



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:38 am GMT

PDB ID : 5AB2
Title : Crystal structure of aminopeptidase ERAP2 with ligand
Authors : Mpakali, A.; Giastas, P.; Saridakis, E.; Mavridis, I.M.; Stratikos, E.
Deposited on : 2015-07-31
Resolution : 2.73 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

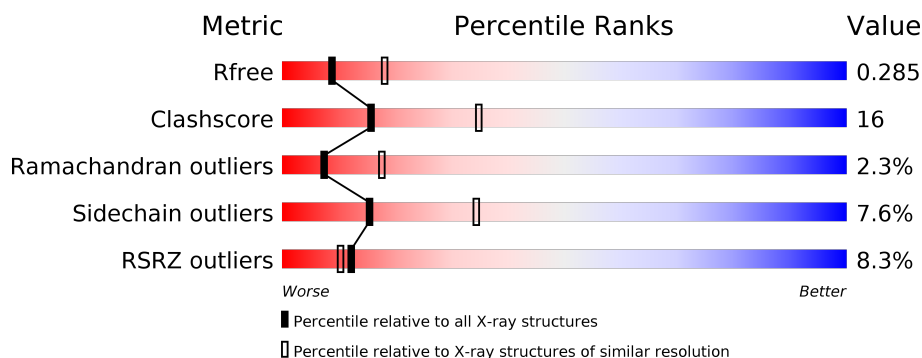
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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}	100719	2649 (2.74-2.70)
Clashscore	112137	2993 (2.74-2.70)
Ramachandran outliers	110173	2946 (2.74-2.70)
Sidechain outliers	110143	2947 (2.74-2.70)
RSRZ outliers	101464	2665 (2.74-2.70)

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	967	<div> <div>2%</div> <div>69%</div> <div>22%</div> <div>7%</div> </div>
1	B	967	<div> <div>13%</div> <div>52%</div> <div>33%</div> <div>6%</div> <div>9%</div> </div>
2	C	6	<div> <div>33%</div> <div>50%</div> <div>33%</div> <div>17%</div> </div>
2	D	6	<div> <div>83%</div> <div>33%</div> <div>50%</div> <div>17%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	B	1010	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15144 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 ENDOPLASMIC RETICULUM AMINOPEPTIDASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	897	Total	C	N	O	S	0	8	1
			7344	4737	1217	1361	29			
1	B	879	Total	C	N	O	S	0	0	1
			7156	4617	1188	1323	28			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	961	ARG	-	CLONING ARTIFACT	UNP Q6P179
A	962	HIS	-	EXPRESSION TAG	UNP Q6P179
A	963	HIS	-	EXPRESSION TAG	UNP Q6P179
A	964	HIS	-	EXPRESSION TAG	UNP Q6P179
A	965	HIS	-	EXPRESSION TAG	UNP Q6P179
A	966	HIS	-	EXPRESSION TAG	UNP Q6P179
A	967	HIS	-	EXPRESSION TAG	UNP Q6P179
B	961	ARG	-	EXPRESSION TAG	UNP Q6P179
B	962	HIS	-	EXPRESSION TAG	UNP Q6P179
B	963	HIS	-	EXPRESSION TAG	UNP Q6P179
B	964	HIS	-	EXPRESSION TAG	UNP Q6P179
B	965	HIS	-	EXPRESSION TAG	UNP Q6P179
B	966	HIS	-	EXPRESSION TAG	UNP Q6P179
B	967	HIS	-	EXPRESSION TAG	UNP Q6P179

- Molecule 2 is a protein called GPI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	5	0
			80	52	17	11			
2	D	6	Total	C	N	O	0	0	0
			42	27	9	6			

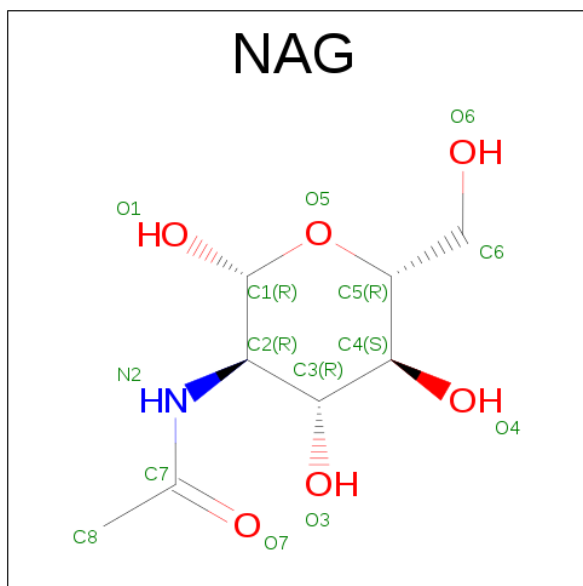
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

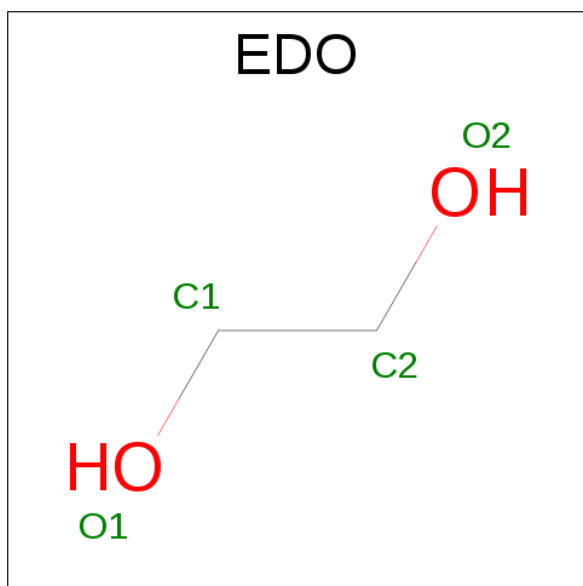


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		
6	A	1	Total	Zn	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	4	Total	C	N	O	0	0
			50	28	2	20		

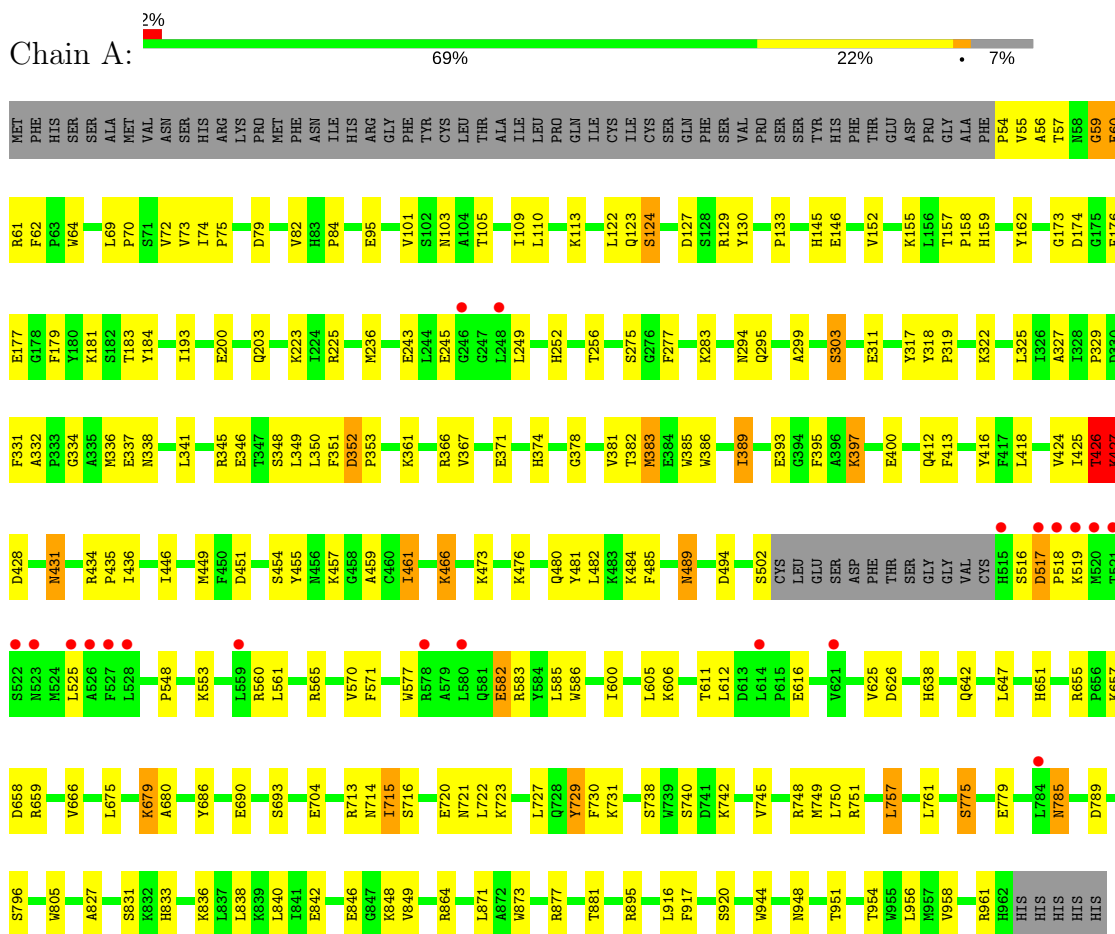
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	82	Total	O	0	0
			82	82		
9	B	20	Total	O	0	0
			20	20		

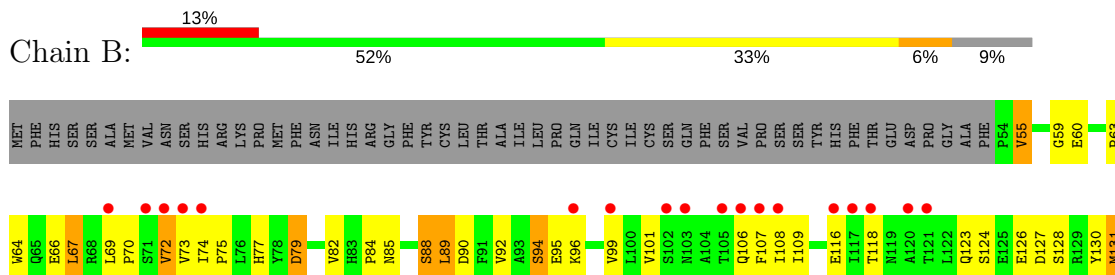
3 Residue-property plots

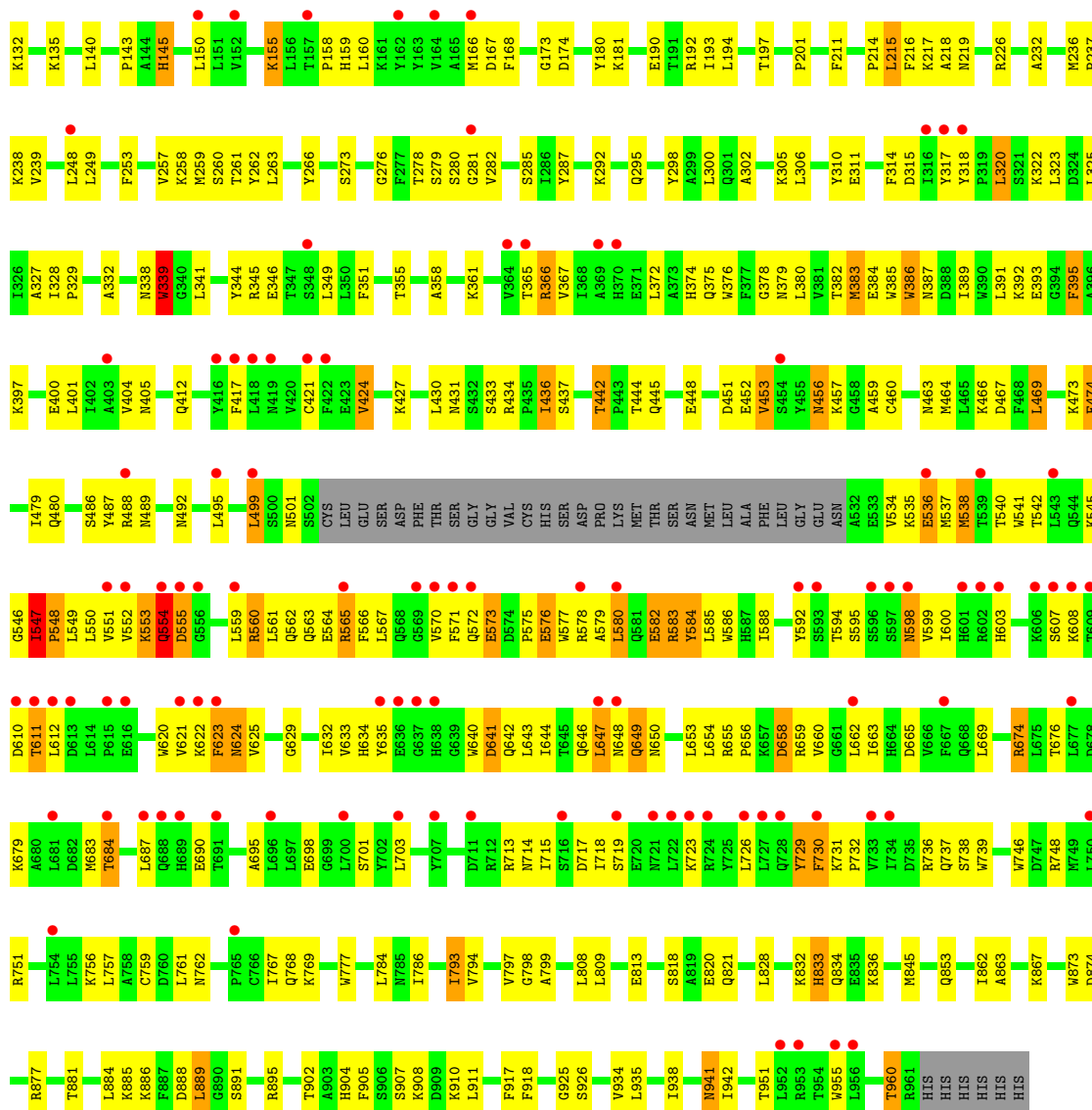
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ENDOPLASMIC RETICULUM AMINOPEPTIDASE 2



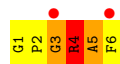
• Molecule 1: ENDOPLASMIC RETICULUM AMINOPEPTIDASE 2





• Molecule 2: GPI

Chain C:



• Molecule 2: GPI

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.65Å 135.47Å 128.21Å 90.00° 90.24° 90.00°	Depositor
Resolution (Å)	49.01 – 2.73 49.01 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.01-2.73) 98.6 (49.01-2.73)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.223 , 0.286 0.223 , 0.285	Depositor DCC
R_{free} test set	6667 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15144	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, BMA, NAG, 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	0.59	1/7550 (0.0%)	0.69	0/10229
1	B	0.40	1/7334 (0.0%)	0.59	1/9939 (0.0%)
2	C	0.84	0/82	1.64	0/106
2	D	0.59	0/43	1.16	0/56
All	All	0.51	2/15009 (0.0%)	0.65	1/20330 (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
2	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLY	C-N	-6.35	1.19	1.34
1	B	548	PRO	N-CD	5.19	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	547	ILE	C-N-CD	5.70	140.37	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	3[A]	GLY	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	7344	0	7297	146	0
1	B	7156	0	7112	330	0
2	C	80	0	79	11	0
2	D	42	0	42	6	0
3	A	78	0	68	0	0
4	A	140	0	125	3	0
4	B	56	0	50	2	0
5	A	28	0	26	0	0
5	B	42	0	39	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	12	0	18	0	0
7	B	12	0	18	0	0
8	B	50	0	43	6	0
9	A	82	0	0	10	0
9	B	20	0	0	7	0
All	All	15144	0	14917	490	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 16.

All (490) 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:B:566:PHE:CE1	1:B:567:LEU:O	1.72	1.40
1:B:554:GLN:CG	1:B:560:ARG:HD2	1.59	1.31
1:B:566:PHE:CD1	1:B:567:LEU:N	2.10	1.18
1:B:554:GLN:HG2	1:B:560:ARG:HD2	1.32	1.12
1:B:554:GLN:HG2	1:B:560:ARG:CD	1.88	1.03
1:B:634:HIS:CD2	1:B:635:TYR:H	1.76	1.02
1:B:566:PHE:HE1	1:B:567:LEU:O	1.43	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:GLN:CB	1:B:560:ARG:HD2	1.90	0.99
1:B:634:HIS:HB2	1:B:669:LEU:HD22	1.47	0.95
1:B:550:LEU:HB3	1:B:633:VAL:HG12	1.45	0.95
1:B:554:GLN:CG	1:B:560:ARG:CD	2.44	0.94
1:B:566:PHE:HD1	1:B:567:LEU:H	1.01	0.93
1:B:549:LEU:HD12	1:B:550:LEU:N	1.84	0.91
1:B:550:LEU:CB	1:B:633:VAL:HG12	2.01	0.90
1:B:552:VAL:N	1:B:634:HIS:O	2.05	0.89
1:B:383:MET:HE1	1:B:392:LYS:HD3	1.55	0.88
1:B:573:GLU:HB3	1:B:674:ARG:NH2	1.87	0.88
1:B:634:HIS:CD2	1:B:635:TYR:N	2.42	0.87
1:A:426:THR:O	1:A:428:ASP:N	2.07	0.86
1:B:566:PHE:O	1:B:567:LEU:HG	1.75	0.84
1:B:554:GLN:HB2	1:B:560:ARG:HG3	1.59	0.84
1:B:554:GLN:HG2	1:B:560:ARG:NE	1.93	0.83
1:B:59:GLY:HA3	1:B:60:GLU:HB2	1.59	0.83
1:B:552:VAL:HB	1:B:635:TYR:CD2	2.15	0.82
1:A:961:ARG:O	9:A:2074:HOH:O	1.97	0.82
1:B:554:GLN:CB	1:B:560:ARG:CD	2.57	0.81
1:B:549:LEU:HB2	1:B:566:PHE:HB2	1.61	0.81
1:B:573:GLU:HB3	1:B:674:ARG:HH21	1.45	0.81
1:B:576:GLU:O	1:B:579:ALA:O	2.00	0.80
1:B:374:HIS:CE1	1:B:392:LYS:HG2	2.17	0.80
1:B:383:MET:H	1:B:383:MET:HE3	1.46	0.80
1:B:549:LEU:HD12	1:B:550:LEU:H	1.44	0.79
1:B:549:LEU:HD13	1:B:632:ILE:HG22	1.64	0.79
1:B:215:LEU:O	1:B:217:LYS:N	2.17	0.78
1:B:553:LYS:O	1:B:560:ARG:HG3	1.84	0.77
1:B:248:LEU:HD21	8:B:1001:NAG:H61	1.67	0.77
1:B:600:ILE:HG12	1:B:625:VAL:HG21	1.65	0.76
1:B:550:LEU:O	1:B:633:VAL:HA	1.85	0.76
1:A:311:GLU:HG2	1:A:317:TYR:HA	1.67	0.76
1:B:554:GLN:HB2	1:B:560:ARG:HD2	1.68	0.74
1:B:554:GLN:HB2	1:B:560:ARG:CG	2.18	0.74
1:B:551:VAL:O	1:B:561:LEU:HD13	1.88	0.74
1:B:565:ARG:HD2	1:B:566:PHE:O	1.87	0.73
1:A:55:VAL:HB	1:A:62:PHE:H	1.53	0.73
1:B:298:TYR:HH	1:B:365:THR:HG1	1.32	0.73
1:B:108:ILE:HG23	1:B:150:LEU:HB2	1.69	0.73
1:B:486:SER:HB3	1:B:487:TYR:HD1	1.53	0.72
1:B:554:GLN:CD	1:B:560:ARG:HD2	2.09	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:SER:HB2	1:B:910:LYS:HB2	1.70	0.72
1:B:60:GLU:HG2	1:B:140:LEU:HD11	1.72	0.72
1:B:374:HIS:HE1	1:B:392:LYS:HG2	1.52	0.72
1:B:166:MET:O	9:B:2002:HOH:O	2.07	0.71
1:B:634:HIS:HD2	1:B:635:TYR:H	1.36	0.71
1:B:548:PRO:HG3	1:B:586:TRP:CE3	2.26	0.71
1:B:549:LEU:HB3	1:B:564:GLU:O	1.91	0.71
1:B:552:VAL:CG1	1:B:635:TYR:CD2	2.74	0.70
1:B:552:VAL:HG11	1:B:635:TYR:CD2	2.26	0.70
1:B:592:TYR:HB3	1:B:623:PHE:HE1	1.56	0.69
1:B:550:LEU:HD23	1:B:562:GLN:O	1.93	0.69
1:A:895:ARG:HG3	1:A:895:ARG:HH11	1.58	0.68
1:A:833:HIS:HB2	1:A:836:LYS:HG3	1.75	0.68
1:B:553:LYS:O	1:B:554:GLN:HB2	1.92	0.68
2:C:4[A]:PRO:HB2	2:C:4[A]:ARG:HG3	1.74	0.68
1:B:124:SER:HB2	1:B:130:TYR:HB2	1.76	0.68
1:B:106:GLN:HB3	1:B:155:LYS:HG2	1.76	0.67
1:A:838:LEU:HD13	1:A:871:LEU:HD11	1.75	0.67
1:B:436:ILE:HG22	1:B:453:VAL:HG12	1.77	0.67
1:B:554:GLN:HB2	1:B:560:ARG:CD	2.24	0.67
1:B:659:ARG:NH1	1:B:690:GLU:OE2	2.27	0.67
1:B:552:VAL:CB	1:B:635:TYR:CD2	2.77	0.67
1:B:69:LEU:HD23	1:B:211:PHE:HD1	1.60	0.67
1:A:659:ARG:NH1	1:A:690:GLU:OE1	2.28	0.66
2:D:4:ARG:H	2:D:4:ARG:HD2	1.61	0.66
1:B:577:TRP:C	1:B:579:ALA:O	2.34	0.66
1:B:95:GLU:O	9:B:2002:HOH:O	2.12	0.65
1:B:566:PHE:CD1	1:B:567:LEU:O	2.45	0.65
1:B:550:LEU:N	1:B:632:ILE:O	2.28	0.65
1:A:714:ASN:O	1:A:716:SER:N	2.30	0.65
1:A:337:GLU:HG3	1:A:374:HIS:HB3	1.78	0.65
1:B:595:SER:HB3	1:B:620:TRP:CE2	2.32	0.65
1:B:563:GLN:OE1	1:B:586:TRP:N	2.23	0.64
1:B:566:PHE:CG	1:B:567:LEU:N	2.65	0.64
1:A:334:GLY:HA3	2:C:4[A]:ARG:H	1.63	0.64
1:B:70:PRO:HB2	1:B:72:VAL:HG23	1.80	0.64
1:B:620:TRP:NE1	1:B:646:GLN:OE1	2.26	0.64
1:A:658:ASP:OD2	9:A:2049:HOH:O	2.15	0.64
1:B:552:VAL:HG11	1:B:635:TYR:CE2	2.33	0.64
1:A:553:LYS:HD2	1:A:560:ARG:HH21	1.62	0.63
1:A:397:LYS:HB3	1:A:459:ALA:HB2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:PRO:HD2	1:B:109:ILE:HG21	1.80	0.63
1:B:562:GLN:HE21	1:B:608:LYS:CD	2.12	0.62
1:B:64:TRP:NE1	1:B:70:PRO:HD3	2.13	0.62
1:B:292:LYS:HG2	1:B:295:GLN:HE21	1.62	0.62
1:B:237:PRO:HG3	1:B:322:LYS:HG2	1.81	0.62
1:B:583:ARG:O	1:B:585:LEU:N	2.33	0.62
1:A:836:LYS:NZ	9:A:2065:HOH:O	2.33	0.62
1:B:95:GLU:HG2	1:B:168:PHE:HE1	1.65	0.62
1:B:273:SER:HB3	1:B:287:TYR:CE1	2.35	0.62
1:B:280:SER:OG	1:B:281:GLY:N	2.32	0.61
1:A:954:THR:O	1:A:958:VAL:HG23	2.01	0.61
1:A:295:GLN:HG2	1:A:352:ASP:HB2	1.83	0.61
1:A:275:SER:OG	9:A:2030:HOH:O	2.16	0.61
1:B:292:LYS:NZ	1:B:346:GLU:OE1	2.32	0.61
1:B:551:VAL:HG12	1:B:553:LYS:HG2	1.81	0.61
1:B:560:ARG:O	1:B:561:LEU:HD22	2.00	0.60
2:C:3[A]:GLY:O	2:C:4[A]:ARG:HB2	2.01	0.60
1:A:517:ASP:HB2	1:A:518:PRO:HD3	1.82	0.60
1:B:173:GLY:H	1:B:180:TYR:HA	1.66	0.60
1:B:655:ARG:HB2	1:B:658:ASP:HB2	1.84	0.60
1:B:310:TYR:O	1:B:314:PHE:HB2	2.02	0.60
1:B:738:SER:OG	1:B:751:ARG:NH1	2.35	0.60
1:B:332:ALA:O	1:B:345:ARG:NH2	2.35	0.59
1:A:200:GLU:HB3	1:A:336:MET:HE1	1.84	0.59
1:B:118:THR:HB	1:B:167:ASP:HB2	1.84	0.59
1:B:549:LEU:CD1	1:B:632:ILE:HG22	2.31	0.59
4:A:1014:NAG:H83	4:A:1014:NAG:H3	1.85	0.59
1:B:397:LYS:HB3	1:B:459:ALA:HB2	1.85	0.59
1:B:684:THR:O	1:B:684:THR:OG1	2.18	0.59
1:A:184:TYR:HB3	1:A:329:PRO:HG2	1.84	0.58
1:B:563:GLN:OE1	1:B:585:LEU:HA	2.03	0.58
1:B:874:ASP:OD1	1:B:877:ARG:NH2	2.34	0.58
1:A:59:GLY:O	1:A:60:GLU:O	2.21	0.58
1:B:594:THR:HG22	1:B:621:VAL:HG23	1.84	0.58
1:A:397:LYS:HD3	1:A:455:TYR:HB3	1.85	0.58
1:A:723:LYS:HG3	1:A:761:LEU:HB3	1.85	0.58
1:B:302:ALA:O	1:B:306:LEU:HB2	2.03	0.58
1:B:738:SER:O	1:B:751:ARG:HD2	2.02	0.58
1:B:257:VAL:HG12	4:B:1009:NAG:H81	1.86	0.58
1:B:552:VAL:HG21	1:B:635:TYR:CE2	2.38	0.58
1:A:72:VAL:HG23	1:A:73:VAL:HG23	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:SER:HB3	1:B:487:TYR:CD1	2.37	0.58
1:B:565:ARG:HD2	1:B:566:PHE:N	2.19	0.58
1:B:226:ARG:HH12	1:B:249:LEU:HD12	1.68	0.58
1:B:881:THR:HG22	1:B:885:LYS:HE3	1.85	0.58
1:A:366:ARG:HH11	1:A:416:TYR:HE2	1.50	0.58
1:A:338:ASN:HB2	1:A:341:LEU:O	2.04	0.58
1:B:338:ASN:HB2	1:B:341:LEU:O	2.04	0.57
1:A:713:ARG:HB2	1:A:715:ILE:HG13	1.85	0.57
1:B:560:ARG:C	1:B:561:LEU:HD22	2.25	0.57
1:B:375:GLN:O	1:B:379:ASN:HB2	2.03	0.57
1:B:376:TRP:HA	1:B:380:LEU:HD12	1.87	0.57
1:B:576:GLU:HB3	1:B:580:LEU:HG	1.87	0.57
1:B:611:THR:OG1	1:B:611:THR:O	2.17	0.57
1:B:214:PRO:HA	1:B:260:SER:HB3	1.85	0.57
1:B:547:ILE:HG23	1:B:547:ILE:O	2.05	0.57
1:A:722:LEU:HG	1:A:956:LEU:HD11	1.86	0.57
1:B:550:LEU:HD22	1:B:561:LEU:HD12	1.86	0.57
1:B:88:SER:OG	1:B:90:ASP:OD1	2.22	0.57
1:B:818:SER:HA	1:B:821:GLN:HB2	1.87	0.56
1:B:886:LYS:NZ	9:B:2019:HOH:O	2.30	0.56
1:A:548:PRO:HB3	1:A:586:TRP:CE3	2.40	0.56
1:B:640:TRP:CD1	1:B:643:LEU:HD13	2.40	0.56
1:A:944:TRP:O	1:A:948:ASN:HB2	2.05	0.56
1:A:158:PRO:HB2	1:A:159:HIS:ND1	2.21	0.55
1:B:217:LYS:HD2	1:B:382:THR:OG1	2.06	0.55
1:A:473:LYS:HG3	1:A:502:SER:HB3	1.88	0.55
1:B:59:GLY:CA	1:B:60:GLU:HB2	2.35	0.55
1:B:756:LYS:HG3	1:B:793:ILE:HG23	1.86	0.55
1:B:579:ALA:C	1:B:580:LEU:HD23	2.26	0.55
1:B:634:HIS:CG	1:B:635:TYR:N	2.73	0.55
1:A:348:SER:HB3	1:A:367:VAL:HG11	1.88	0.55
1:B:566:PHE:O	1:B:567:LEU:CG	2.51	0.55
1:B:833:HIS:HB2	1:B:836:LYS:HB2	1.88	0.55
1:A:332:ALA:O	1:A:345:ARG:NH1	2.39	0.55
1:A:466:LYS:HG2	1:A:466:LYS:O	2.07	0.55
1:B:541:TRP:CZ3	1:B:548:PRO:HD3	2.42	0.55
1:B:622:LYS:HE2	1:B:662:LEU:HG	1.88	0.55
1:B:592:TYR:HB3	1:B:623:PHE:CE1	2.39	0.55
1:A:366:ARG:HD2	1:A:413:PHE:CE1	2.42	0.55
1:A:434:ARG:NH1	1:A:435:PRO:O	2.39	0.55
1:B:873:TRP:CZ2	1:B:877:ARG:HD3	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1006:NAG:O3	4:B:1007:NAG:O5	2.24	0.55
1:A:738:SER:O	1:A:751:ARG:HD3	2.06	0.55
1:B:732:PRO:O	1:B:736:ARG:HB2	2.06	0.54
1:B:550:LEU:HB2	1:B:633:VAL:HG12	1.84	0.54
1:A:176:PHE:CG	1:A:332:ALA:HB2	2.42	0.54
1:B:88:SER:HB3	8:B:1001:NAG:H82	1.89	0.54
1:A:366:ARG:NH1	1:A:416:TYR:HE2	2.05	0.54
1:B:278:THR:OG1	1:B:279:SER:N	2.39	0.54
1:B:554:GLN:CB	1:B:560:ARG:CG	2.85	0.54
1:B:445:GLN:HA	1:B:448:GLU:HB2	1.90	0.54
1:A:383:MET:HG2	1:A:389:ILE:HA	1.90	0.54
1:B:594:THR:HA	1:B:621:VAL:HA	1.89	0.54
1:A:585:LEU:HD21	1:A:606:LYS:O	2.07	0.54
1:B:552:VAL:CG1	1:B:635:TYR:HD2	2.20	0.54
1:B:660:VAL:HG13	1:B:695:ALA:HA	1.90	0.54
1:B:777:TRP:HA	1:B:784:LEU:HB3	1.89	0.54
1:A:451:ASP:HA	2:C:4[A]:ARG:HH22	1.73	0.54
1:B:395:PHE:HE2	1:B:495:LEU:HD21	1.73	0.54
1:B:570:VAL:HG11	1:B:577:TRP:HB2	1.90	0.54
1:B:563:GLN:HB3	1:B:608:LYS:HB3	1.89	0.53
1:B:355:THR:HB	1:B:820:GLU:HB2	1.90	0.53
1:B:541:TRP:HH2	1:B:548:PRO:HG2	1.73	0.53
1:B:541:TRP:HH2	1:B:548:PRO:CD	2.22	0.53
1:A:64:TRP:CD2	1:A:70:PRO:HG3	2.43	0.53
1:B:375:GLN:HA	1:B:379:ASN:ND2	2.24	0.53
1:B:918:PHE:HE2	1:B:934:VAL:HB	1.73	0.53
1:B:384:GLU:HA	1:B:489:ASN:HD22	1.74	0.53
1:B:769:LYS:NZ	9:B:2014:HOH:O	2.21	0.53
1:B:565:ARG:HG2	1:B:584:TYR:CD2	2.43	0.53
1:B:582:GLU:C	1:B:584:TYR:H	2.12	0.53
1:B:748:ARG:HG2	1:B:751:ARG:HH21	1.74	0.53
1:B:634:HIS:HB2	1:B:669:LEU:CD2	2.33	0.52
1:B:676:THR:HG23	1:B:679:LYS:HG2	1.91	0.52
1:B:375:GLN:HA	1:B:379:ASN:HD22	1.75	0.52
1:B:480:GLN:NE2	1:B:501:ASN:O	2.43	0.52
1:B:623:PHE:HD2	1:B:633:VAL:HG11	1.74	0.52
1:A:626:ASP:OD1	1:A:657:LYS:HB2	2.10	0.52
1:A:54:PRO:HG2	1:A:55:VAL:HG13	1.90	0.52
2:C:5[A]:ALA:O	2:C:6[A]:PHE:HB2	2.08	0.52
1:A:647:LEU:HD21	1:A:659:ARG:HG2	1.92	0.52
1:A:704:GLU:HG3	1:A:757:LEU:HD12	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:MET:O	1:B:540:THR:OG1	2.26	0.52
1:B:698:GLU:O	1:B:701:SER:OG	2.25	0.52
1:B:580:LEU:N	1:B:580:LEU:CD2	2.73	0.52
1:B:552:VAL:O	1:B:635:TYR:HA	2.09	0.52
1:B:566:PHE:HD1	1:B:567:LEU:N	1.78	0.52
1:A:236:MET:HE2	1:A:256:THR:HA	1.91	0.51
1:B:845:MET:O	1:B:886:LYS:HE2	2.11	0.51
8:B:1001:NAG:O6	8:B:1002:NAG:O6	2.27	0.51
1:A:223:LYS:HE2	1:A:252:HIS:CD2	2.46	0.51
1:B:124:SER:OG	1:B:127:ASP:HB3	2.11	0.51
1:B:576:GLU:O	1:B:579:ALA:C	2.49	0.51
1:B:634:HIS:CD2	1:B:669:LEU:HD13	2.46	0.51
1:B:474:PHE:HB3	1:B:499:LEU:HD21	1.92	0.51
1:B:809:LEU:HB2	1:B:828:LEU:HD21	1.92	0.51
1:B:541:TRP:CH2	1:B:548:PRO:CD	2.94	0.51
1:B:217:LYS:HE3	1:B:259:MET:HA	1.92	0.51
1:B:541:TRP:CH2	1:B:548:PRO:HG2	2.46	0.50
1:B:808:LEU:HB2	1:B:828:LEU:HD11	1.93	0.50
1:B:442:THR:HG22	1:B:444:THR:H	1.76	0.50
1:B:448:GLU:HA	1:B:895:ARG:NH1	2.26	0.50
1:B:572:GLN:O	1:B:573:GLU:HG3	2.11	0.50
1:A:69:LEU:HD22	1:A:109:ILE:HG22	1.93	0.50
1:B:599:VAL:HG22	1:B:600:ILE:H	1.77	0.50
1:B:79:ASP:HB2	1:B:96:LYS:HG3	1.93	0.50
1:B:566:PHE:CZ	1:B:567:LEU:O	2.52	0.50
1:A:775:SER:O	1:A:779:GLU:HG2	2.11	0.50
1:B:579:ALA:O	1:B:580:LEU:HB2	2.11	0.50
1:A:386:TRP:CD1	1:A:446:ILE:HD13	2.47	0.49
1:A:236:MET:CE	1:A:256:THR:HA	2.42	0.49
1:B:85:ASN:ND2	9:B:2001:HOH:O	2.46	0.49
1:B:127:ASP:OD1	1:B:128:SER:N	2.46	0.49
1:B:77:HIS:HD1	1:B:219:ASN:HB2	1.76	0.49
1:B:647:LEU:HD13	1:B:654:LEU:HD23	1.93	0.49
1:B:717:ASP:OD1	1:B:718:ILE:N	2.45	0.49
1:B:762:ASN:HA	1:B:767:ILE:HD11	1.94	0.49
1:A:659:ARG:HH11	1:A:690:GLU:CD	2.16	0.49
8:B:1003:BMA:H61	8:B:1004:BMA:H2	1.65	0.49
1:B:158:PRO:HB2	1:B:159:HIS:ND1	2.27	0.49
1:B:541:TRP:HH2	1:B:548:PRO:CG	2.26	0.49
1:A:334:GLY:HA3	2:C:4[A]:ARG:N	2.28	0.49
1:B:456:ASN:OD1	1:B:456:ASN:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:ILE:HG23	1:B:683:MET:HG2	1.95	0.48
1:B:737:GLN:HG3	1:B:751:ARG:HG3	1.95	0.48
1:B:232:ALA:O	1:B:253:PHE:HZ	1.96	0.48
1:B:218:ALA:O	1:B:258:LYS:HA	2.14	0.48
1:A:82:VAL:HG12	1:A:84:PRO:HD3	1.95	0.48
1:B:385:TRP:CG	1:B:386:TRP:N	2.82	0.48
1:B:911:LEU:HB2	1:B:942:ILE:HD11	1.95	0.48
1:A:666:VAL:HG11	1:A:680:ALA:HA	1.96	0.48
1:B:375:GLN:OE1	1:B:379:ASN:ND2	2.46	0.48
1:B:665:ASP:O	1:B:669:LEU:HG	2.14	0.48
1:B:687:LEU:HB2	1:B:730:PHE:HE1	1.79	0.48
1:B:345:ARG:HG3	1:B:853:GLN:HE22	1.78	0.48
4:A:1014:NAG:O3	4:A:1015:NAG:H2	2.14	0.48
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.95	0.48
1:B:77:HIS:HD1	1:B:219:ASN:CB	2.26	0.48
1:B:888:ASP:O	1:B:891:SER:N	2.42	0.48
1:A:451:ASP:HA	2:C:4[A]:ARG:NH2	2.28	0.48
1:B:832:LYS:O	1:B:867:LYS:HD2	2.14	0.47
1:B:935:LEU:HD23	1:B:935:LEU:HA	1.71	0.47
1:A:346:GLU:HG2	1:A:350:LEU:HD12	1.95	0.47
1:A:877:ARG:HG2	1:A:917:PHE:CD1	2.49	0.47
1:A:720:GLU:OE1	9:A:2055:HOH:O	2.20	0.47
1:B:236:MET:HE2	1:B:320:LEU:HD22	1.97	0.47
1:B:469:LEU:O	1:B:473:LYS:HB2	2.14	0.47
1:B:554:GLN:OE1	1:B:560:ARG:HD2	2.14	0.47
1:B:562:GLN:HG2	1:B:563:GLN:N	2.30	0.47
1:B:64:TRP:CE2	1:B:70:PRO:HD3	2.49	0.47
1:B:401:LEU:HD13	1:B:417:PHE:HB2	1.96	0.47
1:B:190:GLU:OE1	1:B:192:ARG:NH2	2.46	0.47
1:B:554:GLN:HB3	1:B:555:ASP:H	1.52	0.47
1:B:644:ILE:O	1:B:648:ASN:ND2	2.48	0.47
1:B:451:ASP:C	2:D:4:ARG:HH22	2.18	0.47
1:A:638:HIS:O	1:A:642:GLN:N	2.35	0.47
8:B:1001:NAG:O3	8:B:1001:NAG:O7	2.21	0.47
1:B:535:LYS:HB2	1:B:535:LYS:HE3	1.72	0.47
1:B:739:TRP:O	9:B:2012:HOH:O	2.20	0.47
1:A:184:TYR:HB3	1:A:329:PRO:CG	2.44	0.47
1:A:693:SER:OG	1:A:750:LEU:HD22	2.15	0.47
1:B:310:TYR:HD1	1:B:314:PHE:HE2	1.63	0.47
1:B:731:LYS:N	1:B:732:PRO:HD2	2.29	0.47
1:A:55:VAL:HG21	1:A:61:ARG:HA	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:TYR:CE1	1:B:339:TRP:HZ3	2.32	0.46
2:C:1:GLY:HA2	2:C:2[A]:PRO:HD3	1.57	0.46
1:A:331:PHE:O	1:A:345:ARG:HD2	2.15	0.46
1:A:385:TRP:CG	1:A:386:TRP:N	2.83	0.46
1:B:562:GLN:HE21	1:B:608:LYS:HD3	1.79	0.46
1:A:431:ASN:HA	1:A:565:ARG:NH2	2.31	0.46
1:A:570:VAL:HG12	1:A:577:TRP:HD1	1.80	0.46
1:B:131:MET:HG3	1:B:132:LYS:H	1.80	0.46
1:A:299:ALA:O	1:A:303:SER:OG	2.29	0.46
1:A:805:TRP:CD2	1:A:836:LYS:HD3	2.50	0.46
1:B:89:LEU:HD13	1:B:181:LYS:HD3	1.97	0.46
2:D:5:ALA:O	2:D:6:PHE:HB2	2.16	0.46
1:B:327:ALA:HB2	1:B:349:LEU:HD23	1.98	0.46
1:B:786:ILE:HD13	1:B:794:VAL:HG11	1.96	0.46
1:B:282:VAL:HG22	1:B:318:TYR:HD2	1.80	0.46
1:B:546:GLY:HA3	1:B:586:TRP:CZ2	2.51	0.46
1:B:729:TYR:O	1:B:731:LYS:N	2.48	0.46
1:A:397:LYS:O	1:A:400:GLU:HG3	2.16	0.46
1:B:292:LYS:HG2	1:B:295:GLN:NE2	2.29	0.46
1:B:306:LEU:O	1:B:310:TYR:HD2	1.99	0.46
1:B:397:LYS:HB3	1:B:397:LYS:HE3	1.83	0.46
1:A:740:SER:O	1:A:751:ARG:NE	2.49	0.45
1:B:938:ILE:HA	1:B:941:ASN:HB2	1.97	0.45
2:D:4:ARG:H	2:D:4:ARG:CD	2.25	0.45
1:B:655:ARG:O	1:B:659:ARG:HG3	2.16	0.45
1:B:884:LEU:HD13	1:B:889:LEU:HD23	1.98	0.45
1:B:535:LYS:HB3	1:B:536:GLU:H	1.49	0.45
1:A:351:PHE:CZ	1:A:361:LYS:HE3	2.51	0.45
1:B:424:VAL:HG13	1:B:452:GLU:HB3	1.98	0.45
1:A:481:TYR:O	1:A:485:PHE:HD2	2.00	0.45
1:B:126:GLU:O	1:B:160:LEU:HD13	2.16	0.45
1:B:323:LEU:HD21	1:B:372:LEU:HD22	1.97	0.45
1:A:424:VAL:O	1:A:428:ASP:HB2	2.17	0.45
1:A:489:ASN:N	1:A:489:ASN:OD1	2.50	0.45
1:A:55:VAL:HG11	1:A:61:ARG:HG3	1.97	0.45
1:B:424:VAL:O	1:B:427:LYS:N	2.46	0.45
1:B:538:MET:HE3	1:B:541:TRP:HD1	1.80	0.45
1:B:82:VAL:HG12	1:B:84:PRO:HD3	1.99	0.45
1:A:895:ARG:NH1	1:A:895:ARG:HG3	2.29	0.45
1:B:263:LEU:HD23	1:B:338:ASN:HA	1.98	0.45
1:A:425:ILE:C	1:A:426:THR:O	2.54	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:LYS:HG2	1:A:485:PHE:CE2	2.51	0.45
1:A:55:VAL:O	1:A:56:ALA:HB2	2.16	0.45
1:A:173:GLY:O	1:A:181[A]:LYS:HG2	2.17	0.45
1:A:54:PRO:C	1:A:55:VAL:HG13	2.36	0.45
1:A:951:THR:OG1	9:A:2073:HOH:O	2.21	0.45
1:B:464:MET:CG	1:B:629:GLY:HA2	2.47	0.45
1:B:640:TRP:HB2	1:B:642:GLN:H	1.82	0.44
1:A:294:ASN:HD22	4:A:1016:NAG:C7	2.30	0.44
1:A:366:ARG:HD2	1:A:413:PHE:HE1	1.82	0.44
1:A:877:ARG:HA	1:A:917:PHE:CE1	2.52	0.44
1:B:649:GLN:HA	1:B:650:ASN:HA	1.72	0.44
1:B:106:GLN:HG3	1:B:107:PHE:H	1.80	0.44
1:A:243:GLU:HA	1:A:249:LEU:HD23	1.99	0.44
1:A:393:GLU:OE2	2:C:1:GLY:HA3	2.18	0.44
1:B:400:GLU:O	1:B:404:VAL:HG23	2.17	0.44
1:B:433:SER:OG	1:B:434:ARG:N	2.48	0.44
1:B:541:TRP:HZ3	1:B:548:PRO:HD3	1.82	0.44
1:B:611:THR:O	1:B:612:LEU:HD23	2.18	0.44
1:B:94:SER:HB3	1:B:167:ASP:OD1	2.18	0.44
1:B:548:PRO:HG3	1:B:586:TRP:CD2	2.52	0.44
1:A:582:GLU:HG3	1:A:583:ARG:HG2	2.00	0.44
1:A:679:LYS:HB2	1:A:679:LYS:HE2	1.91	0.44
1:B:314:PHE:O	1:B:479:ILE:HD12	2.17	0.44
1:B:541:TRP:CH2	1:B:548:PRO:CG	3.00	0.44
1:A:127:ASP:OD2	1:A:162:TYR:OH	2.34	0.44
1:B:173:GLY:N	1:B:180:TYR:HA	2.32	0.44
1:B:393:GLU:OE2	2:D:1:GLY:HA3	2.18	0.44
1:A:79:ASP:O	1:A:95:GLU:HA	2.17	0.44
1:B:659:ARG:O	1:B:662:LEU:HB2	2.17	0.44
1:B:75:PRO:HA	1:B:99:VAL:HA	2.00	0.44
1:A:427:LYS:HB3	1:A:427:LYS:HE2	1.84	0.44
1:A:561:LEU:HD11	1:A:612:LEU:HD12	1.98	0.44
1:A:727:LEU:O	1:A:731:LYS:HB2	2.18	0.44
1:B:430:LEU:HD12	1:B:431:ASN:H	1.83	0.44
1:A:159:HIS:O	9:A:2011:HOH:O	2.21	0.43
1:A:412:GLN:OE1	1:A:745:VAL:HB	2.18	0.43
1:B:106:GLN:HG3	1:B:107:PHE:CD1	2.53	0.43
1:B:436:ILE:CG2	1:B:457:LYS:HD2	2.47	0.43
1:B:634:HIS:CE1	1:B:674:ARG:O	2.70	0.43
1:A:183:THR:HG22	1:A:193:ILE:HG12	1.99	0.43
1:A:655:ARG:HG3	9:A:2049:HOH:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:PRO:HA	1:B:659:ARG:NE	2.32	0.43
1:A:655:ARG:H	1:A:655:ARG:HG3	1.58	0.43
1:B:561:LEU:HD13	1:B:561:LEU:HA	1.74	0.43
1:B:391:LEU:O	1:B:395:PHE:HB2	2.19	0.43
1:A:796:SER:HB3	1:A:827:ALA:HA	2.00	0.43
1:B:325:LEU:HG	1:B:344:TYR:HE1	1.83	0.43
1:A:223:LYS:NZ	9:A:2024:HOH:O	2.51	0.43
1:A:378:GLY:O	1:A:382:THR:OG1	2.23	0.43
1:A:431:ASN:HA	1:A:565:ARG:HH21	1.83	0.43
1:B:385:TRP:C	1:B:387:ASN:H	2.22	0.43
1:B:64:TRP:NE1	1:B:66:GLU:HB3	2.33	0.43
1:B:863:ALA:O	1:B:904:HIS:NE2	2.52	0.43
1:A:130:TYR:OH	1:A:152:VAL:HG13	2.18	0.43
1:A:742:LYS:O	1:A:751:ARG:NH2	2.52	0.43
1:A:796:SER:HA	1:A:827:ALA:HB1	2.01	0.43
1:A:600:ILE:HG23	1:A:625:VAL:HG21	2.00	0.43
1:B:374:HIS:CE1	1:B:393:GLU:OE2	2.72	0.43
1:B:640:TRP:HE3	1:B:641:ASP:HA	1.82	0.43
1:B:643:LEU:O	1:B:647:LEU:HB2	2.19	0.43
1:A:327:ALA:HB2	1:A:349:LEU:HD23	2.01	0.43
1:A:418:LEU:HA	1:A:418:LEU:HD23	1.79	0.43
1:B:238:LYS:HE2	1:B:238:LYS:HB3	1.81	0.43
1:A:485:PHE:CZ	1:A:494:ASP:HB3	2.54	0.42
1:A:785:ASN:OD1	9:A:2062:HOH:O	2.22	0.42
1:B:393:GLU:CD	2:D:1:GLY:HA3	2.39	0.42
1:B:358:ALA:HB2	1:B:748:ARG:CZ	2.49	0.42
1:B:925:GLY:HA2	1:B:926:SER:HA	1.68	0.42
1:A:381:VAL:HG21	1:A:482:LEU:HA	2.01	0.42
1:B:261:THR:O	1:B:263:LEU:N	2.52	0.42
1:B:374:HIS:NE2	1:B:393:GLU:OE2	2.52	0.42
1:B:421:CYS:O	1:B:424:VAL:HG23	2.19	0.42
1:A:177:GLU:HG2	1:A:203:GLN:HG2	2.02	0.42
1:B:310:TYR:HD1	1:B:314:PHE:CE2	2.37	0.42
1:B:378:GLY:CA	1:B:392:LYS:HG3	2.49	0.42
1:B:217:LYS:HD3	1:B:488:ARG:HA	2.02	0.42
1:B:550:LEU:O	1:B:634:HIS:N	2.50	0.42
1:B:412:GLN:NE2	1:B:746:TRP:HD1	2.18	0.42
1:A:721:ASN:CB	1:A:956:LEU:HD13	2.49	0.42
1:B:383:MET:HE1	1:B:392:LYS:CD	2.38	0.42
1:B:389:ILE:HG13	1:B:389:ILE:H	1.57	0.42
1:B:392:LYS:HE3	1:B:392:LYS:HB3	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:PHE:CE2	1:A:283:LYS:HB2	2.55	0.42
1:A:393:GLU:CD	2:C:1:GLY:HA3	2.38	0.42
1:B:126:GLU:HB2	1:B:160:LEU:HB3	2.00	0.42
1:B:729:TYR:HB3	1:B:730:PHE:CD2	2.55	0.42
1:B:723:LYS:HG3	1:B:761:LEU:HB3	2.02	0.42
1:B:328:ILE:HA	1:B:329:PRO:HD3	1.79	0.42
1:B:731:LYS:HE2	1:B:731:LYS:HB3	1.75	0.42
1:B:877:ARG:HG2	1:B:917:PHE:CE1	2.55	0.42
1:B:905:PHE:O	1:B:938:ILE:HG23	2.20	0.42
1:A:113:LYS:HB2	1:A:146:GLU:HG2	2.01	0.42
1:A:371:GLU:OE2	2:C:2[B]:PRO:HD2	2.19	0.42
1:A:55:VAL:HG12	1:A:62:PHE:O	2.19	0.42
1:B:135:LYS:HD3	1:B:135:LYS:HA	1.93	0.42
1:B:305:LYS:HE2	1:B:305:LYS:HB3	1.86	0.42
1:B:563:GLN:HG2	1:B:563:GLN:O	2.19	0.42
1:A:157:THR:HA	1:A:158:PRO:HD2	1.80	0.42
1:A:721:ASN:HB2	1:A:956:LEU:HD13	2.02	0.42
1:B:579:ALA:CB	1:B:580:LEU:HD23	2.50	0.42
1:A:476:LYS:O	1:A:480:GLN:HG3	2.20	0.41
1:B:298:TYR:OH	1:B:365:THR:OG1	2.08	0.41
1:A:745:VAL:O	1:A:749:MET:HG3	2.20	0.41
1:B:116:GLU:O	1:B:168:PHE:HA	2.20	0.41
1:B:366:ARG:HG2	1:B:400:GLU:OE1	2.20	0.41
1:B:576:GLU:O	1:B:579:ALA:HB3	2.21	0.41
1:A:64:TRP:CE3	1:A:70:PRO:HG3	2.56	0.41
1:B:545:LYS:HG2	1:B:545:LYS:O	2.20	0.41
1:A:352:ASP:HA	1:A:353:PRO:HD3	1.76	0.41
1:A:840:LEU:HA	1:A:840:LEU:HD23	1.91	0.41
1:B:580:LEU:N	1:B:580:LEU:HD23	2.36	0.41
1:A:647:LEU:HD23	1:A:651:HIS:HB2	2.01	0.41
1:A:748:ARG:HB3	1:A:789:ASP:OD2	2.20	0.41
1:B:538:MET:CE	1:B:541:TRP:HD1	2.32	0.41
1:B:729:TYR:C	1:B:731:LYS:H	2.24	0.41
1:B:314:PHE:O	1:B:315:ASP:HB3	2.20	0.41
1:A:74:ILE:HA	1:A:75:PRO:HD2	1.95	0.41
1:B:797:VAL:O	1:B:799:ALA:N	2.53	0.41
1:A:729:TYR:O	1:A:730:PHE:HB2	2.20	0.41
1:B:748:ARG:HG2	1:B:751:ARG:NH2	2.36	0.41
1:B:351:PHE:CZ	1:B:361:LYS:HD2	2.56	0.41
1:B:372:LEU:HA	1:B:375:GLN:HG2	2.02	0.41
1:B:460:CYS:O	1:B:463:ASN:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:951:THR:O	1:B:955:TRP:HB2	2.21	0.41
1:A:64:TRP:CE2	1:A:70:PRO:HG3	2.56	0.41
1:A:449:MET:O	1:A:454:SER:OG	2.34	0.41
1:B:385:TRP:O	1:B:387:ASN:N	2.54	0.41
1:B:442:THR:O	1:B:445:GLN:HG2	2.21	0.41
1:B:549:LEU:HD13	1:B:632:ILE:CG2	2.43	0.41
1:B:902:THR:O	1:B:905:PHE:HB2	2.21	0.41
1:B:276:GLY:HA3	1:B:300:LEU:HD11	2.02	0.40
1:B:384:GLU:HA	1:B:489:ASN:HB3	2.02	0.40
1:B:703:LEU:HD13	1:B:726:LEU:HD21	2.02	0.40
1:B:226:ARG:NH1	1:B:249:LEU:HD12	2.36	0.40
1:B:464:MET:HG2	1:B:629:GLY:HA2	2.03	0.40
1:B:541:TRP:CH2	1:B:548:PRO:HD3	2.56	0.40
1:B:624:ASN:HD22	1:B:624:ASN:HA	1.63	0.40
1:B:67:LEU:HG	1:B:145:HIS:CD2	2.56	0.40
1:A:124:SER:OG	1:A:127:ASP:N	2.50	0.40
1:A:318:TYR:HA	1:A:319:PRO:HD3	1.93	0.40
1:A:424:VAL:HG21	1:A:457:LYS:HB2	2.03	0.40
1:B:197:THR:HG23	1:B:266:TYR:O	2.22	0.40
1:B:659:ARG:O	1:B:663:ILE:HG13	2.22	0.40
1:A:325:LEU:N	1:A:325:LEU:HD12	2.36	0.40
1:A:722:LEU:HA	1:A:722:LEU:HD23	1.69	0.40
1:A:846:GLU:OE1	1:A:848:LYS:HD2	2.22	0.40
8:B:1001:NAG:C1	9:B:2001:HOH:O	2.69	0.40
1:B:311:GLU:OE1	1:B:317:TYR:HA	2.21	0.40
1:B:560:ARG:HB3	1:B:610:ASP:OD2	2.20	0.40
1:B:550:LEU:HB2	1:B:632:ILE:O	2.22	0.40
1:B:713:ARG:HB2	1:B:715:ILE:HG13	2.04	0.40
1:A:457:LYS:O	1:A:461:ILE:HG23	2.21	0.40
1:A:675:LEU:HA	1:A:675:LEU:HD12	1.67	0.40
1:B:436:ILE:HG21	1:B:457:LYS:HD2	2.02	0.40
1:B:575:PRO:HG2	1:B:576:GLU:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	901/967 (93%)	814 (90%)	75 (8%)	12 (1%)	14	33
1	B	875/967 (90%)	732 (84%)	117 (13%)	26 (3%)	5	11
2	C	8/6 (133%)	4 (50%)	0	4 (50%)	0	0
2	D	4/6 (67%)	4 (100%)	0	0	100	100
All	All	1788/1946 (92%)	1554 (87%)	192 (11%)	42 (2%)	7	18

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	THR
1	A	60	GLU
1	A	245	GLU
1	A	582	GLU
1	A	616	GLU
1	B	216	PHE
1	B	536	GLU
1	B	554	GLN
1	B	571	PHE
1	B	584	TYR
1	A	124	SER
1	A	427	LYS
1	A	605	LEU
1	A	715	ILE
1	B	72	VAL
1	B	89	LEU
1	B	131	MET
1	B	143	PRO
1	B	155	LYS
1	B	598	ASN
1	B	960	THR
2	C	4[A]	ARG
2	C	4[B]	ARG
2	C	5[A]	ALA
2	C	5[B]	ALA
1	A	155	LYS
1	A	426	THR
1	B	63	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	649	GLN
1	B	730	PHE
1	B	262	TYR
1	B	453	VAL
1	B	534	VAL
1	B	607	SER
1	B	215	LEU
1	B	339	TRP
1	B	386	TRP
1	B	436	ILE
1	B	798	GLY
1	B	55	VAL
1	A	133	PRO
1	B	201	PRO

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	813/870 (93%)	768 (94%)	45 (6%)	25	51
1	B	790/870 (91%)	715 (90%)	75 (10%)	10	22
2	C	6/3 (200%)	4 (67%)	2 (33%)	0	0
2	D	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1612/1746 (92%)	1489 (92%)	123 (8%)	15	34

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	VAL
1	A	103	ASN
1	A	105	THR
1	A	110	LEU
1	A	123	GLN
1	A	129	ARG
1	A	145	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	174	ASP
1	A	179	PHE
1	A	225	ARG
1	A	303	SER
1	A	322	LYS
1	A	352	ASP
1	A	383	MET
1	A	389	ILE
1	A	395	PHE
1	A	397	LYS
1	A	426	THR
1	A	427	LYS
1	A	431	ASN
1	A	436	ILE
1	A	461	ILE
1	A	466	LYS
1	A	489	ASN
1	A	516	SER
1	A	517	ASP
1	A	519	LYS
1	A	525	LEU
1	A	571	PHE
1	A	611	THR
1	A	679	LYS
1	A	686	TYR
1	A	729	TYR
1	A	757	LEU
1	A	775	SER
1	A	785	ASN
1	A	831	SER
1	A	842[A]	GLU
1	A	842[B]	GLU
1	A	849	VAL
1	A	864	ARG
1	A	873	TRP
1	A	881	THR
1	A	916	LEU
1	A	920	SER
1	B	55	VAL
1	B	67	LEU
1	B	73	VAL
1	B	74	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	79	ASP
1	B	88	SER
1	B	92	VAL
1	B	94	SER
1	B	101	VAL
1	B	123	GLN
1	B	145	HIS
1	B	174	ASP
1	B	193	ILE
1	B	194	LEU
1	B	239	VAL
1	B	285	SER
1	B	320	LEU
1	B	339	TRP
1	B	366	ARG
1	B	367	VAL
1	B	383	MET
1	B	395	PHE
1	B	405	ASN
1	B	424	VAL
1	B	437	SER
1	B	442	THR
1	B	456	ASN
1	B	466	LYS
1	B	467	ASP
1	B	469	LEU
1	B	474	PHE
1	B	492	ASN
1	B	499	LEU
1	B	538	MET
1	B	542	THR
1	B	547	ILE
1	B	553	LYS
1	B	554	GLN
1	B	555	ASP
1	B	559	LEU
1	B	560	ARG
1	B	565	ARG
1	B	573	GLU
1	B	576	GLU
1	B	578	ARG
1	B	580	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	582	GLU
1	B	583	ARG
1	B	588	ILE
1	B	598	ASN
1	B	603	HIS
1	B	611	THR
1	B	623	PHE
1	B	624	ASN
1	B	641	ASP
1	B	647	LEU
1	B	653	LEU
1	B	658	ASP
1	B	674	ARG
1	B	684	THR
1	B	714	ASN
1	B	719	SER
1	B	729	TYR
1	B	757	LEU
1	B	759	CYS
1	B	768	GLN
1	B	793	ILE
1	B	813	GLU
1	B	833	HIS
1	B	834	GLN
1	B	862	ILE
1	B	889	LEU
1	B	908	LYS
1	B	941	ASN
1	B	960	THR
2	C	4[A]	ARG
2	C	4[B]	ARG
2	D	4	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	562	GLN
1	B	581	GLN
1	B	624	ASN
1	B	634	HIS
1	B	959	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 ⓘ

24 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$
3	NAG	A	1001	3	14,14,15	1.29	1 (7%)	15,19,21	1.76	1 (6%)
3	NAG	A	1002	1,3	14,14,15	0.51	0	15,19,21	0.60	0
3	BMA	A	1003	3	11,11,12	1.20	2 (18%)	13,15,17	1.53	4 (30%)
4	NAG	A	1004	1,4	14,14,15	0.67	0	15,19,21	0.52	0
4	NAG	A	1005	4	14,14,15	0.45	0	15,19,21	0.46	0
3	NAG	A	1006	1,3	14,14,15	1.09	1 (7%)	15,19,21	0.59	0
3	NAG	A	1007	3	14,14,15	0.54	0	15,19,21	0.72	0
3	BMA	A	1008	3	11,11,12	2.05	4 (36%)	13,15,17	2.43	6 (46%)
4	NAG	A	1010	1,4	14,14,15	0.30	0	15,19,21	0.78	0
4	NAG	A	1011	4	14,14,15	0.40	0	15,19,21	0.40	0
4	NAG	A	1012	1,4	14,14,15	0.67	1 (7%)	15,19,21	0.80	1 (6%)
4	NAG	A	1013	4	14,14,15	0.88	1 (7%)	15,19,21	0.91	1 (6%)
4	NAG	A	1014	1,4	14,14,15	0.31	0	15,19,21	1.40	2 (13%)
4	NAG	A	1015	4	14,14,15	0.31	0	15,19,21	0.45	0
4	NAG	A	1016	1,4	14,14,15	0.95	1 (7%)	15,19,21	1.08	1 (6%)
4	NAG	A	1017	4	14,14,15	0.45	0	15,19,21	0.39	0
8	NAG	B	1001	1,8	14,14,15	0.79	0	15,19,21	1.64	2 (13%)
8	NAG	B	1002	8	14,14,15	0.63	0	15,19,21	1.47	1 (6%)
8	BMA	B	1003	8	11,11,12	1.69	1 (9%)	13,15,17	1.30	2 (15%)
8	BMA	B	1004	8	11,11,12	1.03	0	13,15,17	1.58	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1006	1,4	14,14,15	0.38	0	15,19,21	0.63	0
4	NAG	B	1007	4	14,14,15	0.50	0	15,19,21	0.52	0
4	NAG	B	1008	1,4	14,14,15	0.32	0	15,19,21	0.97	0
4	NAG	B	1009	4	14,14,15	0.70	1 (7%)	15,19,21	0.68	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	NAG	A	1001	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1002	1,3	-	0/6/23/26	0/1/1/1
3	BMA	A	1003	3	-	0/2/19/22	0/1/1/1
4	NAG	A	1004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1005	4	-	0/6/23/26	0/1/1/1
3	NAG	A	1006	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1007	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1008	3	-	0/2/19/22	0/1/1/1
4	NAG	A	1010	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1011	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1012	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1013	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1014	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1015	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1016	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1017	4	-	0/6/23/26	0/1/1/1
8	NAG	B	1001	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1002	8	-	0/6/23/26	0/1/1/1
8	BMA	B	1003	8	-	0/2/19/22	0/1/1/1
8	BMA	B	1004	8	-	0/2/19/22	0/1/1/1
4	NAG	B	1006	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1007	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1008	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1009	4	-	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1006	NAG	O5-C1	-3.64	1.37	1.43
4	A	1016	NAG	O5-C1	-3.31	1.38	1.43
4	A	1012	NAG	O5-C1	-2.39	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	BMA	O5-C5	2.31	1.48	1.43
3	A	1008	BMA	C2-C3	2.42	1.55	1.52
4	B	1009	NAG	C1-C2	2.44	1.55	1.52
3	A	1003	BMA	C1-C2	2.47	1.58	1.52
4	A	1013	NAG	O5-C1	2.92	1.48	1.43
3	A	1008	BMA	O5-C1	2.98	1.48	1.43
3	A	1008	BMA	O5-C5	3.61	1.51	1.43
3	A	1008	BMA	C1-C2	3.81	1.61	1.52
8	B	1003	BMA	C2-C3	4.49	1.58	1.52
3	A	1001	NAG	O5-C1	4.70	1.51	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1001	NAG	O4-C4-C3	-4.37	100.85	110.36
3	A	1008	BMA	C3-C4-C5	-2.28	106.20	110.22
4	A	1012	NAG	O4-C4-C3	-2.23	105.50	110.36
3	A	1008	BMA	O2-C2-C3	-2.16	105.94	110.17
8	B	1004	BMA	O2-C2-C3	-2.14	105.98	110.17
8	B	1003	BMA	C1-C2-C3	-2.03	107.08	109.65
3	A	1003	BMA	O2-C2-C3	-2.02	106.21	110.17
3	A	1008	BMA	O2-C2-C1	2.08	113.40	109.18
4	A	1014	NAG	C1-C2-N2	2.21	114.26	110.49
3	A	1003	BMA	C1-C2-C3	2.35	112.64	109.65
3	A	1008	BMA	C1-C2-C3	2.39	112.68	109.65
3	A	1003	BMA	O5-C1-C2	2.41	114.57	110.79
4	A	1016	NAG	C3-C4-C5	2.47	114.56	110.22
3	A	1003	BMA	C1-O5-C5	2.81	116.04	112.17
8	B	1004	BMA	C1-O5-C5	2.91	116.17	112.17
4	A	1013	NAG	C1-O5-C5	3.02	116.33	112.17
8	B	1001	NAG	C4-C3-C2	3.30	115.85	111.02
3	A	1008	BMA	O5-C1-C2	3.46	116.20	110.79
8	B	1003	BMA	O3-C3-C2	3.80	116.94	110.02
4	A	1014	NAG	C2-N2-C7	4.21	129.08	122.94
8	B	1002	NAG	C1-O5-C5	4.72	118.68	112.17
3	A	1008	BMA	C1-O5-C5	6.29	120.83	112.17
3	A	1001	NAG	C1-O5-C5	6.47	121.09	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1014	NAG	2	0
4	A	1015	NAG	1	0
4	A	1016	NAG	1	0
8	B	1001	NAG	5	0
8	B	1002	NAG	1	0
8	B	1003	BMA	1	0
8	B	1004	BMA	1	0
4	B	1006	NAG	1	0
4	B	1007	NAG	1	0
4	B	1009	NAG	1	0

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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	$\# Z > 2$
5	NAG	A	1009	1	14,14,15	0.32	0	15,19,21	0.87	1 (6%)
5	NAG	A	1018	1	14,14,15	0.50	0	15,19,21	0.56	0
7	EDO	A	1962	-	3,3,3	0.67	0	2,2,2	0.15	0
7	EDO	A	1963	-	3,3,3	0.46	0	2,2,2	0.40	0
7	EDO	A	1964	-	3,3,3	0.54	0	2,2,2	0.22	0
5	NAG	B	1005	1	14,14,15	0.53	0	15,19,21	0.64	0
5	NAG	B	1010	1	14,14,15	0.35	0	15,19,21	0.54	0
5	NAG	B	1011	1	14,14,15	0.52	0	15,19,21	0.51	0
7	EDO	B	1961	-	3,3,3	0.50	0	2,2,2	0.17	0
7	EDO	B	1962	-	3,3,3	0.47	0	2,2,2	0.35	0
7	EDO	B	1963	-	3,3,3	0.44	0	2,2,2	0.38	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
5	NAG	A	1009	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1018	1	-	0/6/23/26	0/1/1/1
7	EDO	A	1962	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1963	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1964	-	-	0/1/1/1	0/0/0/0
5	NAG	B	1005	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1011	1	-	0/6/23/26	0/1/1/1
7	EDO	B	1961	-	-	0/1/1/1	0/0/0/0
7	EDO	B	1962	-	-	0/1/1/1	0/0/0/0
7	EDO	B	1963	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1009	NAG	C1-O5-C5	2.26	115.28	112.17

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	897/967 (92%)	-0.04	20 (2%) 62 63	24, 47, 86, 151	0
1	B	879/967 (90%)	0.82	121 (13%) 3 2	30, 100, 150, 170	0
2	C	6/6 (100%)	1.90	2 (33%) 0 0	42, 47, 52, 54	0
2	D	6/6 (100%)	5.31	5 (83%) 0 0	74, 77, 84, 90	6 (100%)
All	All	1788/1946 (91%)	0.41	148 (8%) 12 10	24, 66, 137, 170	6 (0%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	580	LEU	8.6
1	A	520	MET	8.1
1	B	602	ARG	7.6
2	D	6	PHE	7.6
1	B	72	VAL	7.5
2	D	5	ALA	7.0
1	B	727	LEU	6.9
1	B	592	TYR	6.8
1	B	623	PHE	6.6
1	B	571	PHE	6.5
1	B	721	ASN	6.1
2	D	4	ARG	5.9
1	B	723	LYS	5.9
1	B	569	GLY	5.8
1	B	612	LEU	5.8
1	B	647	LEU	5.7
1	A	523	ASN	5.7
1	A	519	LYS	5.5
1	B	621	VAL	5.5
2	D	3	GLY	5.4
1	A	521	THR	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	687	LEU	5.3
1	B	637	GLY	5.2
1	B	556	GLY	5.1
1	B	570	VAL	4.9
1	B	554	GLN	4.6
1	B	99	VAL	4.6
1	B	601	HIS	4.5
1	B	596	SER	4.5
1	B	108	ILE	4.5
1	B	150	LEU	4.4
1	B	610	ASP	4.4
1	A	527	PHE	4.4
1	A	522	SER	4.3
1	B	69	LEU	4.2
1	B	607	SER	4.1
1	B	572	GLN	4.1
1	B	681	LEU	4.1
1	B	722	LEU	4.1
1	B	956	LEU	4.0
2	D	2	PRO	3.9
1	B	635	TYR	3.9
1	B	667	PHE	3.9
1	B	750	LEU	3.9
1	B	611	THR	3.9
1	A	580	LEU	3.9
1	B	952	LEU	3.9
1	B	117	ILE	3.8
1	B	648	ASN	3.8
1	B	96	LYS	3.7
1	B	615	PRO	3.7
1	B	73	VAL	3.7
2	C	3[A]	GLY	3.7
1	B	689	HIS	3.6
1	B	118	THR	3.6
1	B	555	ASP	3.6
1	B	608	LYS	3.6
1	A	559	LEU	3.5
1	B	318	TYR	3.5
1	B	106	GLN	3.4
1	B	716	SER	3.4
1	B	317	TYR	3.3
1	B	107	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	71	SER	3.2
1	B	677	LEU	3.2
1	A	526	ALA	3.1
1	B	609	THR	3.1
1	B	724	ARG	3.1
1	B	164	VAL	3.1
1	B	603	HIS	3.1
1	B	953	ARG	3.1
1	B	551	VAL	3.1
1	A	517	ASP	3.1
1	B	696	LEU	3.0
1	B	597	SER	3.0
1	B	688	GLN	2.9
1	A	784	LEU	2.9
1	B	539	THR	2.9
1	B	622	LYS	2.9
1	B	419	ASN	2.9
1	B	543	LEU	2.9
1	B	700	LEU	2.8
1	B	726	LEU	2.8
1	B	636	GLU	2.8
2	C	6[A]	PHE	2.8
1	B	417	PHE	2.7
1	B	105	THR	2.7
1	B	103	ASN	2.7
1	B	707	TYR	2.6
1	A	246	GLY	2.6
1	B	102	SER	2.6
1	A	614	LEU	2.6
1	B	606	LYS	2.5
1	B	316	ILE	2.5
1	B	616	GLU	2.5
1	B	734	ILE	2.5
1	B	166	MET	2.5
1	B	120	ALA	2.4
1	B	495	LEU	2.4
1	B	638	HIS	2.4
1	B	116	GLU	2.4
1	B	559	LEU	2.4
1	A	515	HIS	2.4
1	B	703	LEU	2.4
1	B	348	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	730	PHE	2.4
1	B	162	TYR	2.4
1	B	662	LEU	2.3
1	B	565	ARG	2.3
1	A	621	VAL	2.3
1	A	518	PRO	2.3
1	A	525	LEU	2.3
1	B	488	ARG	2.3
1	B	719	SER	2.3
1	B	955	TRP	2.2
1	B	416	TYR	2.2
1	B	421	CYS	2.2
1	A	528	LEU	2.2
1	B	499	LEU	2.2
1	B	403	ALA	2.2
1	B	365	THR	2.2
1	B	691	THR	2.2
1	B	754	LEU	2.1
1	B	578	ARG	2.1
1	B	765	PRO	2.1
1	B	536	GLU	2.1
1	B	157	THR	2.1
1	B	552	VAL	2.1
1	B	711	ASP	2.1
1	B	684	THR	2.1
1	B	281	GLY	2.1
1	B	152	VAL	2.1
1	B	364	VAL	2.1
1	B	369	ALA	2.1
1	B	613	ASP	2.1
1	A	248	LEU	2.0
1	B	370	HIS	2.0
1	B	598	ASN	2.0
1	B	593	SER	2.0
1	B	418	LEU	2.0
1	B	74	ILE	2.0
1	B	121	THR	2.0
1	B	422	PHE	2.0
1	A	578	ARG	2.0
1	B	454	SER	2.0
1	B	728	GLN	2.0
1	B	248	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	733	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

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
3	NAG	A	1002	14/15	0.95	0.25	0.80	43,68,77,77	0
3	NAG	A	1006	14/15	0.96	0.13	-0.04	41,46,56,62	0
3	NAG	A	1001	14/15	0.91	0.21	-0.17	79,90,107,113	0
4	NAG	B	1008	14/15	0.83	0.16	-0.26	91,115,128,134	0
3	BMA	A	1008	11/12	0.76	0.15	-	90,97,105,107	0
4	NAG	A	1013	14/15	0.69	0.25	-	112,122,130,132	0
4	NAG	B	1007	14/15	0.77	0.23	-	131,158,162,163	0
4	NAG	A	1005	14/15	0.66	0.39	-	142,155,160,161	0
8	NAG	B	1002	14/15	0.87	0.14	-	50,77,88,88	0
8	BMA	B	1004	11/12	0.82	0.18	-	73,100,109,113	0
8	NAG	B	1001	14/15	0.89	0.23	-	57,67,76,79	0
4	NAG	A	1004	14/15	0.83	0.25	-	91,119,136,146	0
8	BMA	B	1003	11/12	0.79	0.13	-	73,98,104,104	0
4	NAG	A	1014	14/15	0.80	0.19	-	106,127,136,138	0
4	NAG	A	1015	14/15	0.67	0.26	-	119,132,141,141	0
4	NAG	A	1011	14/15	0.80	0.23	-	103,114,118,119	0
4	NAG	A	1010	14/15	0.89	0.12	-	76,84,97,106	0
4	NAG	A	1016	14/15	0.81	0.18	-	57,92,108,122	0
4	NAG	A	1012	14/15	0.87	0.17	-	95,103,114,117	0
4	NAG	B	1009	14/15	0.76	0.25	-	121,133,137,140	0
4	NAG	B	1006	14/15	0.70	0.20	-	138,153,159,164	0
4	NAG	A	1017	14/15	0.77	0.30	-	115,128,133,139	0
3	NAG	A	1007	14/15	0.91	0.12	-	46,66,84,88	0
3	BMA	A	1003	11/12	0.83	0.23	-	109,117,121,122	0

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	B	1010	14/15	0.40	0.46	6.13	112,136,147,147	0
5	NAG	A	1009	14/15	0.91	0.17	0.39	60,84,88,89	0
6	ZN	A	1119	1/1	0.99	0.21	-0.93	28,28,28,28	0
6	ZN	B	1119	1/1	0.97	0.22	-1.17	60,60,60,60	0
7	EDO	A	1962	4/4	0.87	0.11	-1.65	51,56,57,65	0
7	EDO	B	1962	4/4	0.78	0.38	-	96,99,103,116	0
5	NAG	B	1005	14/15	0.69	0.29	-	143,151,154,154	0
7	EDO	B	1963	4/4	0.84	0.27	-	99,99,104,120	0
7	EDO	B	1961	4/4	0.77	0.29	-	81,93,96,97	0
5	NAG	A	1018	14/15	0.80	0.23	-	97,110,122,129	0
7	EDO	A	1964	4/4	0.69	0.31	-	74,80,84,88	0
7	EDO	A	1963	4/4	0.91	0.10	-	83,89,90,96	0
5	NAG	B	1011	14/15	0.66	0.27	-	132,143,148,150	0

6.5 Other polymers [i](#)

There are no such residues in this entry.