



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:13 AM UTC

PDB ID : 3NVQ / pdb_00003nvq
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

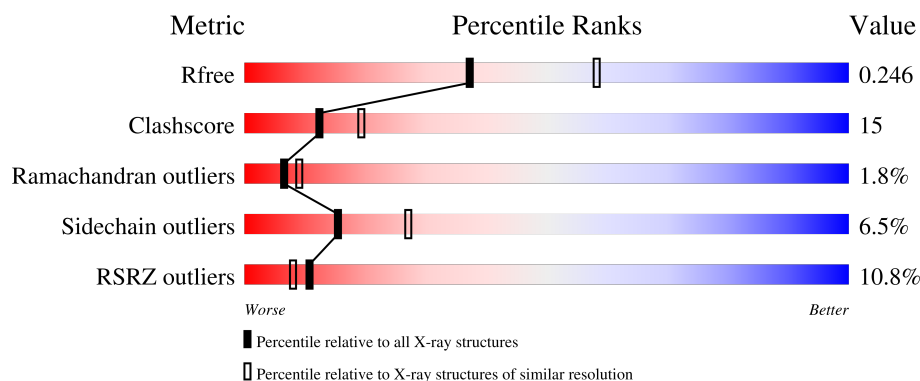
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

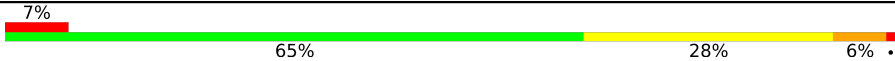
The reported resolution of this entry is 2.40 Å.

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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	
1	E	590	
2	B	476	
2	F	476	

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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



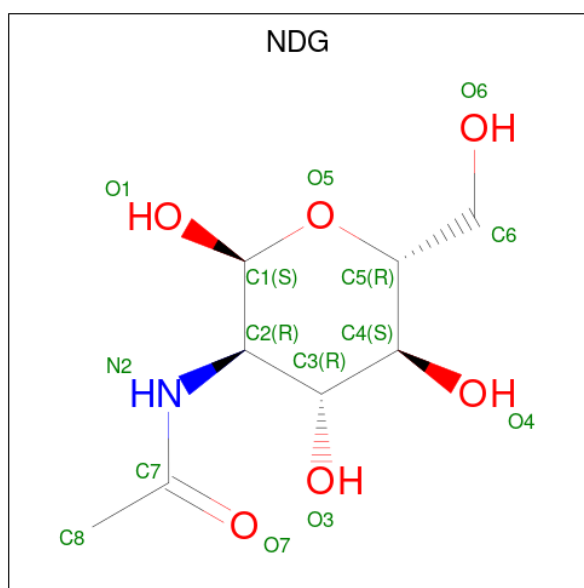
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

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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- α -D-glucopyranose (CCD ID: 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		

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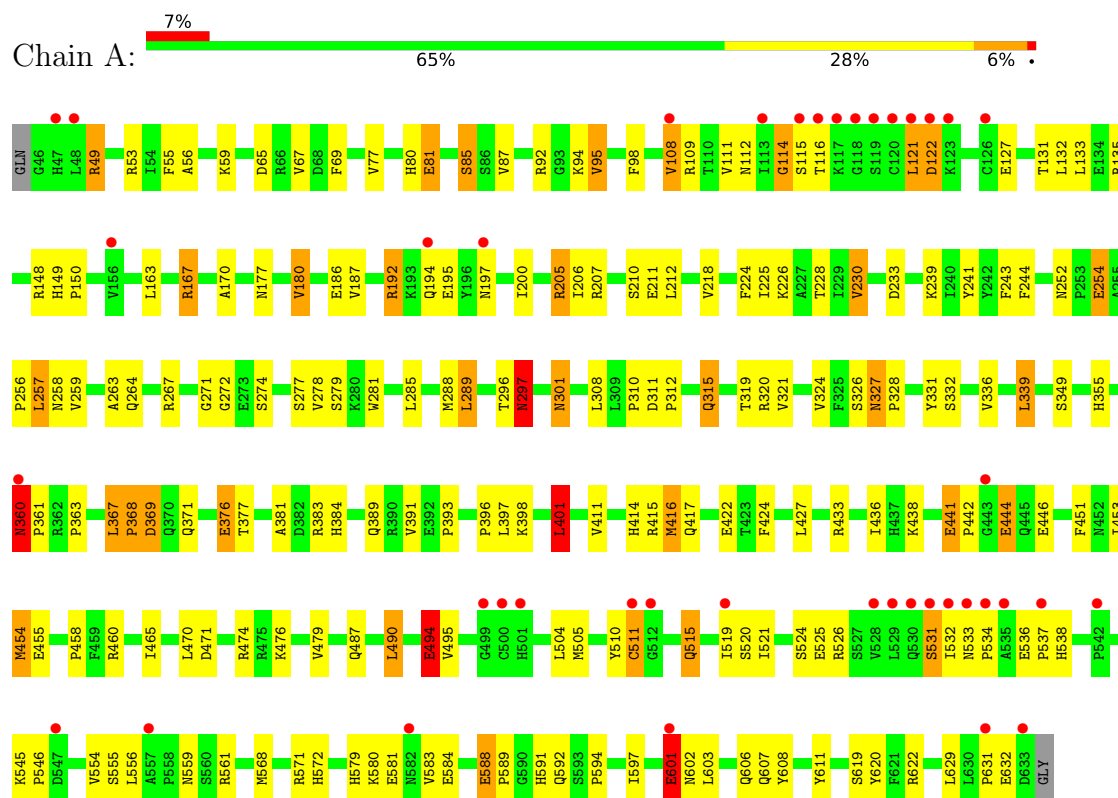
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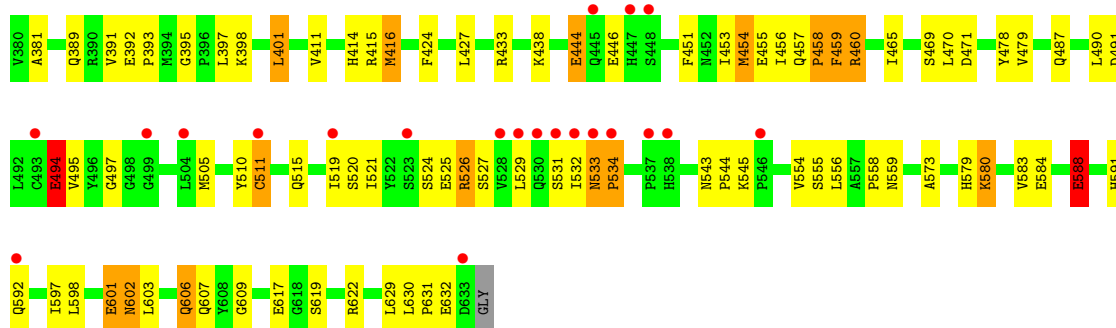
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	162	Total 162	O 162	0	0
5	E	297	Total 297	O 297	0	0
5	F	120	Total 120	O 120	0	0

3 Residue-property plots [i](#)

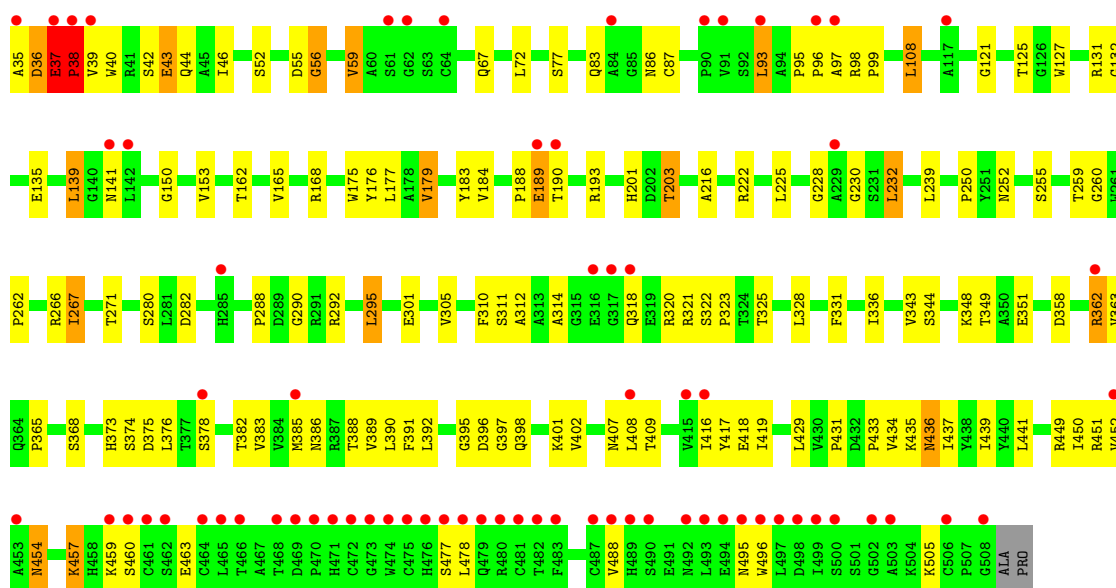
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

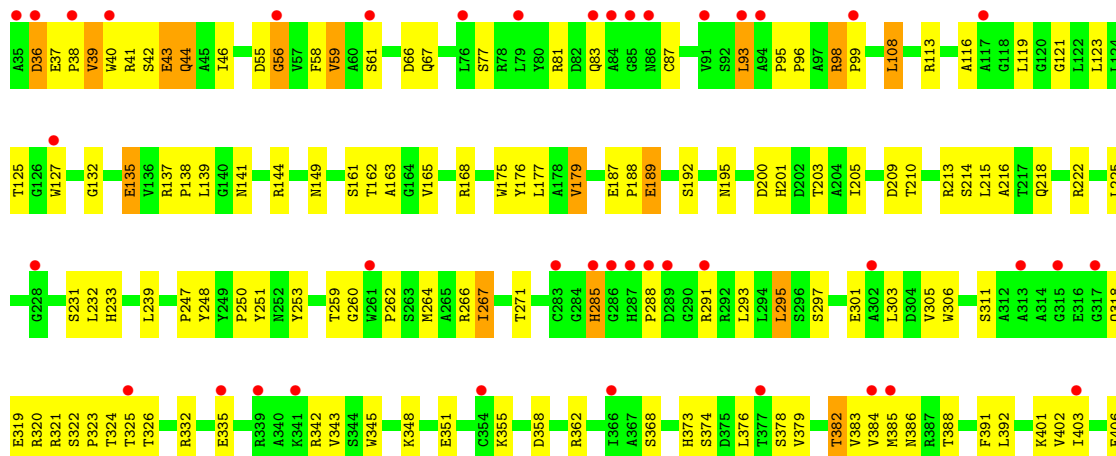


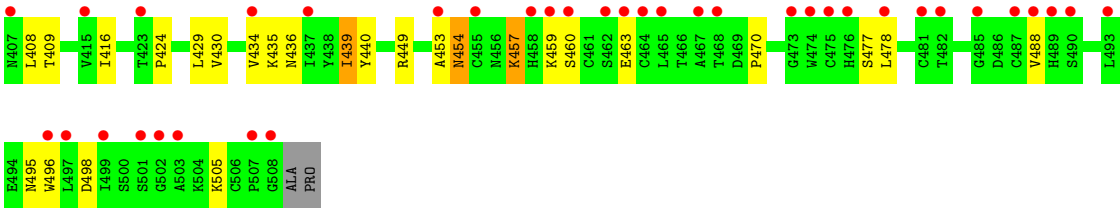


• Molecule 2: Plexin-C1



• 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.50	1/4839 (0.0%)	1.08	39/6568 (0.6%)
1	E	0.51	0/4839	1.05	33/6568 (0.5%)
2	B	0.43	0/3706	0.93	8/5039 (0.2%)
2	F	0.40	1/3706 (0.0%)	0.88	5/5039 (0.1%)
All	All	0.47	2/17090 (0.0%)	1.00	85/23214 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	GLU	C-N	-6.63	1.25	1.33
2	F	382	THR	C-N	-5.38	1.25	1.33

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	THR	N-CA-C	17.86	135.04	112.89
1	A	602	ASN	N-CA-CB	-11.12	93.93	110.84
2	B	37	GLU	N-CA-C	10.81	133.69	109.81
1	A	297	ASN	N-CA-CB	9.40	129.11	114.45
1	E	602	ASN	N-CA-C	-9.34	91.64	107.80
2	B	36	ASP	N-CA-C	9.20	130.40	110.80
1	E	531	SER	N-CA-C	9.02	123.80	110.17
1	A	601	GLU	CB-CA-C	9.00	128.33	110.42
2	B	38	PRO	N-CA-C	-8.66	94.62	112.47
1	E	602	ASN	N-CA-CB	-8.11	98.25	110.90
1	E	121	LEU	N-CA-C	-7.80	97.92	110.32
1	A	69	PHE	N-CA-C	-7.71	100.58	110.53
1	A	602	ASN	N-CA-C	-7.68	94.35	108.02
1	A	494	GLU	N-CA-C	-7.64	103.85	113.01
1	A	121	LEU	N-CA-C	-7.60	98.23	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ARG	N-CA-C	-7.54	103.14	111.36
1	E	511	CYS	N-CA-C	7.53	120.36	109.14
2	B	216	ALA	N-CA-C	7.50	120.85	110.35
1	A	360	ASN	CA-C-N	-7.46	110.52	119.84
1	A	360	ASN	C-N-CA	-7.46	110.52	119.84
1	E	460	ARG	N-CA-C	-7.43	103.27	111.36
1	A	49	ARG	N-CA-C	-7.33	104.37	112.72
2	F	87	CYS	N-CA-C	-7.18	103.68	113.30
1	E	49	ARG	N-CA-C	-7.14	103.67	112.88
1	E	619	SER	N-CA-C	-7.03	103.88	113.30
1	A	257	LEU	N-CA-C	6.95	118.85	111.28
2	F	216	ALA	N-CA-C	6.94	120.02	110.24
1	A	332	SER	N-CA-C	6.92	120.25	109.52
1	E	271	GLY	N-CA-C	-6.71	103.92	111.63
1	A	511	CYS	N-CA-C	6.58	118.77	108.96
1	E	458	PRO	N-CA-C	6.53	122.06	114.03
2	F	430	VAL	N-CA-C	6.48	114.95	107.89
2	B	87	CYS	N-CA-C	-6.47	104.64	113.30
1	A	401	LEU	N-CA-C	-6.45	104.25	111.28
1	E	205	ARG	N-CA-C	-6.35	98.19	108.41
1	E	609	GLY	N-CA-C	6.30	117.92	111.56
1	E	601	GLU	CB-CA-C	6.25	122.85	110.42
1	A	296	THR	CB-CA-C	-6.21	97.01	109.99
1	E	597	ILE	N-CA-C	6.12	116.73	108.17
1	E	601	GLU	N-CA-C	6.07	123.72	110.80
1	A	458	PRO	N-CA-C	6.05	121.91	114.35
2	B	184	VAL	N-CA-C	6.04	116.56	107.80
1	A	65	ASP	N-CA-C	6.01	120.80	112.45
1	A	149	HIS	CA-C-N	6.00	127.35	119.84
1	A	149	HIS	C-N-CA	6.00	127.35	119.84
1	E	395	GLY	CA-C-N	5.95	125.97	119.90
1	E	395	GLY	C-N-CA	5.95	125.97	119.90
1	E	545	LYS	CA-C-N	5.88	127.19	119.84
1	E	545	LYS	C-N-CA	5.88	127.19	119.84
1	E	494	GLU	N-CA-C	-5.85	105.99	113.01
1	E	497	GLY	N-CA-C	-5.79	102.69	112.77
1	E	331	TYR	N-CA-C	-5.75	100.91	110.17
1	A	545	LYS	CA-C-N	5.73	127.01	119.84
1	A	545	LYS	C-N-CA	5.73	127.01	119.84
1	A	218	VAL	N-CA-C	5.70	120.43	112.50
1	A	281	TRP	N-CA-C	-5.70	101.42	109.96
1	E	69	PHE	N-CA-C	-5.70	102.33	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	262	PRO	N-CA-C	-5.65	102.33	111.14
2	B	153	VAL	N-CA-C	-5.64	106.96	111.81
1	E	261	ARG	N-CA-C	5.58	117.67	109.24
1	A	205	ARG	N-CA-C	-5.56	98.70	108.20
1	E	172	PHE	N-CA-C	-5.47	106.78	113.50
1	A	597	ILE	N-CA-C	5.45	115.80	108.17
1	E	262	VAL	N-CA-C	-5.45	100.35	108.46
1	A	619	SER	N-CA-C	-5.36	106.05	112.59
1	A	233	ASP	N-CA-C	5.36	116.80	111.07
2	F	39	VAL	N-CA-C	5.36	117.17	109.51
1	A	271	GLY	N-CA-C	-5.34	103.38	110.97
1	E	588	GLU	CA-C-N	5.34	126.52	119.84
1	E	588	GLU	C-N-CA	5.34	126.52	119.84
1	A	454	MET	N-CA-C	5.30	116.58	108.52
1	A	369	ASP	N-CA-C	5.30	117.74	108.52
1	E	401	LEU	N-CA-C	-5.30	105.51	111.28
1	E	122	ASP	N-CA-C	-5.22	104.80	110.91
1	A	355	HIS	N-CA-C	5.17	119.09	112.26
1	A	367	LEU	CA-C-N	5.12	126.25	119.84
1	A	367	LEU	C-N-CA	5.12	126.25	119.84
1	E	459	PHE	N-CA-C	5.11	118.06	110.14
2	B	262	PRO	N-CA-C	-5.11	103.09	111.21
1	A	531	SER	N-CA-C	5.10	117.39	110.35
1	A	490	LEU	N-CA-C	-5.05	106.62	112.89
1	E	533	ASN	N-CA-C	5.03	120.93	109.81
1	A	85	SER	N-CA-C	-5.02	106.84	113.17
1	E	415	ARG	N-CA-C	-5.02	101.13	109.46
1	A	122	ASP	N-CA-C	-5.01	105.04	110.91

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	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4706	0	4478	149	0
2	B	3623	0	3496	105	0
2	F	3623	0	3497	117	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	15	0
5	F	120	0	0	6	0
All	All	17824	0	16235	510	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 (510) 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
1:A:259:VAL:HG21	1:A:288:MET:HE2	1.25	1.07
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
1:A:416:MET:HE1	1:A:424:PHE:HB2	1.40	1.00
2:F:203:THR:HG22	2:F:222:ARG:HH11	1.29	0.96
1:A:592:GLN:HG3	1:E:592:GLN:CD	1.92	0.95
1:E:259:VAL:HG21	1:E:288:MET:HE2	1.50	0.93
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: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
2:F:385:MET:HE1	2:F:498:ASP:HB2	1.58	0.85
1:A:592:GLN:CG	1:E:592:GLN:CD	2.49	0.84
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:CD	1:E:592:GLN:HG3	2.06	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:416:MET:HE1	1:E:424:PHE:HB2	1.66	0.77
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: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: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
1:A:592:GLN:CD	1:E:592:GLN:CD	2.59	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: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:327:ASN:C	1:A:327:ASN:HD22	2.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:GLN:CD	1:E:592:GLN:CG	2.70	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:E:376:GLU:H	1:E:376:GLU:CD	2.05	0.64
1:E:327:ASN:C	1:E:327:ASN:HD22	2.03	0.63
2:F:385:MET:HE1	2:F:498:ASP:CB	2.28	0.63
2:B:43:GLU:CD	2:B:43:GLU:H	2.04	0.63
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: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
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
1:A:114:GLY:C	1:A:116:THR:H	2.09	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: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
2:F:401:LYS:HB3	2:F:416:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:114:GLY:C	1:E:116:THR:H	2.09	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
1:E:532:ILE:C	1:E:534:PRO:HD2	2.28	0.58
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
1:A:592:GLN:OE1	1:E:592:GLN:CG	2.52	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
2:B:37:GLU:C	2:B:39:VAL:H	2.12	0.57
2:F:401:LYS:HZ3	2:F:453:ALA:HB2	1.68	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
1:A:376:GLU:CD	1:A:376:GLU:H	2.11	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
2:B:373:HIS:ND1	2:B:374:SER:N	2.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:322:SER:C	2:F:324:THR:H	2.14	0.55
2:B:362:ARG:CZ	2:B:362:ARG:HB2	2.37	0.55
2:F:247:PRO:HG3	2:F:264:MET:HE2	1.88	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:A:451:PHE:CD2	1:A:453:ILE:HG22	2.39	0.55
1:A:327:ASN:C	1:A:327:ASN:ND2	2.60	0.55
1:A:148:ARG:HH21	1:A:195:GLU:CD	2.15	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:B:121:GLY:C	2:B:139:LEU:HB2	2.31	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:B:389:VAL:C	2:B:390:LEU:HD12	2.32	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
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
2:F:373:HIS:HB3	2:F:376:LEU:HG	1.91	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:580:LYS:O	1:A:581:GLU:HB2	2.09	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:E:416:MET:CE	1:E:424:PHE:HB2	2.38	0.51
2:F:391:PHE:C	2:F:392:LEU:HD12	2.35	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:327:ASN:C	1:E:327:ASN:ND2	2.68	0.51
1:E:329:TRP:O	1:E:330:ASN:HB2	2.11	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
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
2:F:43:GLU:CD	2:F:43:GLU:H	2.18	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: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
1:A:568:MET:HE1	1:A:591:HIS:ND1	2.27	0.50

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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: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
1:E:259:VAL:HG21	1:E:288:MET:CE	2.34	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
1:A:259:VAL:HG21	1:A:288:MET:CE	2.18	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:A:311:ASP:OD1	1:A:312:PRO:HD2	2.13	0.48
1:A:444:GLU:CD	1:A:444:GLU:H	2.21	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
1:E:444:GLU:CD	1:E:444:GLU:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ILE:HD12	2:B:59:VAL:HG21	1.96	0.48
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:460:SER:HB3	2:F:463:GLU:CB	2.44	0.47
1:E:223:GLN:CD	3:E:3:NAG:H62	2.40	0.47
1:E:293:ASP:O	1:E:296:THR:O	2.31	0.47
1:E:505:MET:HE1	5:E:931:HOH:O	2.14	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:391:PHE:C	2:B:392:LEU:HD12	2.40	0.47
1:E:179:LEU:C	1:E:179:LEU:HD13	2.40	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:A:532:ILE:C	1:A:534:PRO:HD2	2.40	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
2:F:402:VAL:C	2:F:403:ILE:HD12	2.40	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
1:A:505:MET:HE2	1:A:620:TYR:CD2	2.50	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
1:A:77:VAL:HG21	1:A:131:THR:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:525:GLU:C	1:E:527:SER:H	2.23	0.46
2:F:478:LEU:HD23	2:F:478:LEU:H	1.81	0.46
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:43:GLU:CD	2:B:43:GLU:N	2.72	0.45
2:B:434:VAL:HG12	2:B:435:LYS:HD2	1.98	0.45
1:E:114:GLY:C	1:E:116:THR:N	2.75	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:B:401:LYS:HB2	2:B:416:ILE:HD11	1.97	0.45
2:B:441:LEU:HD23	2:B:441:LEU:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:323:PRO:HA	2:F:374:SER:CB	2.47	0.44
2:B:351:GLU:H	2:B:351:GLU:CD	2.25	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
1:A:92:ARG:HD3	1:A:127:GLU:CD	2.42	0.44
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
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
1:E:598:LEU:C	1:E:598:LEU:HD23	2.42	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
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:E:224:PHE:C	1:E:225:ILE:HD13	2.43	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:228:GLY:C	2:B:230:GLY:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:319:GLU:C	2:F:321:ARG:H	2.27	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
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:B:437:ILE:C	2:B:452:VAL:HG13	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:LEU:C	1:E:78:LEU:HD23	2.44	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
2:F:161:SER:HB3	2:F:233:HIS:CE1	2.55	0.42
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
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
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:E:392:GLU:CD	1:E:398:LYS:HD3	2.45	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
3:E:4:NAG:H4	5:E:715:HOH:O	2.20	0.41
1:A:416:MET:CE	1:A:424:PHE:HB2	2.29	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:36:ASP:C	2:F:38:PRO:HD3	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:322:SER:C	2:F:324:THR:N	2.76	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
2:F:81:ARG:HH21	2:F:135:GLU:CD	2.28	0.40
1:A:114:GLY:C	1:A:116:THR:N	2.75	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
1:A:589:PRO:C	1:A:591:HIS:H	2.29	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
1:E:558:PRO:O	1:E:559:ASN:HB2	2.21	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

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	586/590 (99%)	530 (90%)	47 (8%)	9 (2%)	8	12
1	E	586/590 (99%)	529 (90%)	46 (8%)	11 (2%)	6	8
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%)	6	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

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Mol	Chain	Res	Type
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
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%)	484 (93%)	34 (7%)	15	26
1	E	518/519 (100%)	480 (93%)	38 (7%)	13	22
2	B	389/390 (100%)	364 (94%)	25 (6%)	16	28
2	F	389/390 (100%)	368 (95%)	21 (5%)	20	35
All	All	1814/1818 (100%)	1696 (94%)	118 (6%)	15	27

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	81	GLU
1	A	95	VAL
1	A	108	VAL

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Mol	Chain	Res	Type
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	285	LEU
1	A	289	LEU
1	A	297	ASN
1	A	301	ASN
1	A	315	GLN
1	A	327	ASN
1	A	339	LEU
1	A	376	GLU
1	A	401	LEU
1	A	416	MET
1	A	446	GLU
1	A	494	GLU
1	A	515	GLN
1	A	559	ASN
1	A	584	GLU
1	A	588	GLU
1	A	606	GLN
1	A	622	ARG
2	B	37	GLU
2	B	43	GLU
2	B	44	GLN
2	B	59	VAL
2	B	86	ASN
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

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Mol	Chain	Res	Type
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	382	THR
2	B	396	ASP
2	B	436	ASN
2	B	454	ASN
2	B	457	LYS
2	B	496	TRP
1	E	59	LYS
1	E	72	THR
1	E	81	GLU
1	E	95	VAL
1	E	108	VAL
1	E	109	ARG
1	E	110	THR
1	E	187	VAL
1	E	190	THR
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	304	GLN
1	E	315	GLN
1	E	320	ARG
1	E	327	ASN
1	E	332	SER
1	E	339	LEU
1	E	376	GLU
1	E	401	LEU
1	E	416	MET
1	E	427	LEU
1	E	446	GLU
1	E	454	MET

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Mol	Chain	Res	Type
1	E	458	PRO
1	E	469	SER
1	E	494	GLU
1	E	515	GLN
1	E	580	LYS
1	E	584	GLU
1	E	588	GLU
1	E	606	GLN
1	E	622	ARG
2	F	36	ASP
2	F	43	GLU
2	F	44	GLN
2	F	59	VAL
2	F	93	LEU
2	F	98	ARG
2	F	108	LEU
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	295	LEU
2	F	362	ARG
2	F	382	THR
2	F	439	ILE
2	F	454	ASN
2	F	457	LYS
2	F	496	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	71	GLN
1	A	80	HIS
1	A	149	HIS
1	A	154	ASN
1	A	177	ASN
1	A	194	GLN
1	A	234	GLN

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Mol	Chain	Res	Type
1	A	264	GLN
1	A	270	GLN
1	A	301	ASN
1	A	304	GLN
1	A	327	ASN
1	A	371	GLN
1	A	384	HIS
1	A	389	GLN
1	A	414	HIS
1	A	417	GLN
1	A	457	GLN
1	A	466	GLN
1	A	482	GLN
1	A	487	GLN
1	A	515	GLN
1	A	552	GLN
1	A	559	ASN
1	A	579	HIS
1	A	582	ASN
1	A	602	ASN
1	A	606	GLN
1	A	625	GLN
1	A	628	GLN
2	B	44	GLN
2	B	67	GLN
2	B	172	ASN
2	B	173	ASN
2	B	276	GLN
2	B	285	HIS
2	B	318	GLN
2	B	359	GLN
2	B	364	GLN
2	B	398	GLN
2	B	436	ASN
2	B	456	ASN
2	B	471	HIS
1	E	64	GLN
1	E	71	GLN
1	E	80	HIS
1	E	154	ASN
1	E	177	ASN
1	E	194	GLN

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Mol	Chain	Res	Type
1	E	220	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	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
1	E	616	GLN
2	F	44	GLN
2	F	67	GLN
2	F	172	ASN
2	F	173	ASN
2	F	201	HIS
2	F	269	GLN
2	F	285	HIS
2	F	287	HIS
2	F	359	GLN
2	F	398	GLN
2	F	436	ASN
2	F	454	ASN
2	F	456	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 ⓘ

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

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	F	1	2	-	4/6/23/26	0/1/1/1
3	NAG	F	2	2	-	4/6/23/26	0/1/1/1
3	NAG	B	4	2	-	2/6/23/26	0/1/1/1
3	NAG	B	5	2	-	2/6/23/26	0/1/1/1
3	NAG	A	2	1	-	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
3	NAG	F	6	2	1/1/5/7	4/6/23/26	0/1/1/1
4	NDG	A	4	-	-	3/6/23/26	0/1/1/1
3	NAG	E	4	1	-	2/6/23/26	0/1/1/1
3	NAG	B	7	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	A	1	1	-	4/6/23/26	0/1/1/1
3	NAG	B	6	2	-	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
3	NAG	E	2	1	-	4/6/23/26	0/1/1/1
3	NAG	F	4	2	-	4/6/23/26	0/1/1/1
3	NAG	F	7	2	-	4/6/23/26	0/1/1/1
3	NAG	F	3	2	-	4/6/23/26	0/1/1/1
3	NAG	E	1	1	-	5/6/23/26	0/1/1/1
3	NAG	F	5	2	-	2/6/23/26	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
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
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

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Mol	Chain	Res	Type	Atoms
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
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	F	1	NAG	1	0
3	B	3	NAG	1	0
3	E	4	NAG	1	0
3	E	3	NAG	5	0
3	B	1	NAG	1	0
3	E	2	NAG	2	0
3	F	7	NAG	1	0
3	F	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%)	0.39	41 (6%) 22 19	25, 55, 113, 150	0
1	E	588/590 (99%)	0.41	40 (6%) 23 20	27, 53, 107, 140	0
2	B	474/476 (99%)	0.92	71 (14%) 5 4	34, 70, 129, 150	0
2	F	474/476 (99%)	0.98	78 (16%) 4 3	37, 72, 131, 150	0
All	All	2124/2132 (99%)	0.64	230 (10%) 11 8	25, 62, 125, 150	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	465	LEU	6.0
2	F	488	VAL	5.6
2	B	493	LEU	5.0
2	F	468	THR	4.8
1	A	121	LEU	4.6
1	E	633	ASP	4.4
2	F	503	ALA	4.4
2	B	499	ILE	4.2
2	B	481	CYS	4.2
2	B	470	PRO	4.1
1	A	116	THR	4.1
1	A	117	LYS	4.1
2	B	488	VAL	4.0
1	A	542	PRO	4.0
1	E	533	ASN	3.8
1	E	532	ILE	3.8
2	B	474	TRP	3.8
2	F	497	LEU	3.8
2	B	472	CYS	3.8
2	B	508	GLY	3.8
2	B	475	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	F	465	LEU	3.7
1	E	117	LYS	3.7
2	B	487	CYS	3.6
1	A	531	SER	3.6
2	B	318	GLN	3.6
1	A	48	LEU	3.6
2	F	94	ALA	3.5
1	A	535	ALA	3.5
1	E	519	ILE	3.5
2	B	483	PHE	3.5
2	F	507	PRO	3.4
2	B	141	ASN	3.4
1	E	531	SER	3.4
1	A	119	SER	3.4
2	F	38	PRO	3.4
2	F	482	THR	3.4
2	F	35	ALA	3.4
2	F	499	ILE	3.3
2	F	36	ASP	3.3
2	B	480	ARG	3.2
2	B	229	ALA	3.2
1	A	530	GLN	3.2
1	E	537	PRO	3.2
2	B	415	VAL	3.2
2	F	475	CYS	3.2
2	B	490	SER	3.2
1	E	122	ASP	3.1
2	F	474	TRP	3.1
2	F	496	TRP	3.1
2	B	502	GLY	3.1
1	E	194	GLN	3.1
1	E	126	CYS	3.1
1	E	530	GLN	3.1
2	F	83	GLN	3.0
1	A	113	ILE	3.0
1	E	48	LEU	3.0
1	A	533	ASN	3.0
2	F	313	ALA	3.0
2	B	489	HIS	3.0
2	B	496	TRP	3.0
1	A	534	PRO	3.0
2	B	35	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	592	GLN	2.9
2	B	362	ARG	2.9
2	F	490	SER	2.9
2	B	464	CYS	2.9
2	B	462	SER	2.9
2	B	495	ASN	2.9
2	B	64	CYS	2.9
2	F	464	CYS	2.9
2	B	482	THR	2.9
2	B	503	ALA	2.9
2	F	508	GLY	2.9
1	A	108	VAL	2.8
1	E	528	VAL	2.8
2	F	481	CYS	2.8
1	A	532	ILE	2.8
2	B	492	ASN	2.8
2	F	501	SER	2.8
1	E	534	PRO	2.8
2	F	493	LEU	2.8
2	F	127	TRP	2.8
1	A	123	LYS	2.8
2	F	462	SER	2.7
2	B	97	ALA	2.7
2	B	461	CYS	2.7
1	A	47	HIS	2.7
1	E	197	ASN	2.7
1	A	156	VAL	2.7
2	F	283	CYS	2.7
1	A	512	GLY	2.7
1	E	499	GLY	2.7
2	B	285	HIS	2.7
1	A	443	GLY	2.7
2	F	502	GLY	2.7
1	E	206	ILE	2.7
2	B	452	VAL	2.7
2	F	91	VAL	2.7
2	F	478	LEU	2.7
2	B	316	GLU	2.7
2	B	468	THR	2.7
2	F	489	HIS	2.7
2	F	228	GLY	2.6
2	B	91	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	115	SER	2.6
2	B	476	HIS	2.6
2	F	315	GLY	2.6
1	A	120	CYS	2.6
1	E	360	ASN	2.6
1	E	445	GLN	2.6
2	B	471	HIS	2.6
2	F	485	GLY	2.6
1	A	528	VAL	2.6
2	F	460	SER	2.6
1	E	448	SER	2.6
2	B	498	ASP	2.5
1	E	529	LEU	2.5
2	B	39	VAL	2.5
2	F	459	LYS	2.5
2	B	317	GLY	2.5
2	B	416	ILE	2.5
2	F	335	GLU	2.5
2	B	478	LEU	2.5
1	E	523	SER	2.5
1	A	511	CYS	2.5
1	A	529	LEU	2.5
2	B	497	LEU	2.5
2	F	291	ARG	2.5
2	F	377	THR	2.5
2	F	487	CYS	2.5
2	F	463	GLU	2.5
1	E	447	HIS	2.5
2	B	61	SER	2.5
1	E	511	CYS	2.4
2	B	62	GLY	2.4
1	A	122	ASP	2.4
1	A	360	ASN	2.4
2	F	99	PRO	2.4
2	B	142	LEU	2.4
2	F	93	LEU	2.4
1	E	196	TYR	2.4
2	F	385	MET	2.4
2	F	40	TRP	2.4
2	F	467	ALA	2.4
2	B	378	SER	2.4
2	B	460	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	93	LEU	2.4
2	B	408	LEU	2.4
1	E	95	VAL	2.4
2	F	415	VAL	2.4
2	B	117	ALA	2.4
1	E	70	GLY	2.3
2	B	473	GLY	2.3
1	E	113	ILE	2.3
2	F	86	ASN	2.3
2	F	288	PRO	2.3
2	F	61	SER	2.3
2	F	85	GLY	2.3
2	F	317	GLY	2.3
1	E	493	CYS	2.3
2	F	56	GLY	2.3
2	F	261	TRP	2.3
2	B	37	GLU	2.3
1	A	194	GLN	2.3
2	F	473	GLY	2.3
1	E	115	SER	2.3
2	F	79	LEU	2.3
2	B	90	PRO	2.3
1	A	582	ASN	2.2
1	E	116	THR	2.2
2	B	190	THR	2.2
2	B	466	THR	2.2
2	F	325	THR	2.2
1	A	633	ASP	2.2
2	B	494	GLU	2.2
2	B	96	PRO	2.2
2	F	117	ALA	2.2
2	F	458	HIS	2.2
2	F	341	LYS	2.2
2	F	289	ASP	2.2
2	B	453	ALA	2.2
2	F	302	ALA	2.2
1	A	500	CYS	2.2
1	A	118	GLY	2.2
1	A	499	GLY	2.2
1	E	504	LEU	2.2
2	F	286	GLY	2.2
1	A	519	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	175	ASP	2.2
1	A	197	ASN	2.2
2	F	84	ALA	2.2
2	F	423	THR	2.2
2	F	354	CYS	2.2
1	E	178	SER	2.2
1	A	547	ASP	2.2
1	E	546	PRO	2.2
2	B	459	LYS	2.2
1	A	557	ALA	2.1
2	F	437	ILE	2.1
1	A	126	CYS	2.1
2	B	506	CYS	2.1
2	F	455	CYS	2.1
2	F	407	ASN	2.1
2	F	366	ILE	2.1
1	E	167	ARG	2.1
2	B	500	SER	2.1
2	F	403	ILE	2.1
2	B	38	PRO	2.1
2	F	384	VAL	2.1
2	F	76	LEU	2.1
1	A	537	PRO	2.1
2	F	434	VAL	2.0
2	B	84	ALA	2.0
2	F	453	ALA	2.0
1	A	601	GLU	2.0
2	B	189	GLU	2.0
2	B	477	SER	2.0
1	E	538	HIS	2.0
2	F	285	HIS	2.0
2	F	287	HIS	2.0
2	B	479	GLN	2.0
2	F	339	ARG	2.0
1	E	176	GLU	2.0
1	E	118	GLY	2.0
1	A	631	PRO	2.0
2	B	385	MET	2.0
2	B	469	ASP	2.0
1	A	501	HIS	2.0
2	F	476	HIS	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 oligosaccharides 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($\text{\AA}^2$)	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
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 [i](#)

There are no such residues in this entry.