



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2024 – 10:46 PM EST

PDB ID : 3NVQ
Title : Molecular mechanism of guidance cue recognition
Authors : Juo, Z.; Liu, H.; Shim, A.; Focia, P.; Chen, X.; Garcia, C.; He, X.
Deposited on : 2010-07-08
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

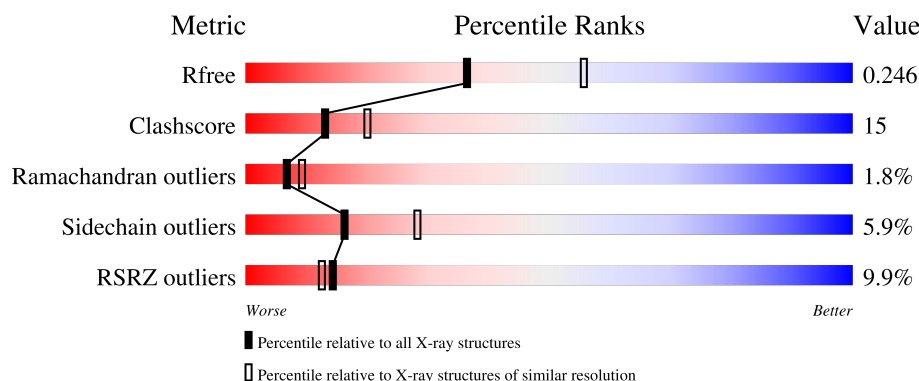
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	590	<div> <div>6%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	E	590	<div> <div>6%</div> <div>70%</div> <div>25%</div> <div>.</div> </div>
2	B	476	<div> <div>14%</div> <div>70%</div> <div>26%</div> <div>.</div> </div>
2	F	476	<div> <div>15%</div> <div>67%</div> <div>29%</div> <div>.</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	3	X	-	-	-
3	NAG	E	3	X	-	-	-
3	NAG	F	6	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17824 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 Semaphorin-7A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4706	2957	840	882	27			
1	E	588	Total	C	N	O	S	0	0	0
			4706	2957	840	882	27			

- Molecule 2 is a protein called Plexin-C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	474	Total	C	N	O	S	0	0	0
			3623	2261	645	696	21			
2	F	474	Total	C	N	O	S	0	0	0
			3623	2261	645	696	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	508	GLY	-	expression tag	UNP O60486
B	509	ALA	-	expression tag	UNP O60486
B	510	PRO	-	expression tag	UNP O60486
F	508	GLY	-	expression tag	UNP O60486
F	509	ALA	-	expression tag	UNP O60486
F	510	PRO	-	expression tag	UNP O60486

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



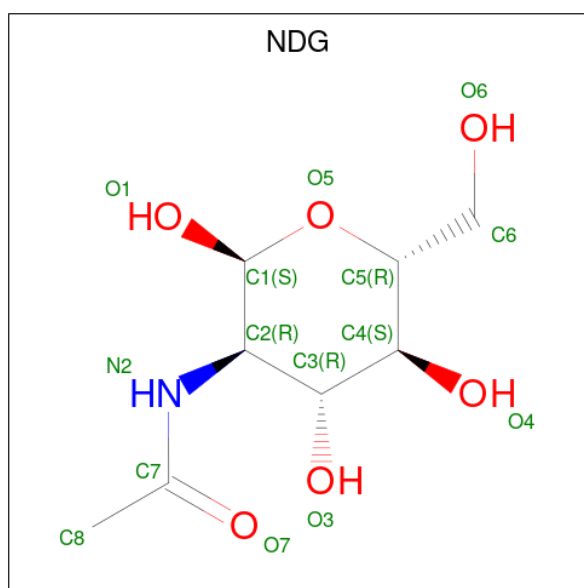
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	279	Total	O	0	0
			279	279		

Continued on next page...

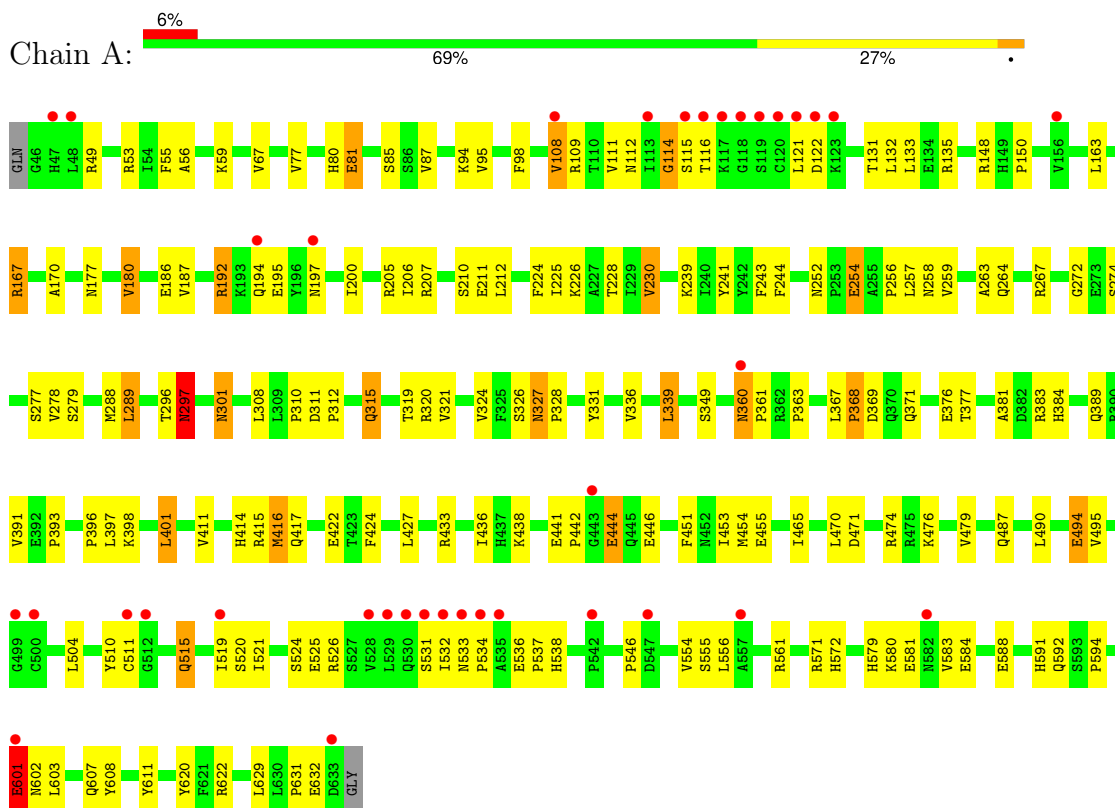
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	162	Total 162	O 162	0	0
5	E	297	Total 297	O 297	0	0
5	F	120	Total 120	O 120	0	0

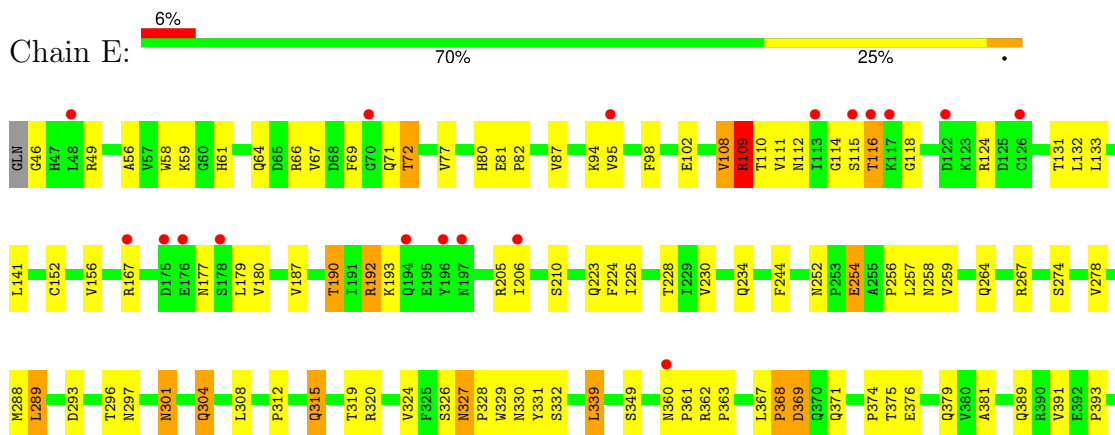
3 Residue-property plots [i](#)

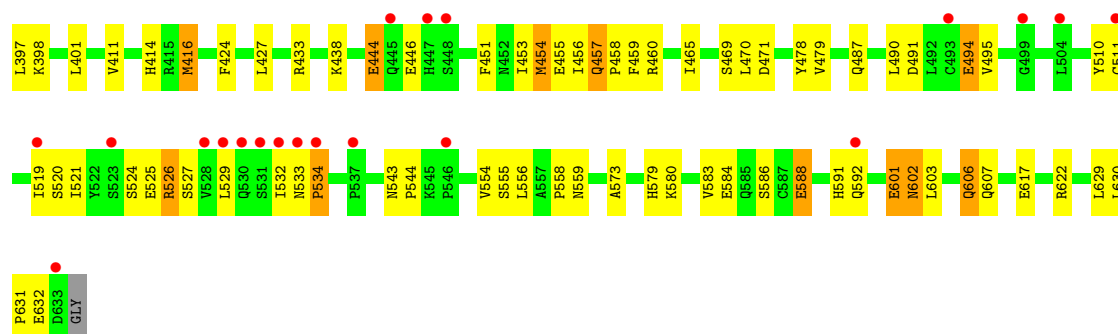
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Semaphorin-7A

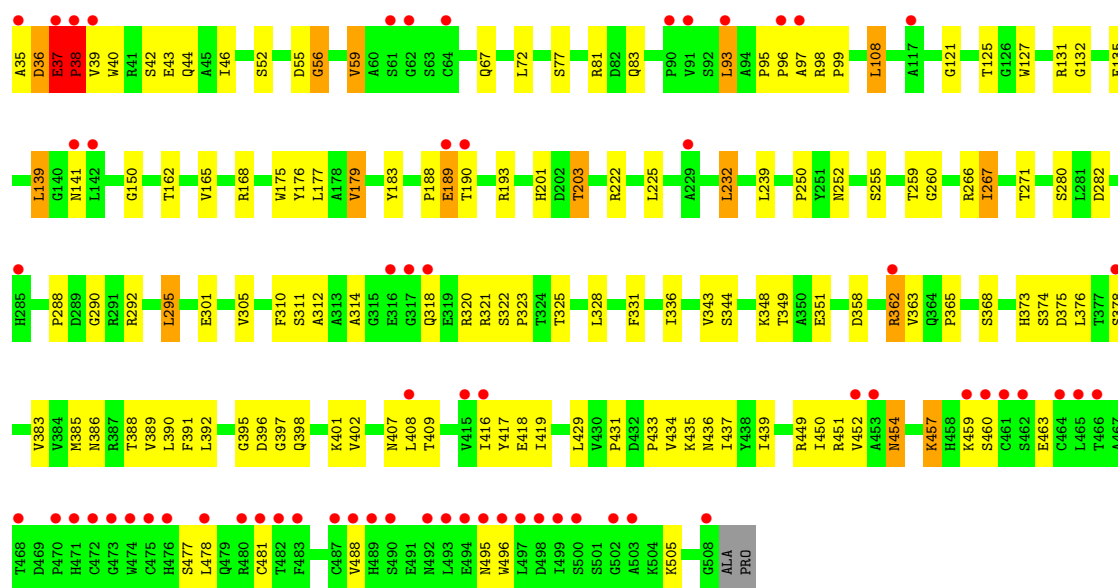


• Molecule 1: Semaphorin-7A

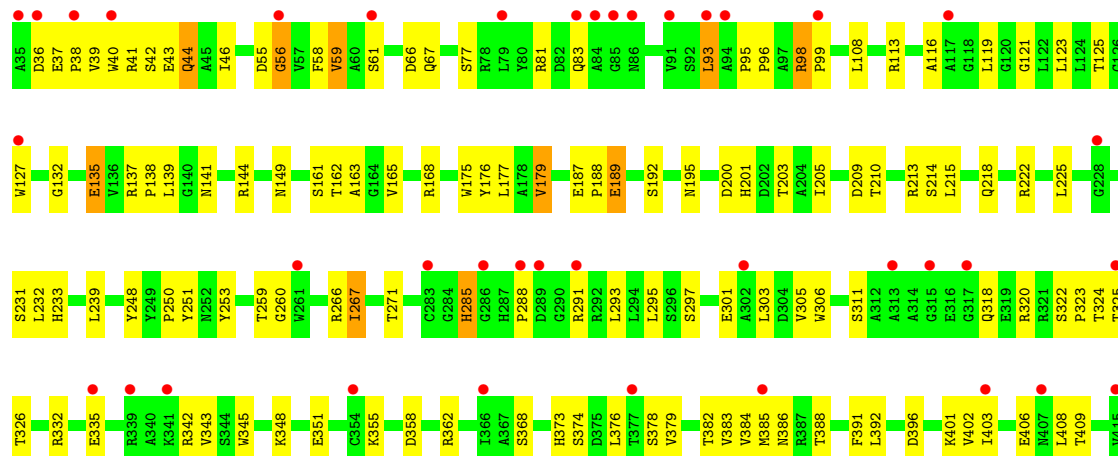


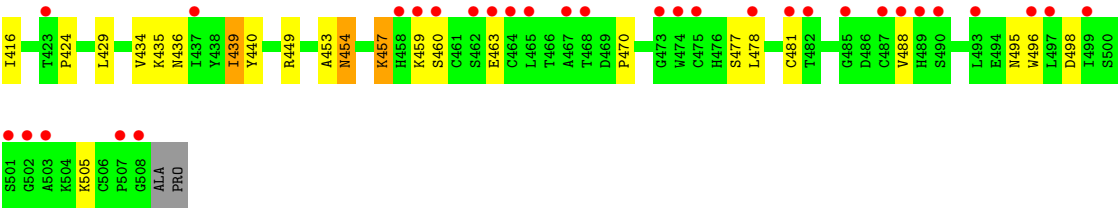


• Molecule 2: Plexin-C1



• Molecule 2: Plexin-C1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.64Å 126.08Å 236.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.40 – 2.40 25.40 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.7 (25.40-2.40) 98.3 (25.40-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.277 0.249 , 0.246	Depositor DCC
R_{free} test set	5760 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17824	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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

5.1 Standard geometry

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

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	0.43	0/4839	0.73	6/6568 (0.1%)
1	E	0.42	0/4839	0.71	3/6568 (0.0%)
2	B	0.37	0/3706	0.66	4/5039 (0.1%)
2	F	0.36	0/3706	0.60	0/5039
All	All	0.40	0/17090	0.68	13/23214 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASN	N-CA-CB	10.29	129.11	110.60
1	A	602	ASN	N-CA-CB	-9.26	93.93	110.60
1	A	601	GLU	CB-CA-C	8.97	128.33	110.40
1	A	296	THR	N-CA-C	8.90	135.04	111.00
2	B	37	GLU	N-CA-C	8.40	133.69	111.00
2	B	36	ASP	N-CA-C	7.19	130.40	111.00
1	E	602	ASN	N-CA-C	-7.17	91.64	111.00
1	E	602	ASN	N-CA-CB	-6.86	98.25	110.60
2	B	38	PRO	N-CA-C	-6.72	94.62	112.10
1	E	601	GLU	CB-CA-C	6.22	122.85	110.40
1	A	602	ASN	N-CA-C	-6.17	94.35	111.00
1	A	296	THR	CB-CA-C	-5.40	97.01	111.60
2	B	36	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4706	0	4479	148	0
1	E	4706	0	4478	143	0
2	B	3623	0	3496	100	0
2	F	3623	0	3497	111	0
3	A	42	0	39	0	0
3	B	98	0	91	2	0
3	E	56	0	52	8	0
3	F	98	0	91	3	0
4	A	14	0	12	0	0
5	A	279	0	0	11	0
5	B	162	0	0	8	0
5	E	297	0	0	14	0
5	F	120	0	0	6	0
All	All	17824	0	16235	488	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 15.

All (488) 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:A:592:GLN:HG3	1:E:592:GLN:NE2	1.63	1.11
2:B:35:ALA:N	2:B:451:ARG:HB2	1.72	1.04
1:E:360:ASN:HB3	1:E:361:PRO:HD3	1.39	1.02
2:F:203:THR:HG22	2:F:222:ARG:HH11	1.29	0.96
2:B:459:LYS:HD3	5:B:805:HOH:O	1.71	0.91
1:E:228:THR:HG21	1:E:308:LEU:HD12	1.53	0.91
1:A:592:GLN:HG3	1:E:592:GLN:CD	1.92	0.90
1:E:319:THR:HB	1:E:339:LEU:HD22	1.52	0.90
1:E:274:SER:O	1:E:278:VAL:HG23	1.72	0.89
2:F:203:THR:HG22	2:F:222:ARG:NH1	1.88	0.87
1:E:603:LEU:HD12	1:E:607:GLN:HG3	1.57	0.85
1:E:156:VAL:HG11	3:E:2:NAG:C7	2.08	0.83
1:A:349:SER:HB2	1:A:389:GLN:HG2	1.60	0.83
1:A:592:GLN:CG	1:E:592:GLN:CD	2.49	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:THR:HB	1:A:339:LEU:HD22	1.64	0.80
1:E:349:SER:HB2	1:E:389:GLN:HG2	1.64	0.79
1:A:603:LEU:HD12	1:A:607:GLN:HG3	1.65	0.78
2:F:295:LEU:HD21	2:F:311:SER:HB3	1.64	0.77
1:A:228:THR:HG21	1:A:308:LEU:HD11	1.65	0.77
1:A:416:MET:HE1	1:A:424:PHE:HB2	1.67	0.76
1:E:360:ASN:HB3	1:E:361:PRO:CD	2.15	0.76
1:A:470:LEU:HD11	1:A:490:LEU:HD21	1.66	0.76
1:A:592:GLN:CD	1:E:592:GLN:HG3	2.06	0.75
1:A:393:PRO:HD2	1:A:398:LYS:HB3	1.68	0.75
2:F:200:ASP:O	2:F:203:THR:HG23	1.86	0.74
2:F:250:PRO:HB2	2:F:259:THR:HB	1.69	0.74
1:A:259:VAL:HG21	1:A:288:MET:CE	2.18	0.74
1:A:592:GLN:OE1	1:E:592:GLN:HG3	1.88	0.73
1:E:457:GLN:HE22	1:E:459:PHE:H	1.34	0.73
1:E:465:ILE:HG23	1:E:479:VAL:HG13	1.70	0.73
1:A:49:ARG:HD3	1:A:451:PHE:CE1	2.24	0.73
1:A:187:VAL:HG23	1:A:206:ILE:HB	1.71	0.72
1:E:555:SER:HB3	1:E:632:GLU:HB2	1.70	0.72
1:E:580:LYS:HB3	5:E:662:HOH:O	1.90	0.72
1:E:304:GLN:HE21	1:E:304:GLN:HA	1.55	0.71
1:A:67:VAL:HG11	1:A:108:VAL:HG22	1.71	0.71
2:F:343:VAL:HG21	2:F:358:ASP:O	1.90	0.71
1:A:451:PHE:HD2	1:A:453:ILE:HG22	1.57	0.70
1:A:465:ILE:HG23	1:A:479:VAL:HG13	1.74	0.69
2:F:406:GLU:HG3	3:F:7:NAG:H5	1.74	0.69
1:E:67:VAL:HG11	1:E:108:VAL:HG22	1.73	0.69
1:A:259:VAL:HG21	1:A:288:MET:HE2	1.74	0.69
1:A:592:GLN:HB2	1:E:592:GLN:OE1	1.92	0.68
2:B:398:GLN:HG2	2:B:418:GLU:HG2	1.73	0.68
2:F:165:VAL:HG21	2:F:239:LEU:HD13	1.74	0.68
1:E:532:ILE:HG22	1:E:534:PRO:HD2	1.75	0.68
1:A:274:SER:O	1:A:278:VAL:HG23	1.93	0.68
1:E:320:ARG:HD3	5:E:650:HOH:O	1.93	0.67
1:E:369:ASP:N	1:E:371:GLN:HE21	1.92	0.67
1:A:360:ASN:HB3	1:A:361:PRO:CD	2.24	0.67
1:A:631:PRO:O	1:A:632:GLU:HG2	1.94	0.67
1:E:393:PRO:HD2	1:E:398:LYS:HB3	1.77	0.67
1:A:454:MET:HG2	1:A:455:GLU:N	2.10	0.67
2:B:176:TYR:CE2	2:B:271:THR:HG22	2.30	0.67
1:E:457:GLN:NE2	1:E:459:PHE:H	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:VAL:HG22	1:A:207:ARG:HB3	1.77	0.66
2:F:401:LYS:CB	2:F:416:ILE:HD11	2.25	0.65
1:E:132:LEU:HD12	1:E:133:LEU:N	2.12	0.65
2:B:401:LYS:HD2	2:B:416:ILE:HD11	1.78	0.64
1:A:532:ILE:HG22	1:A:534:PRO:HD2	1.79	0.64
1:A:369:ASP:N	1:A:371:GLN:HE21	1.96	0.64
2:B:177:LEU:HG	2:B:179:VAL:HG22	1.80	0.64
1:E:414:HIS:HD2	1:E:510:TYR:OH	1.79	0.64
2:B:322:SER:HB3	2:B:325:THR:HG23	1.80	0.64
1:A:225:ILE:HD13	1:A:244:PHE:HA	1.79	0.63
2:B:328:LEU:HD21	2:B:390:LEU:HD23	1.80	0.63
2:B:165:VAL:HG21	2:B:239:LEU:HD13	1.80	0.63
2:F:141:ASN:HB3	2:F:144:ARG:HG3	1.81	0.63
2:F:213:ARG:HG3	2:F:213:ARG:HH11	1.61	0.63
1:A:327:ASN:C	1:A:327:ASN:HD22	2.00	0.63
1:A:416:MET:CE	1:A:424:PHE:HB2	2.29	0.63
1:E:228:THR:HG21	1:E:308:LEU:CD1	2.28	0.63
2:F:322:SER:HB3	2:F:325:THR:HG23	1.79	0.62
1:E:223:GLN:OE1	3:E:3:NAG:H62	2.00	0.62
1:E:588:GLU:O	1:E:591:HIS:HB2	1.99	0.62
1:A:177:ASN:HD21	1:A:224:PHE:H	1.47	0.62
1:A:579:HIS:HE1	1:A:607:GLN:HA	1.63	0.62
1:A:519:ILE:HG13	1:A:520:SER:N	2.15	0.61
1:E:132:LEU:HD12	1:E:133:LEU:H	1.65	0.61
1:A:414:HIS:HD2	1:A:510:TYR:OH	1.83	0.61
2:B:46:ILE:HG23	2:B:59:VAL:HG23	1.81	0.61
2:B:83:GLN:HE21	3:B:1:NAG:HN2	1.47	0.61
1:A:592:GLN:CD	1:E:592:GLN:CD	2.59	0.61
2:F:149:ASN:O	2:F:214:SER:HA	2.00	0.61
1:E:579:HIS:HE1	1:E:607:GLN:HA	1.65	0.61
1:E:98:PHE:CE1	1:E:108:VAL:HG13	2.36	0.60
1:E:349:SER:HB2	1:E:389:GLN:HE21	1.66	0.60
2:B:188:PRO:HG2	2:B:189:GLU:H	1.67	0.60
2:B:250:PRO:HB2	2:B:259:THR:HB	1.82	0.60
2:B:343:VAL:HG21	2:B:358:ASP:O	2.01	0.60
2:B:407:ASN:HB2	2:B:409:THR:HG23	1.84	0.60
2:F:291:ARG:HD3	2:F:311:SER:HA	1.81	0.60
1:A:349:SER:CB	1:A:389:GLN:HG2	2.30	0.60
1:E:327:ASN:C	1:E:327:ASN:HD22	2.03	0.60
1:A:592:GLN:CG	1:E:592:GLN:NE2	2.51	0.60
2:B:328:LEU:HD22	2:B:392:LEU:HD21	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:GLN:CD	1:E:592:GLN:CG	2.70	0.60
2:F:401:LYS:HB3	2:F:416:ILE:HD11	1.82	0.60
1:A:49:ARG:HD3	1:A:451:PHE:HE1	1.66	0.59
1:A:327:ASN:HD21	1:A:331:TYR:H	1.48	0.59
1:E:177:ASN:HD21	1:E:224:PHE:H	1.49	0.59
2:F:168:ARG:HD2	2:F:175:TRP:CZ2	2.37	0.59
1:E:223:GLN:HE22	3:E:3:NAG:H61	1.66	0.59
1:E:376:GLU:H	1:E:376:GLU:CD	2.05	0.59
1:E:470:LEU:HD11	1:E:490:LEU:HD21	1.84	0.59
2:B:125:THR:HB	2:B:127:TRP:CH2	2.38	0.59
2:B:436:ASN:N	2:B:436:ASN:HD22	2.01	0.59
2:F:378:SER:OG	2:F:429:LEU:HG	2.03	0.59
1:A:327:ASN:ND2	1:A:331:TYR:H	2.00	0.59
2:B:43:GLU:CD	2:B:43:GLU:H	2.04	0.59
1:A:592:GLN:HG3	1:E:592:GLN:HE22	1.59	0.58
1:A:536:GLU:N	1:A:537:PRO:HD3	2.18	0.58
2:B:323:PRO:HA	2:B:374:SER:HB3	1.86	0.58
1:A:555:SER:HB3	1:A:632:GLU:HB2	1.86	0.58
1:A:583:VAL:HG22	5:A:923:HOH:O	2.03	0.58
2:F:401:LYS:HZ3	2:F:453:ALA:HB2	1.68	0.58
1:A:592:GLN:OE1	1:E:592:GLN:CG	2.52	0.57
1:E:259:VAL:HG21	1:E:288:MET:CE	2.34	0.57
2:F:323:PRO:HA	2:F:374:SER:HB3	1.86	0.57
1:E:156:VAL:HG11	3:E:2:NAG:N2	2.19	0.57
2:F:99:PRO:HB2	2:F:293:LEU:HD13	1.86	0.57
1:E:80:HIS:HE1	1:E:471:ASP:OD2	1.86	0.57
1:A:98:PHE:CE1	1:A:108:VAL:HG13	2.39	0.57
2:B:203:THR:OG1	2:B:222:ARG:HD2	2.04	0.57
2:B:378:SER:OG	2:B:429:LEU:HG	2.05	0.57
1:E:320:ARG:HD2	5:E:869:HOH:O	2.04	0.57
2:F:203:THR:HG22	2:F:222:ARG:HD2	1.85	0.57
1:A:519:ILE:HG13	1:A:520:SER:H	1.69	0.56
2:F:98:ARG:N	2:F:99:PRO:HD2	2.21	0.56
2:F:401:LYS:HB2	2:F:416:ILE:HD11	1.87	0.56
1:A:132:LEU:HD12	1:A:133:LEU:N	2.21	0.56
1:E:46:GLY:HA2	5:E:835:HOH:O	2.04	0.56
1:E:49:ARG:HD3	1:E:451:PHE:CE1	2.40	0.56
1:A:414:HIS:HB2	1:A:470:LEU:HD21	1.88	0.56
1:A:588:GLU:O	1:A:591:HIS:HB2	2.06	0.56
1:E:109:ARG:NH1	5:E:697:HOH:O	2.38	0.56
2:F:177:LEU:HG	2:F:179:VAL:HG22	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:373:HIS:ND1	2:B:374:SER:N	2.51	0.56
1:E:454:MET:HG2	1:E:455:GLU:N	2.21	0.56
1:A:301:ASN:H	1:A:301:ASN:HD22	1.54	0.55
2:B:97:ALA:HB1	2:B:99:PRO:HD2	1.86	0.55
2:B:362:ARG:CZ	2:B:362:ARG:HB2	2.37	0.55
1:A:288:MET:SD	1:E:254:GLU:HG2	2.46	0.55
1:E:66:ARG:NH2	1:E:460:ARG:HA	2.20	0.55
1:E:397:LEU:HB2	5:E:930:HOH:O	2.06	0.55
1:E:114:GLY:C	1:E:116:THR:H	2.09	0.55
1:A:451:PHE:CD2	1:A:453:ILE:HG22	2.39	0.55
1:A:114:GLY:C	1:A:116:THR:H	2.09	0.55
1:A:230:VAL:HG13	1:A:239:LYS:HB2	1.89	0.55
1:A:95:VAL:HG13	1:A:111:VAL:HB	1.89	0.55
2:F:225:LEU:O	2:F:348:LYS:HE3	2.07	0.55
1:A:433:ARG:HG3	1:A:433:ARG:HH11	1.71	0.55
1:E:368:PRO:HB2	1:E:371:GLN:HE22	1.72	0.55
2:F:39:VAL:HG13	2:F:41:ARG:HH12	1.71	0.55
2:B:108:LEU:HD13	2:B:162:THR:HG22	1.88	0.54
1:A:256:PRO:HA	1:E:297:ASN:OD1	2.08	0.54
2:F:83:GLN:HE21	3:F:1:NAG:HN2	1.55	0.54
1:E:327:ASN:HB2	1:E:328:PRO:CD	2.37	0.54
1:E:532:ILE:C	1:E:534:PRO:HD2	2.28	0.54
1:E:416:MET:CE	1:E:424:PHE:HB2	2.38	0.54
2:F:439:ILE:HD13	2:F:440:TYR:N	2.23	0.54
1:A:327:ASN:HB2	1:A:328:PRO:CD	2.37	0.54
2:F:373:HIS:ND1	2:F:374:SER:N	2.56	0.54
1:A:438:LYS:HE2	1:A:453:ILE:HD11	1.90	0.53
1:A:504:LEU:HB3	1:A:531:SER:HB3	1.89	0.53
2:B:190:THR:HG22	2:B:193:ARG:NH2	2.24	0.53
1:A:187:VAL:HG22	1:A:207:ARG:CB	2.37	0.53
2:B:362:ARG:HB2	2:B:362:ARG:NH1	2.24	0.53
2:B:392:LEU:HD12	2:B:392:LEU:N	2.23	0.53
1:E:631:PRO:O	1:E:632:GLU:HG2	2.08	0.53
2:F:46:ILE:HG23	2:F:59:VAL:HG23	1.89	0.53
1:A:369:ASP:N	1:A:371:GLN:NE2	2.56	0.53
2:F:41:ARG:HG3	2:F:41:ARG:HH11	1.73	0.53
1:A:252:ASN:HB3	1:A:254:GLU:OE1	2.09	0.53
1:A:580:LYS:O	1:A:581:GLU:HB2	2.09	0.52
2:B:37:GLU:C	2:B:39:VAL:H	2.12	0.52
2:F:373:HIS:HB3	2:F:376:LEU:HG	1.91	0.52
1:A:376:GLU:CD	1:A:376:GLU:H	2.11	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:ASN:HB3	1:E:254:GLU:OE1	2.10	0.52
2:F:384:VAL:HB	2:F:470:PRO:HB2	1.91	0.52
2:F:251:TYR:CE1	2:F:253:TYR:HA	2.44	0.52
1:E:327:ASN:ND2	1:E:331:TYR:H	2.08	0.52
1:A:53:ARG:HB2	1:A:572:HIS:CE1	2.44	0.52
1:A:397:LEU:HA	5:A:917:HOH:O	2.09	0.52
1:E:301:ASN:HD22	1:E:301:ASN:H	1.56	0.52
1:E:433:ARG:HH11	1:E:433:ARG:HG2	1.74	0.52
2:F:209:ASP:O	2:F:215:LEU:HA	2.10	0.52
2:F:403:ILE:HD12	2:F:403:ILE:N	2.25	0.52
1:A:531:SER:HB2	1:A:537:PRO:HB3	1.92	0.52
2:B:436:ASN:N	2:B:436:ASN:ND2	2.58	0.52
1:E:519:ILE:HG13	1:E:520:SER:H	1.75	0.52
2:B:343:VAL:HG23	5:B:710:HOH:O	2.09	0.52
1:E:124:ARG:HA	5:E:878:HOH:O	2.08	0.52
2:B:168:ARG:HD2	2:B:175:TRP:CZ2	2.44	0.51
1:A:561:ARG:HA	1:A:601:GLU:O	2.10	0.51
1:E:363:PRO:HB3	1:E:381:ALA:HB2	1.92	0.51
1:E:451:PHE:CD2	1:E:453:ILE:HG22	2.45	0.51
2:B:295:LEU:HD21	2:B:311:SER:CB	2.41	0.51
1:E:141:LEU:HD11	1:E:152:CYS:HB3	1.92	0.51
1:E:329:TRP:O	1:E:330:ASN:HB2	2.11	0.51
2:F:322:SER:C	2:F:324:THR:H	2.14	0.51
2:B:121:GLY:C	2:B:139:LEU:HB2	2.31	0.51
1:E:555:SER:HB3	1:E:632:GLU:CB	2.41	0.51
2:B:93:LEU:O	2:B:95:PRO:HD3	2.10	0.51
2:B:401:LYS:CD	2:B:416:ILE:HD11	2.40	0.51
2:F:436:ASN:N	2:F:436:ASN:HD22	2.09	0.51
1:A:327:ASN:C	1:A:327:ASN:ND2	2.60	0.51
2:B:125:THR:HB	2:B:127:TRP:CZ3	2.45	0.51
2:B:225:LEU:O	2:B:348:LYS:HE3	2.10	0.51
1:E:72:THR:HG21	5:E:696:HOH:O	2.11	0.50
1:A:187:VAL:CG2	1:A:206:ILE:HB	2.41	0.50
3:B:3:NAG:H2	5:B:740:HOH:O	2.11	0.50
1:E:451:PHE:HD2	1:E:453:ILE:HG22	1.75	0.50
2:F:251:TYR:HE1	2:F:253:TYR:HA	1.76	0.50
2:B:38:PRO:O	2:B:72:LEU:HB2	2.11	0.50
1:E:519:ILE:HG13	1:E:520:SER:N	2.26	0.50
1:A:148:ARG:HH21	1:A:195:GLU:CD	2.15	0.50
1:E:369:ASP:N	1:E:371:GLN:NE2	2.58	0.50
1:A:308:LEU:CD2	1:A:321:VAL:HG22	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:PRO:HA	2:B:439:ILE:HD12	1.94	0.50
2:F:93:LEU:N	2:F:93:LEU:HD22	2.26	0.50
1:A:592:GLN:CB	1:E:592:GLN:OE1	2.57	0.50
1:E:61:HIS:HB3	1:E:64:GLN:NE2	2.27	0.50
2:F:210:THR:HA	2:F:215:LEU:HD22	1.93	0.50
2:F:125:THR:HB	2:F:127:TRP:CH2	2.47	0.50
1:A:85:SER:HA	1:A:474:ARG:NH1	2.26	0.50
2:B:389:VAL:C	2:B:390:LEU:HD12	2.32	0.50
2:B:397:GLY:O	2:B:419:ILE:HG12	2.11	0.50
1:A:327:ASN:HB2	1:A:328:PRO:HD2	1.94	0.49
2:F:93:LEU:O	2:F:95:PRO:HD3	2.12	0.49
1:A:77:VAL:HG21	1:A:131:THR:O	2.12	0.49
1:A:80:HIS:HE1	1:A:471:ASP:OD2	1.94	0.49
1:A:211:GLU:HB3	5:A:821:HOH:O	2.12	0.49
2:B:131:ARG:HD3	5:B:657:HOH:O	2.12	0.49
2:B:375:ASP:OD1	2:B:395:GLY:HA3	2.12	0.49
1:E:234:GLN:HG3	5:E:924:HOH:O	2.12	0.49
2:B:266:ARG:O	2:B:267:ILE:HD12	2.13	0.49
2:B:505:LYS:HD3	2:B:505:LYS:O	2.12	0.49
2:F:41:ARG:HG3	2:F:41:ARG:NH1	2.27	0.49
2:F:505:LYS:O	2:F:505:LYS:HD3	2.11	0.49
2:B:368:SER:HB3	2:B:409:THR:HG22	1.95	0.49
2:B:40:TRP:CZ3	2:B:42:SER:HB2	2.48	0.49
1:E:375:THR:O	1:E:379:GLN:HG3	2.13	0.49
1:E:438:LYS:HG2	1:E:453:ILE:HD11	1.95	0.49
2:F:416:ILE:HD12	2:F:416:ILE:N	2.27	0.49
2:B:93:LEU:N	2:B:93:LEU:HD22	2.27	0.49
2:B:260:GLY:O	2:B:292:ARG:HD3	2.12	0.49
1:E:259:VAL:HG21	1:E:288:MET:HE2	1.94	0.49
1:E:416:MET:HE1	1:E:424:PHE:HB2	1.94	0.49
1:A:311:ASP:OD1	1:A:312:PRO:HD2	2.13	0.48
1:E:95:VAL:HG13	1:E:111:VAL:HB	1.95	0.48
2:F:37:GLU:N	2:F:38:PRO:CD	2.76	0.48
1:A:533:ASN:N	1:A:534:PRO:HD2	2.27	0.48
1:A:556:LEU:HD12	1:A:629:LEU:HD12	1.96	0.48
1:A:581:GLU:HB2	5:A:864:HOH:O	2.11	0.48
1:E:349:SER:CB	1:E:389:GLN:HG2	2.40	0.48
2:B:336:ILE:HD13	2:B:363:VAL:HG11	1.95	0.48
1:A:170:ALA:HA	5:A:691:HOH:O	2.13	0.48
1:A:369:ASP:H	1:A:371:GLN:NE2	2.11	0.48
2:B:46:ILE:HD12	2:B:59:VAL:HG21	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:434:VAL:HG12	2:F:435:LYS:HD2	1.96	0.48
2:B:460:SER:HB3	2:B:463:GLU:CB	2.44	0.48
2:F:285:HIS:HB2	5:F:676:HOH:O	2.14	0.48
2:B:295:LEU:HD21	2:B:311:SER:HB3	1.94	0.47
1:E:312:PRO:HB2	5:E:822:HOH:O	2.14	0.47
2:B:55:ASP:O	2:B:56:GLY:O	2.32	0.47
1:E:187:VAL:CG2	1:E:206:ILE:HB	2.43	0.47
1:A:194:GLN:HG2	1:A:197:ASN:HD22	1.79	0.47
1:A:310:PRO:O	1:A:415:ARG:NH2	2.46	0.47
1:A:433:ARG:HG3	1:A:433:ARG:NH1	2.30	0.47
2:F:391:PHE:C	2:F:392:LEU:HD12	2.35	0.47
2:F:460:SER:HB3	2:F:463:GLU:CB	2.44	0.47
1:E:293:ASP:O	1:E:296:THR:O	2.31	0.47
1:A:132:LEU:CD2	1:A:180:VAL:HG21	2.45	0.47
2:B:225:LEU:CD2	2:B:232:LEU:HD22	2.45	0.47
2:B:385:MET:N	5:B:702:HOH:O	2.41	0.46
1:E:360:ASN:O	1:E:362:ARG:N	2.47	0.46
1:A:465:ILE:HG23	1:A:479:VAL:CG1	2.43	0.46
1:E:327:ASN:C	1:E:327:ASN:ND2	2.68	0.46
1:A:546:PRO:HB3	1:A:620:TYR:OH	2.15	0.46
1:E:529:LEU:N	1:E:529:LEU:HD12	2.31	0.46
2:F:40:TRP:CZ3	2:F:42:SER:HB2	2.51	0.46
1:E:132:LEU:HD22	1:E:180:VAL:HG21	1.98	0.46
1:E:179:LEU:HB3	1:E:190:THR:HB	1.97	0.46
1:E:583:VAL:HG23	1:E:583:VAL:O	2.15	0.46
1:A:81:GLU:H	1:A:81:GLU:HG2	1.50	0.46
1:A:361:PRO:HG2	1:A:377:THR:OG1	2.15	0.46
2:B:459:LYS:HD2	2:B:459:LYS:N	2.31	0.46
2:B:478:LEU:H	2:B:478:LEU:HD23	1.81	0.46
1:E:205:ARG:HD2	1:E:210:SER:O	2.15	0.46
2:F:43:GLU:CD	2:F:43:GLU:H	2.18	0.46
1:A:383:ARG:HG2	1:A:384:HIS:CE1	2.51	0.46
2:B:52:SER:HB3	2:B:55:ASP:O	2.16	0.46
2:B:383:VAL:HG12	2:B:388:THR:HG22	1.98	0.46
2:F:213:ARG:HG3	2:F:213:ARG:NH1	2.28	0.46
1:A:476:LYS:HD2	1:A:487:GLN:HG2	1.98	0.46
1:E:573:ALA:HB2	1:E:617:GLU:HG3	1.98	0.46
1:A:132:LEU:HD12	1:A:133:LEU:H	1.81	0.46
1:A:319:THR:CB	1:A:339:LEU:HD22	2.42	0.46
1:A:427:LEU:HD12	1:A:427:LEU:N	2.31	0.46
2:F:478:LEU:HD23	2:F:478:LEU:H	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:TYR:CD2	2:B:203:THR:HG22	2.51	0.46
1:E:192:ARG:H	1:E:192:ARG:HD3	1.81	0.46
2:F:266:ARG:O	2:F:267:ILE:HD12	2.16	0.46
1:A:200:ILE:HD12	1:A:200:ILE:N	2.31	0.45
1:A:417:GLN:HA	1:A:422:GLU:O	2.16	0.45
1:E:601:GLU:HG2	1:E:602:ASN:ND2	2.30	0.45
1:A:192:ARG:HH21	1:A:195:GLU:HA	1.81	0.45
1:A:554:VAL:HG13	1:A:629:LEU:HD13	1.99	0.45
2:F:459:LYS:HD2	2:F:459:LYS:N	2.31	0.45
1:A:326:SER:HA	1:A:331:TYR:O	2.16	0.45
1:A:368:PRO:HD2	1:A:371:GLN:HE22	1.81	0.45
2:B:434:VAL:HG12	2:B:435:LYS:HD2	1.98	0.45
2:F:188:PRO:HG2	2:F:189:GLU:H	1.81	0.45
2:B:417:TYR:HE2	2:B:419:ILE:HD13	1.82	0.45
2:B:450:ILE:HD12	2:B:450:ILE:N	2.31	0.45
1:A:336:VAL:HG23	1:A:401:LEU:HD13	1.97	0.45
2:F:383:VAL:HG12	2:F:388:THR:HG22	1.98	0.45
2:F:392:LEU:HD12	2:F:392:LEU:N	2.30	0.45
2:B:98:ARG:N	2:B:99:PRO:CD	2.79	0.45
1:E:511:CYS:HA	1:E:521:ILE:HG23	1.98	0.45
2:F:385:MET:CE	2:F:498:ASP:HB2	2.47	0.45
2:B:401:LYS:HB2	2:B:416:ILE:HD11	1.97	0.45
1:E:82:PRO:HG2	5:E:890:HOH:O	2.17	0.45
2:F:232:LEU:HG	2:F:248:TYR:CD1	2.52	0.45
2:B:314:ALA:HB3	5:B:678:HOH:O	2.17	0.45
1:A:87:VAL:HB	1:A:98:PHE:HB2	1.99	0.45
1:A:186:GLU:HA	1:A:207:ARG:O	2.17	0.45
1:A:571:ARG:HH22	1:A:594:PRO:HB3	1.82	0.45
2:F:113:ARG:O	2:F:121:GLY:HA2	2.17	0.45
2:F:267:ILE:HG23	5:F:669:HOH:O	2.16	0.45
1:E:278:VAL:HG21	2:F:214:SER:OG	2.18	0.44
1:E:451:PHE:HD2	1:E:453:ILE:CG2	2.31	0.44
2:F:323:PRO:HA	2:F:374:SER:CB	2.47	0.44
1:E:223:GLN:NE2	3:E:3:NAG:C6	2.81	0.44
2:B:93:LEU:HD22	2:B:93:LEU:H	1.82	0.44
1:E:58:TRP:HB2	1:E:456:ILE:HD11	2.00	0.44
2:F:203:THR:CG2	2:F:222:ARG:NH1	2.71	0.44
1:E:87:VAL:HB	1:E:98:PHE:HB2	1.98	0.44
1:E:554:VAL:HG13	1:E:629:LEU:HD13	2.00	0.44
2:F:379:VAL:HA	2:F:391:PHE:O	2.18	0.44
1:E:361:PRO:HG2	1:E:374:PRO:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:VAL:HG22	2:B:40:TRP:N	2.32	0.44
1:E:494:GLU:H	1:E:494:GLU:HG3	1.39	0.44
1:E:327:ASN:HD21	1:E:331:TYR:H	1.66	0.44
2:F:58:PHE:HA	2:F:66:ASP:O	2.18	0.44
1:A:441:GLU:HG3	1:A:442:PRO:HD2	2.00	0.44
1:A:611:TYR:CD2	1:A:629:LEU:HD23	2.53	0.44
1:E:588:GLU:H	1:E:588:GLU:HG2	1.61	0.44
3:F:3:NAG:H83	3:F:3:NAG:O3	2.18	0.44
1:A:320:ARG:HD3	5:A:849:HOH:O	2.17	0.44
1:E:444:GLU:CD	1:E:444:GLU:H	2.21	0.44
2:F:303:LEU:HG	2:F:305:VAL:HG23	2.00	0.44
1:A:205:ARG:HD2	1:A:210:SER:O	2.17	0.43
1:A:592:GLN:CG	1:E:592:GLN:OE1	2.66	0.43
2:B:457:LYS:NZ	2:B:457:LYS:HB2	2.33	0.43
1:E:56:ALA:CB	1:E:495:VAL:HG11	2.48	0.43
2:F:108:LEU:HD13	2:F:162:THR:HG22	1.99	0.43
2:F:311:SER:HB2	2:F:326:THR:HG22	2.00	0.43
1:A:444:GLU:CD	1:A:444:GLU:H	2.21	0.43
2:B:390:LEU:HB2	2:B:402:VAL:CG2	2.49	0.43
1:E:495:VAL:HG13	5:E:698:HOH:O	2.18	0.43
2:F:93:LEU:HD22	2:F:93:LEU:H	1.82	0.43
1:A:368:PRO:HB2	1:A:371:GLN:HE22	1.83	0.43
2:F:187:GLU:HG3	2:F:195:ASN:ND2	2.34	0.43
2:B:454:ASN:O	2:B:457:LYS:HG2	2.18	0.43
1:A:297:ASN:OD1	1:E:256:PRO:HA	2.19	0.43
2:B:343:VAL:HG22	2:B:344:SER:N	2.34	0.43
2:F:176:TYR:CE2	2:F:271:THR:HG22	2.53	0.43
2:F:297:SER:HB2	2:F:306:TRP:HZ2	1.84	0.43
1:A:243:PHE:CD1	1:A:243:PHE:N	2.87	0.43
2:B:310:PHE:CD2	2:B:310:PHE:N	2.85	0.43
2:B:349:THR:HB	2:B:351:GLU:OE1	2.18	0.43
2:F:303:LEU:HD22	2:F:388:THR:HG21	2.00	0.43
2:F:303:LEU:HG	2:F:305:VAL:CG2	2.49	0.43
2:F:454:ASN:O	2:F:457:LYS:HG2	2.18	0.43
1:A:167:ARG:HG3	5:A:750:HOH:O	2.17	0.43
2:B:67:GLN:NE2	2:B:77:SER:OG	2.51	0.43
2:B:282:ASP:O	2:B:365:PRO:HD3	2.19	0.43
1:E:225:ILE:HG12	1:E:244:PHE:HA	2.00	0.43
2:F:55:ASP:O	2:F:56:GLY:O	2.37	0.43
2:F:342:ARG:HD3	5:F:723:HOH:O	2.18	0.43
2:F:436:ASN:N	2:F:436:ASN:ND2	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:PHE:HB2	1:E:71:GLN:O	2.18	0.43
1:E:223:GLN:HE22	3:E:3:NAG:C6	2.30	0.43
1:E:289:LEU:HD12	1:E:391:VAL:HB	2.01	0.43
1:E:367:LEU:HA	1:E:368:PRO:HD3	1.90	0.43
2:F:408:LEU:HD12	2:F:408:LEU:N	2.34	0.43
2:F:460:SER:HB3	2:F:463:GLU:HB2	2.00	0.43
1:A:94:LYS:HB3	1:A:112:ASN:HA	2.00	0.42
2:F:127:TRP:O	2:F:132:GLY:HA2	2.19	0.42
2:F:457:LYS:HB2	2:F:457:LYS:NZ	2.33	0.42
1:A:579:HIS:NE2	1:A:580:LYS:HD3	2.34	0.42
1:A:511:CYS:HA	1:A:521:ILE:HG23	2.00	0.42
2:B:460:SER:HB3	2:B:463:GLU:HB2	2.00	0.42
1:A:315:GLN:HG2	5:A:717:HOH:O	2.20	0.42
1:A:324:VAL:CG2	1:A:411:VAL:HB	2.49	0.42
1:A:367:LEU:HA	1:A:368:PRO:HD3	1.87	0.42
2:B:52:SER:O	2:B:433:PRO:HG3	2.19	0.42
2:F:44:GLN:HE21	2:F:61:SER:HB3	1.83	0.42
2:F:295:LEU:N	2:F:295:LEU:HD22	2.34	0.42
2:B:290:GLY:O	2:B:312:ALA:HB2	2.20	0.42
2:B:305:VAL:HG13	2:B:331:PHE:O	2.20	0.42
1:E:77:VAL:HG21	1:E:131:THR:O	2.19	0.42
1:E:167:ARG:HD2	1:E:193:LYS:HB3	2.00	0.42
2:F:138:PRO:HG2	5:F:675:HOH:O	2.19	0.42
1:E:94:LYS:HB3	1:E:112:ASN:HA	2.01	0.42
1:E:223:GLN:CD	3:E:3:NAG:H62	2.40	0.42
1:E:606:GLN:CA	1:E:606:GLN:HE21	2.33	0.42
2:F:38:PRO:HG3	2:F:449:ARG:HB3	2.02	0.42
2:B:203:THR:HG22	2:B:203:THR:O	2.20	0.42
2:B:391:PHE:C	2:B:392:LEU:HD12	2.40	0.42
1:E:179:LEU:C	1:E:179:LEU:HD13	2.40	0.42
1:E:555:SER:HA	1:E:630:LEU:O	2.20	0.42
2:F:345:TRP:CE3	2:F:355:LYS:HA	2.55	0.42
1:A:515:GLN:HE21	1:A:515:GLN:HB3	1.58	0.42
1:A:81:GLU:OE1	1:A:135:ARG:HD2	2.19	0.42
1:A:194:GLN:O	1:A:197:ASN:HB2	2.19	0.42
1:A:360:ASN:HB3	1:A:361:PRO:HD3	2.00	0.42
1:A:494:GLU:H	1:A:494:GLU:HG3	1.51	0.42
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.84	0.42
2:B:373:HIS:HB3	2:B:376:LEU:HG	2.01	0.42
1:E:326:SER:HA	1:E:331:TYR:O	2.20	0.42
1:E:327:ASN:ND2	1:E:329:TRP:H	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:161:SER:HB3	2:F:233:HIS:CE1	2.55	0.42
1:A:532:ILE:C	1:A:534:PRO:HD2	2.40	0.41
2:B:190:THR:HG23	5:B:706:HOH:O	2.20	0.41
2:B:321:ARG:HH21	2:B:375:ASP:CB	2.33	0.41
2:F:116:ALA:HB3	2:F:119:LEU:O	2.20	0.41
2:F:368:SER:HB3	2:F:409:THR:HG22	2.01	0.41
2:F:402:VAL:C	2:F:403:ILE:HD12	2.40	0.41
1:A:55:PHE:HE1	1:A:571:ARG:HG3	1.85	0.41
1:A:241:TYR:HA	1:A:263:ALA:O	2.19	0.41
1:A:272:GLY:HA3	1:A:277:SER:OG	2.20	0.41
1:E:558:PRO:O	1:E:559:ASN:HB2	2.21	0.41
2:F:478:LEU:HD23	2:F:478:LEU:N	2.36	0.41
1:A:289:LEU:HD12	1:A:391:VAL:HB	2.02	0.41
2:B:295:LEU:H	2:B:295:LEU:HD22	1.84	0.41
1:E:102:GLU:OE1	1:E:102:GLU:HA	2.21	0.41
2:B:176:TYR:CZ	2:B:271:THR:HG22	2.56	0.41
1:E:324:VAL:CG2	1:E:411:VAL:HB	2.50	0.41
1:E:526:ARG:HG3	1:E:526:ARG:HH11	1.85	0.41
1:E:556:LEU:HD12	1:E:629:LEU:HD12	2.02	0.41
1:A:77:VAL:HG21	1:A:131:THR:C	2.41	0.41
2:F:401:LYS:NZ	2:F:453:ALA:HB2	2.35	0.41
1:E:478:TYR:OH	1:E:487:GLN:NE2	2.51	0.41
2:F:135:GLU:HG3	2:F:137:ARG:NH2	2.35	0.41
2:B:408:LEU:N	2:B:408:LEU:HD12	2.36	0.41
1:E:525:GLU:C	1:E:527:SER:H	2.23	0.41
3:E:4:NAG:H4	5:E:715:HOH:O	2.20	0.41
5:A:686:HOH:O	2:B:150:GLY:HA2	2.20	0.41
2:B:437:ILE:O	2:B:452:VAL:HG13	2.20	0.41
2:F:189:GLU:HB3	2:F:192:SER:OG	2.20	0.41
1:A:49:ARG:CZ	5:A:776:HOH:O	2.68	0.41
1:A:212:LEU:HA	1:A:279:SER:O	2.21	0.41
1:A:363:PRO:HB3	1:A:381:ALA:HB2	2.03	0.41
1:A:396:PRO:O	1:A:397:LEU:HB2	2.20	0.41
1:A:436:ILE:HD11	1:A:479:VAL:HG21	2.03	0.41
2:B:127:TRP:O	2:B:132:GLY:HA2	2.21	0.41
1:E:67:VAL:CG1	1:E:108:VAL:HG22	2.48	0.41
2:F:67:GLN:NE2	2:F:77:SER:OG	2.52	0.41
2:F:179:VAL:O	2:F:205:ILE:HG23	2.21	0.41
2:F:231:SER:HB2	2:F:251:TYR:O	2.20	0.41
2:F:250:PRO:HG2	2:F:260:GLY:H	1.85	0.41
1:A:536:GLU:HB3	1:A:538:HIS:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:PRO:HG3	2:B:449:ARG:HB3	2.03	0.41
2:F:163:ALA:HA	5:F:728:HOH:O	2.21	0.41
2:F:351:GLU:OE2	2:F:351:GLU:N	2.53	0.41
1:E:315:GLN:N	1:E:315:GLN:HE21	2.18	0.40
1:E:491:ASP:HB2	1:E:520:SER:HB2	2.03	0.40
2:F:125:THR:HB	2:F:127:TRP:CZ3	2.56	0.40
1:A:608:TYR:HB2	5:A:700:HOH:O	2.20	0.40
1:E:192:ARG:NH1	5:E:858:HOH:O	2.52	0.40
1:E:543:ASN:HA	1:E:544:PRO:HD2	1.96	0.40
2:F:37:GLU:N	2:F:38:PRO:HD3	2.35	0.40
2:F:332:ARG:HD2	2:F:335:GLU:OE2	2.22	0.40
2:B:477:SER:HB2	2:B:495:ASN:HD22	1.86	0.40
1:E:315:GLN:HE21	1:E:315:GLN:CA	2.34	0.40
1:A:121:LEU:O	1:A:122:ASP:HB3	2.20	0.40
1:A:225:ILE:CD1	1:A:244:PHE:HA	2.48	0.40
2:B:97:ALA:HB1	5:B:678:HOH:O	2.21	0.40
2:B:188:PRO:HG2	2:B:189:GLU:N	2.34	0.40
1:A:56:ALA:CB	1:A:495:VAL:HG11	2.51	0.40
2:B:252:ASN:HB3	2:B:255:SER:HB3	2.03	0.40
2:B:460:SER:HB3	2:B:463:GLU:HB3	2.04	0.40
2:F:123:LEU:HG	2:F:125:THR:HG23	2.02	0.40
2:F:424:PRO:HG2	5:F:695:HOH:O	2.20	0.40
2:F:477:SER:HB2	2:F:495:ASN:HD22	1.86	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	586/590 (99%)	530 (90%)	47 (8%)	9 (2%)	8 12
1	E	586/590 (99%)	529 (90%)	46 (8%)	11 (2%)	6 8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	472/476 (99%)	422 (89%)	40 (8%)	10 (2%)	5	7
2	F	472/476 (99%)	417 (88%)	46 (10%)	9 (2%)	6	8
All	All	2116/2132 (99%)	1898 (90%)	179 (8%)	39 (2%)	7	9

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	PRO
1	A	444	GLU
2	B	36	ASP
2	B	301	GLU
1	E	368	PRO
1	E	444	GLU
2	F	301	GLU
1	A	601	GLU
2	B	56	GLY
2	B	318	GLN
1	E	526	ARG
2	F	56	GLY
2	F	288	PRO
2	F	318	GLN
2	B	386	ASN
1	E	115	SER
1	E	369	ASP
2	F	386	ASN
1	A	115	SER
2	B	288	PRO
2	B	320	ARG
1	E	116	THR
2	F	320	ARG
1	A	524	SER
1	A	525	GLU
2	B	38	PRO
1	E	109	ARG
1	E	524	SER
2	F	96	PRO
2	F	285	HIS
1	A	150	PRO
1	A	114	GLY
1	E	533	ASN
2	B	96	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	488	VAL
1	E	118	GLY
2	F	488	VAL
1	A	360	ASN
1	E	534	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	518/519 (100%)	490 (95%)	28 (5%)	18	32
1	E	518/519 (100%)	483 (93%)	35 (7%)	13	22
2	B	389/390 (100%)	366 (94%)	23 (6%)	16	28
2	F	389/390 (100%)	368 (95%)	21 (5%)	18	32
All	All	1814/1818 (100%)	1707 (94%)	107 (6%)	16	28

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	81	GLU
1	A	108	VAL
1	A	109	ARG
1	A	163	LEU
1	A	167	ARG
1	A	180	VAL
1	A	192	ARG
1	A	226	LYS
1	A	230	VAL
1	A	254	GLU
1	A	257	LEU
1	A	258	ASN
1	A	264	GLN
1	A	267	ARG
1	A	289	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	297	ASN
1	A	301	ASN
1	A	315	GLN
1	A	327	ASN
1	A	339	LEU
1	A	401	LEU
1	A	416	MET
1	A	446	GLU
1	A	494	GLU
1	A	515	GLN
1	A	584	GLU
1	A	622	ARG
2	B	37	GLU
2	B	44	GLN
2	B	59	VAL
2	B	81	ARG
2	B	93	LEU
2	B	108	LEU
2	B	135	GLU
2	B	139	LEU
2	B	141	ASN
2	B	179	VAL
2	B	189	GLU
2	B	201	HIS
2	B	203	THR
2	B	232	LEU
2	B	267	ILE
2	B	280	SER
2	B	295	LEU
2	B	362	ARG
2	B	396	ASP
2	B	454	ASN
2	B	457	LYS
2	B	481	CYS
2	B	496	TRP
1	E	59	LYS
1	E	72	THR
1	E	81	GLU
1	E	108	VAL
1	E	109	ARG
1	E	110	THR
1	E	190	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	192	ARG
1	E	230	VAL
1	E	254	GLU
1	E	257	LEU
1	E	258	ASN
1	E	264	GLN
1	E	267	ARG
1	E	289	LEU
1	E	301	ASN
1	E	304	GLN
1	E	315	GLN
1	E	327	ASN
1	E	332	SER
1	E	339	LEU
1	E	401	LEU
1	E	416	MET
1	E	427	LEU
1	E	446	GLU
1	E	454	MET
1	E	457	GLN
1	E	458	PRO
1	E	469	SER
1	E	494	GLU
1	E	584	GLU
1	E	586	SER
1	E	588	GLU
1	E	606	GLN
1	E	622	ARG
2	F	36	ASP
2	F	44	GLN
2	F	59	VAL
2	F	81	ARG
2	F	93	LEU
2	F	98	ARG
2	F	135	GLU
2	F	139	LEU
2	F	179	VAL
2	F	189	GLU
2	F	201	HIS
2	F	218	GLN
2	F	267	ILE
2	F	362	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	382	THR
2	F	396	ASP
2	F	439	ILE
2	F	454	ASN
2	F	457	LYS
2	F	481	CYS
2	F	496	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	71	GLN
1	A	80	HIS
1	A	177	ASN
1	A	194	GLN
1	A	234	GLN
1	A	301	ASN
1	A	327	ASN
1	A	371	GLN
1	A	384	HIS
1	A	389	GLN
1	A	407	HIS
1	A	414	HIS
1	A	417	GLN
1	A	457	GLN
1	A	482	GLN
1	A	487	GLN
1	A	515	GLN
1	A	559	ASN
1	A	579	HIS
1	A	602	ASN
1	A	606	GLN
1	A	628	GLN
2	B	44	GLN
2	B	67	GLN
2	B	172	ASN
2	B	173	ASN
2	B	285	HIS
2	B	359	GLN
2	B	364	GLN
2	B	398	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	436	ASN
2	B	471	HIS
1	E	64	GLN
1	E	71	GLN
1	E	80	HIS
1	E	177	ASN
1	E	194	GLN
1	E	234	GLN
1	E	301	ASN
1	E	304	GLN
1	E	315	GLN
1	E	327	ASN
1	E	371	GLN
1	E	384	HIS
1	E	389	GLN
1	E	407	HIS
1	E	414	HIS
1	E	457	GLN
1	E	482	GLN
1	E	487	GLN
1	E	515	GLN
1	E	559	ASN
1	E	579	HIS
1	E	582	ASN
1	E	602	ASN
1	E	606	GLN
2	F	44	GLN
2	F	67	GLN
2	F	172	ASN
2	F	173	ASN
2	F	218	GLN
2	F	287	HIS
2	F	359	GLN
2	F	398	GLN
2	F	436	ASN
2	F	471	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 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	NAG	E	2	1	14,14,15	0.60	0	17,19,21	0.66	0
3	NAG	B	6	2	14,14,15	0.59	0	17,19,21	0.66	0
3	NAG	A	2	1	14,14,15	0.59	0	17,19,21	0.67	0
3	NAG	B	2	2	14,14,15	0.59	0	17,19,21	0.65	0
3	NAG	B	1	2	14,14,15	0.52	0	17,19,21	0.65	0
4	NDG	A	4	-	14,14,15	0.73	0	17,19,21	1.12	2 (11%)
3	NAG	F	6	2	14,14,15	0.60	0	17,19,21	0.66	0
3	NAG	B	5	2	14,14,15	0.48	0	17,19,21	0.81	1 (5%)
3	NAG	F	4	2	14,14,15	0.57	0	17,19,21	0.83	1 (5%)
3	NAG	A	1	1	14,14,15	0.60	0	17,19,21	0.66	0
3	NAG	F	1	2	14,14,15	0.63	0	17,19,21	0.69	0
3	NAG	E	1	1	14,14,15	0.59	0	17,19,21	0.79	0
3	NAG	B	4	2	14,14,15	0.60	0	17,19,21	1.07	1 (5%)
3	NAG	F	2	2	14,14,15	0.59	0	17,19,21	0.66	0
3	NAG	F	5	2	14,14,15	0.53	0	17,19,21	0.73	1 (5%)
3	NAG	F	3	2	14,14,15	0.62	0	17,19,21	0.70	0
3	NAG	E	3	1	14,14,15	0.60	0	17,19,21	0.66	0
3	NAG	E	4	1	14,14,15	0.56	0	17,19,21	0.73	0
3	NAG	F	7	2	14,14,15	0.59	0	17,19,21	0.66	0
3	NAG	B	7	2	14,14,15	0.61	0	17,19,21	0.66	0
3	NAG	B	3	2	14,14,15	0.69	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	3	1	14,14,15	0.60	0	17,19,21	0.66	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	E	2	1	-	4/6/23/26	0/1/1/1
3	NAG	B	6	2	-	4/6/23/26	0/1/1/1
3	NAG	A	2	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2	2	-	4/6/23/26	0/1/1/1
3	NAG	B	1	2	-	3/6/23/26	0/1/1/1
4	NDG	A	4	-	-	3/6/23/26	0/1/1/1
3	NAG	F	6	2	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	B	5	2	-	2/6/23/26	0/1/1/1
3	NAG	F	4	2	-	4/6/23/26	0/1/1/1
3	NAG	A	1	1	-	4/6/23/26	0/1/1/1
3	NAG	F	1	2	-	4/6/23/26	0/1/1/1
3	NAG	E	1	1	-	5/6/23/26	0/1/1/1
3	NAG	B	4	2	-	2/6/23/26	0/1/1/1
3	NAG	F	2	2	-	4/6/23/26	0/1/1/1
3	NAG	F	5	2	-	2/6/23/26	0/1/1/1
3	NAG	F	3	2	-	4/6/23/26	0/1/1/1
3	NAG	E	3	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	E	4	1	-	2/6/23/26	0/1/1/1
3	NAG	F	7	2	-	4/6/23/26	0/1/1/1
3	NAG	B	7	2	-	4/6/23/26	0/1/1/1
3	NAG	B	3	2	-	2/6/23/26	0/1/1/1
3	NAG	A	3	1	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4	NAG	C2-N2-C7	-2.68	119.31	122.90
3	F	4	NAG	C2-N2-C7	-2.57	119.46	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4	NDG	C4-C3-C2	2.29	114.38	111.02
3	B	5	NAG	C2-N2-C7	-2.27	119.86	122.90
4	A	4	NDG	C2-N2-C7	-2.26	119.87	122.90
3	F	5	NAG	C2-N2-C7	-2.21	119.94	122.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	3	NAG	C1
3	E	3	NAG	C1
3	F	6	NAG	C1

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
3	B	3	NAG	C8-C7-N2-C2
3	B	3	NAG	O7-C7-N2-C2
3	B	5	NAG	C8-C7-N2-C2
3	B	5	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	4	NAG	C8-C7-N2-C2
3	E	4	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	3	NAG	C8-C7-N2-C2
3	F	3	NAG	O7-C7-N2-C2
3	F	4	NAG	C8-C7-N2-C2
3	F	4	NAG	O7-C7-N2-C2
3	F	5	NAG	C8-C7-N2-C2
3	F	5	NAG	O7-C7-N2-C2
4	A	4	NDG	C8-C7-N2-C2
4	A	4	NDG	O7-C7-N2-C2
3	E	1	NAG	O5-C5-C6-O6
3	A	1	NAG	C8-C7-N2-C2
3	A	1	NAG	O7-C7-N2-C2
3	A	2	NAG	C8-C7-N2-C2
3	A	2	NAG	O7-C7-N2-C2
3	A	3	NAG	C8-C7-N2-C2
3	A	3	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	2	NAG	C8-C7-N2-C2
3	B	2	NAG	O7-C7-N2-C2
3	B	6	NAG	C8-C7-N2-C2
3	B	6	NAG	O7-C7-N2-C2
3	B	7	NAG	C8-C7-N2-C2
3	B	7	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	3	NAG	C8-C7-N2-C2
3	E	3	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	6	NAG	C8-C7-N2-C2
3	F	6	NAG	O7-C7-N2-C2
3	F	7	NAG	C8-C7-N2-C2
3	F	7	NAG	O7-C7-N2-C2
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	3	NAG	O5-C5-C6-O6
3	F	3	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	A	1	NAG	O5-C5-C6-O6
3	A	2	NAG	O5-C5-C6-O6
3	A	3	NAG	O5-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
3	B	6	NAG	O5-C5-C6-O6
3	B	7	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	3	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	F	6	NAG	O5-C5-C6-O6
3	F	7	NAG	O5-C5-C6-O6
3	A	1	NAG	C4-C5-C6-O6
3	A	2	NAG	C4-C5-C6-O6
3	A	3	NAG	C4-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
3	B	6	NAG	C4-C5-C6-O6
3	B	7	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	3	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	6	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	F	7	NAG	C4-C5-C6-O6
3	F	4	NAG	O5-C5-C6-O6
3	B	4	NAG	C4-C5-C6-O6
3	B	4	NAG	O5-C5-C6-O6
3	B	1	NAG	C3-C2-N2-C7
3	E	1	NAG	C3-C2-N2-C7
4	A	4	NDG	C3-C2-N2-C7
3	F	4	NAG	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	2	0
3	B	1	NAG	1	0
3	F	1	NAG	1	0
3	F	3	NAG	1	0
3	E	3	NAG	5	0
3	E	4	NAG	1	0
3	F	7	NAG	1	0
3	B	3	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	588/590 (99%)	0.30	37 (6%) 27 25	25, 55, 113, 150	0
1	E	588/590 (99%)	0.31	38 (6%) 26 24	27, 53, 107, 140	0
2	B	474/476 (99%)	0.83	65 (13%) 8 7	34, 70, 129, 150	0
2	F	474/476 (99%)	0.89	70 (14%) 7 6	37, 72, 131, 150	0
All	All	2124/2132 (99%)	0.55	210 (9%) 14 12	25, 62, 125, 150	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	465	LEU	5.9
2	F	488	VAL	5.6
2	B	493	LEU	4.9
2	F	468	THR	4.7
1	E	633	ASP	4.5
1	A	121	LEU	4.5
2	F	503	ALA	4.4
1	A	117	LYS	4.1
2	B	499	ILE	4.1
2	B	470	PRO	4.1
1	A	116	THR	4.0
2	B	481	CYS	4.0
1	A	542	PRO	3.9
2	B	488	VAL	3.9
1	E	533	ASN	3.8
1	E	532	ILE	3.8
2	F	497	LEU	3.7
2	B	508	GLY	3.7
1	E	117	LYS	3.7
2	B	474	TRP	3.7
2	B	472	CYS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	465	LEU	3.6
1	A	531	SER	3.6
2	B	475	CYS	3.6
2	B	318	GLN	3.6
2	B	487	CYS	3.5
1	A	48	LEU	3.5
2	F	94	ALA	3.5
1	A	535	ALA	3.4
1	E	519	ILE	3.4
2	F	507	PRO	3.4
2	B	141	ASN	3.4
2	B	483	PHE	3.4
1	E	531	SER	3.3
1	A	119	SER	3.3
2	F	38	PRO	3.3
2	F	36	ASP	3.3
2	B	480	ARG	3.3
2	F	35	ALA	3.3
2	F	482	THR	3.3
2	F	499	ILE	3.2
1	A	530	GLN	3.2
2	B	229	ALA	3.2
1	E	537	PRO	3.1
1	E	122	ASP	3.1
2	B	415	VAL	3.1
2	B	490	SER	3.1
1	E	194	GLN	3.1
2	B	502	GLY	3.0
2	F	475	CYS	3.0
1	E	530	GLN	3.0
2	F	83	GLN	3.0
2	F	474	TRP	3.0
2	F	496	TRP	3.0
2	B	362	ARG	3.0
1	A	533	ASN	3.0
1	E	126	CYS	2.9
1	A	113	ILE	2.9
2	B	489	HIS	2.9
2	F	313	ALA	2.9
1	E	48	LEU	2.9
1	A	534	PRO	2.9
1	E	592	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	35	ALA	2.9
2	F	490	SER	2.8
2	B	496	TRP	2.8
2	B	495	ASN	2.8
2	B	462	SER	2.8
2	B	503	ALA	2.8
2	B	482	THR	2.8
2	F	508	GLY	2.8
1	A	108	VAL	2.8
1	E	528	VAL	2.8
2	B	492	ASN	2.8
1	A	123	LYS	2.8
2	F	501	SER	2.8
2	B	464	CYS	2.8
1	A	532	ILE	2.7
1	E	534	PRO	2.7
2	B	64	CYS	2.7
2	F	464	CYS	2.7
2	F	481	CYS	2.7
2	F	493	LEU	2.7
2	B	316	GLU	2.7
2	F	462	SER	2.7
2	B	97	ALA	2.7
1	A	47	HIS	2.7
1	E	197	ASN	2.7
1	A	156	VAL	2.6
1	A	512	GLY	2.6
1	E	499	GLY	2.6
2	F	127	TRP	2.6
2	B	285	HIS	2.6
1	A	443	GLY	2.6
2	F	502	GLY	2.6
2	B	452	VAL	2.6
2	F	91	VAL	2.6
2	F	489	HIS	2.6
1	E	206	ILE	2.6
2	B	468	THR	2.6
2	B	461	CYS	2.6
2	F	228	GLY	2.6
2	F	478	LEU	2.6
1	A	115	SER	2.6
2	B	91	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	476	HIS	2.6
1	E	360	ASN	2.6
1	E	445	GLN	2.6
2	F	283	CYS	2.6
2	F	315	GLY	2.6
2	B	471	HIS	2.5
2	F	335	GLU	2.5
2	B	498	ASP	2.5
2	F	485	GLY	2.5
2	F	459	LYS	2.5
1	A	528	VAL	2.5
2	F	460	SER	2.5
2	F	291	ARG	2.5
1	E	448	SER	2.5
2	F	463	GLU	2.5
1	A	120	CYS	2.5
2	B	39	VAL	2.5
2	B	317	GLY	2.5
1	E	529	LEU	2.4
1	E	523	SER	2.4
2	B	416	ILE	2.4
1	A	122	ASP	2.4
2	B	478	LEU	2.4
2	F	377	THR	2.4
1	A	529	LEU	2.4
2	B	497	LEU	2.4
1	E	447	HIS	2.4
2	B	61	SER	2.4
2	B	62	GLY	2.4
1	A	360	ASN	2.4
1	A	511	CYS	2.4
2	F	99	PRO	2.3
2	F	487	CYS	2.3
2	F	385	MET	2.3
1	E	511	CYS	2.3
2	F	467	ALA	2.3
2	B	378	SER	2.3
2	B	460	SER	2.3
2	B	142	LEU	2.3
2	F	93	LEU	2.3
1	E	196	TYR	2.3
2	B	37	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	95	VAL	2.3
2	F	415	VAL	2.3
2	B	117	ALA	2.3
1	E	70	GLY	2.3
2	B	93	LEU	2.3
2	B	408	LEU	2.3
2	B	473	GLY	2.3
2	F	86	ASN	2.3
2	F	288	PRO	2.3
1	E	113	ILE	2.3
2	F	85	GLY	2.2
2	F	317	GLY	2.2
2	F	61	SER	2.2
2	F	40	TRP	2.2
2	B	494	GLU	2.2
2	F	56	GLY	2.2
1	A	633	ASP	2.2
1	A	194	GLN	2.2
2	F	341	LYS	2.2
2	F	473	GLY	2.2
1	E	115	SER	2.2
2	B	90	PRO	2.2
1	A	582	ASN	2.2
2	F	289	ASP	2.2
2	F	79	LEU	2.2
1	E	116	THR	2.2
1	E	493	CYS	2.2
2	B	190	THR	2.2
2	B	466	THR	2.2
2	F	325	THR	2.2
2	B	96	PRO	2.2
1	E	175	ASP	2.2
2	F	261	TRP	2.2
2	F	117	ALA	2.2
2	F	458	HIS	2.2
1	A	547	ASP	2.1
2	B	459	LYS	2.1
2	B	453	ALA	2.1
2	F	302	ALA	2.1
1	A	118	GLY	2.1
1	A	499	GLY	2.1
1	E	167	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	286	GLY	2.1
1	A	197	ASN	2.1
1	A	519	ILE	2.1
1	E	504	LEU	2.1
2	F	84	ALA	2.1
2	F	423	THR	2.1
1	E	546	PRO	2.1
1	E	178	SER	2.1
1	A	557	ALA	2.1
1	A	500	CYS	2.1
2	F	407	ASN	2.1
2	F	437	ILE	2.1
1	A	601	GLU	2.0
2	B	189	GLU	2.0
2	B	500	SER	2.0
2	F	354	CYS	2.0
2	F	366	ILE	2.0
2	F	339	ARG	2.0
2	B	38	PRO	2.0
1	E	176	GLU	2.0
2	F	403	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(\AA^2)	Q<0.9
3	NAG	B	7	14/15	0.01	0.20	150,150,150,150	0
3	NAG	F	7	14/15	0.24	0.18	150,150,150,150	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	E	2	14/15	0.35	0.17	150,150,150,150	0
3	NAG	F	6	14/15	0.36	0.16	149,150,150,150	0
3	NAG	B	1	14/15	0.38	0.14	112,113,113,114	0
3	NAG	A	2	14/15	0.40	0.20	149,150,150,150	0
3	NAG	A	3	14/15	0.47	0.28	93,95,96,96	0
3	NAG	F	1	14/15	0.47	0.15	115,118,119,119	0
3	NAG	B	2	14/15	0.55	0.20	136,138,139,139	0
3	NAG	E	3	14/15	0.57	0.29	114,117,118,118	0
3	NAG	B	6	14/15	0.57	0.23	150,150,150,150	0
3	NAG	F	2	14/15	0.63	0.22	132,135,136,136	0
3	NAG	F	4	14/15	0.63	0.13	81,85,86,86	0
3	NAG	E	1	14/15	0.64	0.13	94,95,98,98	0
3	NAG	B	3	14/15	0.66	0.12	81,86,87,88	0
3	NAG	E	4	14/15	0.76	0.12	65,71,73,75	0
3	NAG	A	1	14/15	0.77	0.13	83,85,86,86	0
4	NDG	A	4	14/15	0.77	0.12	59,64,66,66	0
3	NAG	B	5	14/15	0.79	0.12	78,82,83,83	0
3	NAG	F	3	14/15	0.80	0.12	77,80,81,83	0
3	NAG	F	5	14/15	0.82	0.11	79,82,85,86	0
3	NAG	B	4	14/15	0.89	0.09	51,58,60,62	0

6.5 Other polymers

There are no such residues in this entry.