIS
1	F	485	GLY
1	A	357	ILE
1	B	297	TYR
1	B	357	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	357	ILE
1	D	297	TYR
1	D	357	ILE
1	D	449	ARG
1	E	357	ILE
1	F	297	TYR
1	F	357	ILE
1	B	469	GLY
1	C	310	GLU
1	F	469	GLY
1	E	354	ILE
1	F	354	ILE

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	428/450 (95%)	400 (94%)	28 (6%)	21	46
1	B	427/450 (95%)	397 (93%)	30 (7%)	19	42
1	C	428/450 (95%)	395 (92%)	33 (8%)	16	36
1	D	428/450 (95%)	400 (94%)	28 (6%)	21	46
1	E	415/450 (92%)	392 (94%)	23 (6%)	27	55
1	F	425/450 (94%)	396 (93%)	29 (7%)	20	43
All	All	2551/2700 (94%)	2380 (93%)	171 (7%)	20	44

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	12	TYR
1	A	13	LYS
1	A	44	LYS
1	A	47	GLU
1	A	73	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	87	GLU
1	A	98	LYS
1	A	107	ILE
1	A	160	LYS
1	A	179	GLN
1	A	290	PHE
1	A	365	ASN
1	A	395	ASN
1	A	410	ILE
1	A	413	VAL
1	A	415	ILE
1	A	418	GLU
1	A	430	ARG
1	A	432	ILE
1	A	445	MET
1	A	463	ILE
1	A	470	GLU
1	A	477	SER
1	A	482	PHE
1	A	483	ASP
1	A	484	ASP
1	A	488	THR
1	B	10	LYS
1	B	12	TYR
1	B	13	LYS
1	B	44	LYS
1	B	46	ASP
1	B	47	GLU
1	B	87	GLU
1	B	98	LYS
1	B	107	ILE
1	B	160	LYS
1	B	179	GLN
1	B	290	PHE
1	B	364	ARG
1	B	365	ASN
1	B	393	VAL
1	B	395	ASN
1	B	410	ILE
1	B	413	VAL
1	B	415	ILE
1	B	430	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	432	ILE
1	B	443	ARG
1	B	445	MET
1	B	449	ARG
1	B	450	LEU
1	B	459	GLN
1	B	463	ILE
1	B	468	ASN
1	B	480	SER
1	B	493	ARG
1	C	12	TYR
1	C	13	LYS
1	C	44	LYS
1	C	47	GLU
1	C	87	GLU
1	C	98	LYS
1	C	107	ILE
1	C	160	LYS
1	C	179	GLN
1	C	290	PHE
1	C	308	GLN
1	C	365	ASN
1	C	393	VAL
1	C	395	ASN
1	C	410	ILE
1	C	413	VAL
1	C	415	ILE
1	C	419	GLU
1	C	432	ILE
1	C	434	GLU
1	C	442	VAL
1	C	449	ARG
1	C	451	LEU
1	C	459	GLN
1	C	461	LEU
1	C	463	ILE
1	C	468	ASN
1	C	470	GLU
1	C	477	SER
1	C	480	SER
1	C	483	ASP
1	C	492	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	493	ARG
1	D	7	THR
1	D	10	LYS
1	D	12	TYR
1	D	13	LYS
1	D	44	LYS
1	D	47	GLU
1	D	87	GLU
1	D	98	LYS
1	D	107	ILE
1	D	160	LYS
1	D	179	GLN
1	D	290	PHE
1	D	306	ILE
1	D	354	ILE
1	D	365	ASN
1	D	395	ASN
1	D	410	ILE
1	D	413	VAL
1	D	415	ILE
1	D	429	ASN
1	D	430	ARG
1	D	432	ILE
1	D	445	MET
1	D	459	GLN
1	D	463	ILE
1	D	468	ASN
1	D	470	GLU
1	D	480	SER
1	E	8	VAL
1	E	12	TYR
1	E	13	LYS
1	E	44	LYS
1	E	47	GLU
1	E	87	GLU
1	E	98	LYS
1	E	107	ILE
1	E	160	LYS
1	E	179	GLN
1	E	290	PHE
1	E	365	ASN
1	E	395	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	410	ILE
1	E	413	VAL
1	E	415	ILE
1	E	432	ILE
1	E	451	LEU
1	E	463	ILE
1	E	468	ASN
1	E	470	GLU
1	E	480	SER
1	E	486	ILE
1	F	12	TYR
1	F	13	LYS
1	F	44	LYS
1	F	47	GLU
1	F	87	GLU
1	F	98	LYS
1	F	107	ILE
1	F	160	LYS
1	F	179	GLN
1	F	290	PHE
1	F	310	GLU
1	F	365	ASN
1	F	395	ASN
1	F	398	LEU
1	F	410	ILE
1	F	413	VAL
1	F	415	ILE
1	F	430	ARG
1	F	432	ILE
1	F	446	LYS
1	F	449	ARG
1	F	461	LEU
1	F	463	ILE
1	F	468	ASN
1	F	470	GLU
1	F	481	SER
1	F	484	ASP
1	F	489	SER
1	F	493	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	242	HIS
1	A	243	GLN
1	A	380	HIS
1	A	458	HIS
1	B	72	ASN
1	B	242	HIS
1	B	243	GLN
1	B	380	HIS
1	B	433	HIS
1	B	458	HIS
1	C	242	HIS
1	C	243	GLN
1	C	308	GLN
1	C	309	ASN
1	C	380	HIS
1	C	431	ASN
1	C	458	HIS
1	D	242	HIS
1	D	243	GLN
1	D	309	ASN
1	D	380	HIS
1	D	458	HIS
1	E	72	ASN
1	E	242	HIS
1	E	243	GLN
1	E	380	HIS
1	E	458	HIS
1	E	468	ASN
1	F	72	ASN
1	F	242	HIS
1	F	243	GLN
1	F	380	HIS
1	F	431	ASN
1	F	433	HIS
1	F	453	HIS
1	F	458	HIS
1	F	497	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 ⓘ

16 carbohydrates 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
2	AHR	A	1503	2	9,9,10	0.69	0	11,13,14	1.38	2 (18%)
2	AHR	A	1504	2	9,9,10	0.60	0	11,13,14	1.22	1 (9%)
2	AHR	A	1505	2	10,10,10	1.56	1 (10%)	12,14,14	2.06	3 (25%)
4	AHR	B	1503	4	10,10,10	1.58	1 (10%)	12,14,14	2.11	3 (25%)
4	AHR	B	1504	4	9,9,10	0.58	0	11,13,14	1.26	1 (9%)
2	AHR	C	1503	2	10,10,10	1.59	1 (10%)	12,14,14	2.21	2 (16%)
2	AHR	C	1504	2	9,9,10	0.61	0	11,13,14	1.29	1 (9%)
2	AHR	C	1505	2	9,9,10	0.67	0	11,13,14	1.28	2 (18%)
2	AHR	D	1503	2	10,10,10	1.59	1 (10%)	12,14,14	2.25	2 (16%)
2	AHR	D	1504	2	9,9,10	0.65	0	11,13,14	1.35	1 (9%)
2	AHR	D	1505	2	9,9,10	0.68	0	11,13,14	1.46	2 (18%)
2	AHR	E	1503	2	10,10,10	1.60	1 (10%)	12,14,14	2.27	2 (16%)
2	AHR	E	1504	2	9,9,10	0.64	0	11,13,14	1.48	3 (27%)
2	AHR	E	1505	2	9,9,10	0.64	0	11,13,14	1.68	2 (18%)
4	AHR	F	1503	4	10,10,10	1.55	1 (10%)	12,14,14	2.10	2 (16%)
4	AHR	F	1504	4	9,9,10	0.63	0	11,13,14	1.28	2 (18%)

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
2	AHR	A	1503	2	-	0/0/16/18	0/1/1/1
2	AHR	A	1504	2	-	0/0/16/18	0/1/1/1
2	AHR	A	1505	2	-	0/2/18/18	0/1/1/1
4	AHR	B	1503	4	-	0/2/18/18	0/1/1/1
4	AHR	B	1504	4	-	0/0/16/18	0/1/1/1
2	AHR	C	1503	2	-	0/2/18/18	0/1/1/1
2	AHR	C	1504	2	-	0/0/16/18	0/1/1/1
2	AHR	C	1505	2	-	0/0/16/18	0/1/1/1
2	AHR	D	1503	2	-	0/2/18/18	0/1/1/1
2	AHR	D	1504	2	-	0/0/16/18	0/1/1/1
2	AHR	D	1505	2	-	0/0/16/18	0/1/1/1
2	AHR	E	1503	2	-	0/2/18/18	0/1/1/1
2	AHR	E	1504	2	-	0/0/16/18	0/1/1/1
2	AHR	E	1505	2	-	0/0/16/18	0/1/1/1
4	AHR	F	1503	4	-	0/2/18/18	0/1/1/1
4	AHR	F	1504	4	-	0/0/16/18	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1505	AHR	O5'-C5'	-4.60	1.22	1.42
2	C	1503	AHR	O5'-C5'	-4.58	1.22	1.42
4	B	1503	AHR	O5'-C5'	-4.58	1.22	1.42
2	D	1503	AHR	O5'-C5'	-4.58	1.22	1.42
2	E	1503	AHR	O5'-C5'	-4.55	1.22	1.42
4	F	1503	AHR	O5'-C5'	-4.53	1.22	1.42

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1505	AHR	C5'-C4'-C3'	-4.07	111.55	115.80
2	D	1505	AHR	C5'-C4'-C3'	-3.07	112.59	115.80
2	A	1503	AHR	C5'-C4'-C3'	-2.71	112.96	115.80
2	E	1504	AHR	O4'-C4'-C5'	-2.38	105.00	109.48
2	E	1504	AHR	C5'-C4'-C3'	-2.19	113.51	115.80
2	C	1505	AHR	C5'-C4'-C3'	-2.15	113.55	115.80
4	F	1504	AHR	C1'-O4'-C4'	2.06	112.27	107.82
4	B	1503	AHR	C1'-C2'-C3'	2.15	105.29	102.45
2	A	1505	AHR	C1'-C2'-C3'	2.21	105.38	102.45
2	C	1504	AHR	C1'-C2'-C3'	2.33	105.54	102.45
2	A	1504	AHR	C1'-C2'-C3'	2.37	105.59	102.45
4	F	1504	AHR	C1'-C2'-C3'	2.41	105.64	102.45
4	B	1504	AHR	C1'-C2'-C3'	2.43	105.67	102.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1505	AHR	C1'-C2'-C3'	2.52	105.78	102.45
2	E	1504	AHR	C1'-C2'-C3'	2.52	105.79	102.45
2	D	1504	AHR	C1'-C2'-C3'	2.57	105.85	102.45
2	A	1503	AHR	C1'-C2'-C3'	2.60	105.89	102.45
2	D	1505	AHR	C1'-C2'-C3'	2.66	105.97	102.45
2	C	1505	AHR	C1'-C2'-C3'	2.66	105.97	102.45
2	C	1503	AHR	O5'-C5'-C4'	3.14	121.71	111.33
2	A	1505	AHR	O5'-C5'-C4'	3.20	121.91	111.33
4	B	1503	AHR	O5'-C5'-C4'	3.24	122.04	111.33
2	D	1503	AHR	O5'-C5'-C4'	3.25	122.08	111.33
2	E	1503	AHR	O5'-C5'-C4'	3.28	122.16	111.33
4	F	1503	AHR	O5'-C5'-C4'	3.29	122.20	111.33
2	A	1505	AHR	O1'-C1'-O4'	5.23	118.08	111.22
4	B	1503	AHR	O1'-C1'-O4'	5.42	118.34	111.22
4	F	1503	AHR	O1'-C1'-O4'	5.43	118.34	111.22
2	C	1503	AHR	O1'-C1'-O4'	6.03	119.14	111.22
2	D	1503	AHR	O1'-C1'-O4'	6.18	119.34	111.22
2	E	1503	AHR	O1'-C1'-O4'	6.27	119.45	111.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1504	AHR	1	0
2	D	1505	AHR	1	0

5.6 Ligand geometry

9 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	EDO	A	1506	-	3,3,3	0.47	0	2,2,2	0.43	0
3	EDO	B	1505	-	3,3,3	0.52	0	2,2,2	0.30	0
3	EDO	B	1506	-	3,3,3	0.50	0	2,2,2	0.32	0
3	EDO	C	1506	-	3,3,3	0.46	0	2,2,2	0.45	0
3	EDO	D	1506	-	3,3,3	0.50	0	2,2,2	0.36	0
3	EDO	D	1507	-	3,3,3	0.47	0	2,2,2	0.44	0
3	EDO	E	1506	-	3,3,3	0.51	0	2,2,2	0.34	0
3	EDO	E	1507	-	3,3,3	0.57	0	2,2,2	0.50	0
3	EDO	F	1505	-	3,3,3	0.81	0	2,2,2	0.77	0

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	EDO	A	1506	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1505	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1506	-	-	0/1/1/1	0/0/0/0
3	EDO	C	1506	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1506	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1507	-	-	0/1/1/1	0/0/0/0
3	EDO	E	1506	-	-	0/1/1/1	0/0/0/0
3	EDO	E	1507	-	-	0/1/1/1	0/0/0/0
3	EDO	F	1505	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	496/513 (96%)	0.72	46 (9%) 11 8	23, 46, 46, 48	0
1	B	497/513 (96%)	0.66	28 (5%) 28 26	22, 46, 46, 47	0
1	C	496/513 (96%)	0.75	53 (10%) 8 6	22, 46, 46, 48	0
1	D	499/513 (97%)	0.73	37 (7%) 17 15	22, 46, 46, 47	0
1	E	492/513 (95%)	0.78	42 (8%) 13 10	23, 46, 46, 48	0
1	F	496/513 (96%)	0.75	44 (8%) 12 9	23, 46, 46, 48	0
All	All	2976/3078 (96%)	0.73	250 (8%) 14 11	22, 46, 46, 48	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	439	VAL	5.8
1	B	12	TYR	5.5
1	C	501	ILE	5.4
1	C	484	ASP	5.4
1	A	12	TYR	5.2
1	C	12	TYR	4.8
1	F	443	ARG	4.7
1	D	431	ASN	4.6
1	D	12	TYR	4.6
1	E	487	LEU	4.6
1	F	12	TYR	4.5
1	F	484	ASP	4.5
1	B	437	VAL	4.4
1	C	483	ASP	4.4
1	D	443	ARG	4.4
1	C	423	VAL	4.4
1	A	11	ASP	4.3
1	A	482	PHE	4.2
1	F	416	TYR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	441	ASP	4.0
1	B	431	ASN	4.0
1	F	483	ASP	4.0
1	D	485	GLY	4.0
1	B	443	ARG	4.0
1	A	476	ASN	3.9
1	A	464	ARG	3.9
1	D	410	ILE	3.9
1	E	442	VAL	3.9
1	B	410	ILE	3.8
1	F	481	SER	3.8
1	A	433	HIS	3.8
1	E	501	ILE	3.8
1	C	476	ASN	3.8
1	E	480	SER	3.7
1	A	484	ASP	3.7
1	A	416	TYR	3.7
1	E	435	ASP	3.6
1	A	487	LEU	3.6
1	A	443	ARG	3.6
1	E	426	PHE	3.5
1	D	433	HIS	3.5
1	C	499	ILE	3.5
1	A	445	MET	3.5
1	E	441	ASP	3.5
1	C	478	ASP	3.4
1	E	107	ILE	3.4
1	A	490	MET	3.4
1	C	442	VAL	3.4
1	C	487	LEU	3.4
1	D	416	TYR	3.4
1	F	310	GLU	3.4
1	C	414	ALA	3.4
1	F	486	ILE	3.4
1	A	431	ASN	3.4
1	C	497	ASN	3.4
1	C	436	ILE	3.3
1	E	11	ASP	3.3
1	F	306	ILE	3.3
1	D	437	VAL	3.3
1	A	398	LEU	3.3
1	E	12	TYR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	436	ILE	3.3
1	D	484	ASP	3.2
1	D	11	ASP	3.2
1	E	9	ASP	3.2
1	B	494	ALA	3.2
1	C	457	GLU	3.2
1	C	464	ARG	3.2
1	F	419	GLU	3.1
1	C	490	MET	3.1
1	A	483	ASP	3.1
1	C	398	LEU	3.1
1	E	498	VAL	3.1
1	F	451	LEU	3.1
1	D	246	GLY	3.0
1	D	41	GLY	3.0
1	F	9	ASP	3.0
1	F	47	GLU	3.0
1	E	6	MET	3.0
1	F	450	LEU	3.0
1	F	11	ASP	3.0
1	D	488	THR	3.0
1	E	488	THR	3.0
1	E	431	ASN	3.0
1	C	493	ARG	2.9
1	A	408	THR	2.9
1	E	481	SER	2.9
1	D	436	ILE	2.9
1	F	437	VAL	2.9
1	F	304	ALA	2.9
1	B	399	HIS	2.9
1	F	414	ALA	2.9
1	B	430	ARG	2.9
1	E	478	ASP	2.9
1	B	485	GLY	2.9
1	E	48	ASP	2.9
1	B	433	HIS	2.9
1	F	442	VAL	2.9
1	E	490	MET	2.9
1	F	365	ASN	2.8
1	F	8	VAL	2.8
1	C	410	ILE	2.8
1	E	437	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	416	TYR	2.8
1	C	495	SER	2.8
1	D	368	ALA	2.8
1	A	493	ARG	2.8
1	A	457	GLU	2.8
1	B	461	LEU	2.8
1	C	394	ILE	2.8
1	C	480	SER	2.8
1	B	490	MET	2.8
1	D	309	ASN	2.8
1	C	445	MET	2.7
1	A	459	GLN	2.7
1	A	432	ILE	2.7
1	A	302	GLU	2.7
1	E	40	PRO	2.7
1	E	47	GLU	2.7
1	E	310	GLU	2.7
1	F	40	PRO	2.7
1	A	439	VAL	2.7
1	A	421	GLU	2.7
1	A	436	ILE	2.7
1	A	478	ASP	2.7
1	C	432	ILE	2.7
1	A	178	TRP	2.6
1	C	178	TRP	2.6
1	A	428	VAL	2.6
1	B	8	VAL	2.6
1	D	432	ILE	2.6
1	E	4	ALA	2.6
1	B	3	LYS	2.6
1	F	309	ASN	2.6
1	C	439	VAL	2.6
1	E	440	SER	2.6
1	F	7	THR	2.6
1	E	450	LEU	2.6
1	A	309	ASN	2.6
1	B	478	ASP	2.6
1	B	308	GLN	2.6
1	F	308	GLN	2.6
1	C	437	VAL	2.6
1	C	482	PHE	2.6
1	D	304	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	444	GLY	2.6
1	A	5	ARG	2.6
1	A	501	ILE	2.6
1	B	436	ILE	2.6
1	E	5	ARG	2.6
1	B	481	SER	2.6
1	E	425	ILE	2.6
1	A	368	ALA	2.5
1	B	476	ASN	2.5
1	C	438	LEU	2.5
1	D	302	GLU	2.5
1	F	498	VAL	2.5
1	C	309	ASN	2.5
1	C	429	ASN	2.5
1	B	487	LEU	2.5
1	F	6	MET	2.5
1	C	440	SER	2.5
1	B	409	ASP	2.5
1	F	497	ASN	2.5
1	F	501	ILE	2.5
1	E	432	ILE	2.5
1	C	5	ARG	2.5
1	C	486	ILE	2.4
1	B	302	GLU	2.4
1	E	477	SER	2.4
1	D	446	LYS	2.4
1	F	487	LEU	2.4
1	A	423	VAL	2.4
1	F	410	ILE	2.4
1	F	392	PRO	2.4
1	D	392	PRO	2.4
1	F	499	ILE	2.4
1	B	438	LEU	2.4
1	A	4	ALA	2.4
1	A	14	ILE	2.4
1	F	14	ILE	2.4
1	C	401	THR	2.3
1	C	397	PRO	2.3
1	F	107	ILE	2.3
1	E	451	LEU	2.3
1	D	490	MET	2.3
1	F	500	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	477	SER	2.3
1	E	499	ILE	2.3
1	D	325	PHE	2.3
1	B	441	ASP	2.3
1	B	434	GLU	2.3
1	C	469	GLY	2.3
1	A	475	LYS	2.3
1	D	406	ASP	2.3
1	D	107	ILE	2.3
1	D	499	ILE	2.3
1	A	495	SER	2.3
1	F	478	ASP	2.3
1	A	430	ARG	2.3
1	C	393	VAL	2.3
1	F	439	VAL	2.2
1	E	14	ILE	2.2
1	D	461	LEU	2.2
1	E	469	GLY	2.2
1	E	36	GLY	2.2
1	F	104	GLN	2.2
1	C	488	THR	2.2
1	C	492	ARG	2.2
1	A	410	ILE	2.2
1	E	3	LYS	2.2
1	D	430	ARG	2.2
1	B	439	VAL	2.2
1	D	448	TYR	2.2
1	F	485	GLY	2.2
1	C	4	ALA	2.2
1	D	487	LEU	2.1
1	C	449	ARG	2.1
1	D	418	GLU	2.1
1	C	425	ILE	2.1
1	E	496	TRP	2.1
1	C	329	LEU	2.1
1	C	477	SER	2.1
1	E	500	ARG	2.1
1	F	384	TYR	2.1
1	C	450	LEU	2.1
1	C	325	PHE	2.1
1	A	453	HIS	2.1
1	E	384	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	368	ALA	2.1
1	A	442	VAL	2.1
1	D	442	VAL	2.1
1	E	405	GLU	2.1
1	B	464	ARG	2.1
1	A	392	PRO	2.1
1	C	13	LYS	2.0
1	D	482	PHE	2.0
1	D	155	ILE	2.0
1	D	152	ASP	2.0
1	D	457	GLU	2.0
1	F	421	GLU	2.0
1	F	445	MET	2.0
1	C	433	HIS	2.0
1	A	304	ALA	2.0
1	D	47	GLU	2.0
1	A	429	ASN	2.0
1	A	450	LEU	2.0
1	C	422	GLU	2.0
1	C	472	VAL	2.0
1	B	426	PHE	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 ⓘ

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(Å ²)	Q<0.9
4	AHR	B	1504	9/10	0.83	0.30	5.46	46,46,47,48	0
2	AHR	E	1504	9/10	0.76	0.28	2.24	46,46,47,48	0
2	AHR	A	1504	9/10	0.75	0.35	2.16	46,46,47,48	0
2	AHR	D	1504	9/10	0.76	0.24	1.82	46,46,47,48	0
2	AHR	D	1503	10/10	0.96	0.23	1.68	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	AHR	F	1504	9/10	0.82	0.26	1.59	46,46,47,48	0
4	AHR	B	1503	10/10	0.94	0.23	1.45	46,46,46,46	0
2	AHR	C	1504	9/10	0.74	0.27	0.86	46,46,47,48	0
2	AHR	E	1503	10/10	0.96	0.22	0.56	45,46,46,46	0
2	AHR	A	1505	10/10	0.93	0.23	0.54	45,46,46,46	0
2	AHR	C	1503	10/10	0.93	0.23	0.18	46,46,46,46	0
4	AHR	F	1503	10/10	0.96	0.17	-1.10	46,46,46,46	0
2	AHR	C	1505	9/10	0.22	0.68	-	52,56,57,57	0
2	AHR	D	1505	9/10	0.35	0.57	-	52,56,57,57	0
2	AHR	A	1503	9/10	0.43	0.57	-	53,57,58,58	0
2	AHR	E	1505	9/10	0.65	0.48	-	52,55,55,55	0

6.4 Ligands ⓘ

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
3	EDO	E	1506	4/4	0.54	0.48	15.35	52,52,52,53	0
3	EDO	B	1505	4/4	0.37	0.53	8.26	54,54,55,55	0
3	EDO	D	1506	4/4	0.72	0.36	7.56	47,47,47,48	0
3	EDO	D	1507	4/4	0.90	0.24	4.73	66,66,66,66	0
3	EDO	B	1506	4/4	0.92	0.21	0.93	57,57,57,57	0
3	EDO	C	1506	4/4	0.93	0.18	-1.12	51,51,51,51	0
3	EDO	A	1506	4/4	0.92	0.15	-1.85	50,50,50,50	0
3	EDO	E	1507	4/4	0.94	0.11	-3.79	57,57,57,57	0
3	EDO	F	1505	4/4	0.84	0.23	-	62,62,63,63	0

6.5 Other polymers ⓘ

There are no such residues in this entry.