



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:20 PM UTC

PDB ID : 7ZFB / pdb_00007zfb
Title : SARS-CoV-2 Omicron RBD in complex with nanobody C1, Omi-18 and Omi-31 Fabs
Authors : Zhou, D.; Huo, J.; Ren, J.; Stuart, D.I.
Deposited on : 2022-04-01
Resolution : 3.08 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:

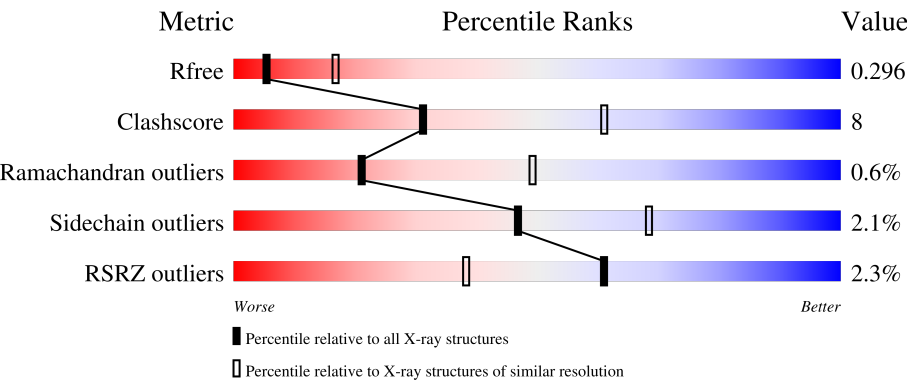
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	M	131	83%11%6%
1	N	131	2% 80%15%5%
2	E	202	3% 72%21%. .
2	F	202	9% 74%19%... .
3	A	233	% 82%16%. .

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Mol	Chain	Length	Quality of chain
3	C	233	%82%16%.
4	B	216	2%81%16%..
4	D	216	2%80%18%..
5	H	222	4%79%17%..
5	J	222	%77%18%. .
6	K	213	2%82%15%..
6	L	213	77%20%. .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17936 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 Nanobody C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	123	Total	C	N	O	S	0	2	0
			967	609	166	188	4			
1	N	124	Total	C	N	O	S	0	2	0
			973	612	167	190	4			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	195	Total	C	N	O	S	0	0	0
			1563	1007	264	284	8			
2	F	195	Total	C	N	O	S	0	0	0
			1563	1007	264	284	8			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
E	331	HIS	-	expression tag	UNP P0DTC2
E	332	HIS	-	expression tag	UNP P0DTC2
E	339	ASP	GLY	variant	UNP P0DTC2
E	371	LEU	SER	variant	UNP P0DTC2
E	373	PRO	SER	variant	UNP P0DTC2
E	375	PHE	SER	variant	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	440	LYS	ASN	variant	UNP P0DTC2
E	446	SER	GLY	variant	UNP P0DTC2
E	477	ASN	SER	variant	UNP P0DTC2
E	478	LYS	THR	variant	UNP P0DTC2
E	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	493	ARG	GLN	variant	UNP P0DTC2
E	496	SER	GLY	variant	UNP P0DTC2
E	498	ARG	GLN	conflict	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	505	HIS	TYR	variant	UNP P0DTC2
E	527	LYS	-	expression tag	UNP P0DTC2
E	528	LYS	-	expression tag	UNP P0DTC2
F	327	HIS	-	expression tag	UNP P0DTC2
F	328	HIS	-	expression tag	UNP P0DTC2
F	329	HIS	-	expression tag	UNP P0DTC2
F	330	HIS	-	expression tag	UNP P0DTC2
F	331	HIS	-	expression tag	UNP P0DTC2
F	332	HIS	-	expression tag	UNP P0DTC2
F	339	ASP	GLY	variant	UNP P0DTC2
F	371	LEU	SER	variant	UNP P0DTC2
F	373	PRO	SER	variant	UNP P0DTC2
F	375	PHE	SER	variant	UNP P0DTC2
F	417	ASN	LYS	variant	UNP P0DTC2
F	440	LYS	ASN	variant	UNP P0DTC2
F	446	SER	GLY	variant	UNP P0DTC2
F	477	ASN	SER	variant	UNP P0DTC2
F	478	LYS	THR	variant	UNP P0DTC2
F	484	ALA	GLU	variant	UNP P0DTC2
F	493	ARG	GLN	variant	UNP P0DTC2
F	496	SER	GLY	variant	UNP P0DTC2
F	498	ARG	GLN	conflict	UNP P0DTC2
F	501	TYR	ASN	variant	UNP P0DTC2
F	505	HIS	TYR	variant	UNP P0DTC2
F	527	LYS	-	expression tag	UNP P0DTC2
F	528	LYS	-	expression tag	UNP P0DTC2

- Molecule 3 is a protein called Omi-31 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	228	Total	C	N	O	S	0	0	0
			1704	1075	288	334	7			
3	C	228	Total	C	N	O	S	0	0	0
			1704	1075	288	334	7			

- Molecule 4 is a protein called Omi-31 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	212	Total	C	N	O	S	0	1	0
			1573	978	266	325	4			
4	D	213	Total	C	N	O	S	0	1	0
			1578	981	267	326	4			

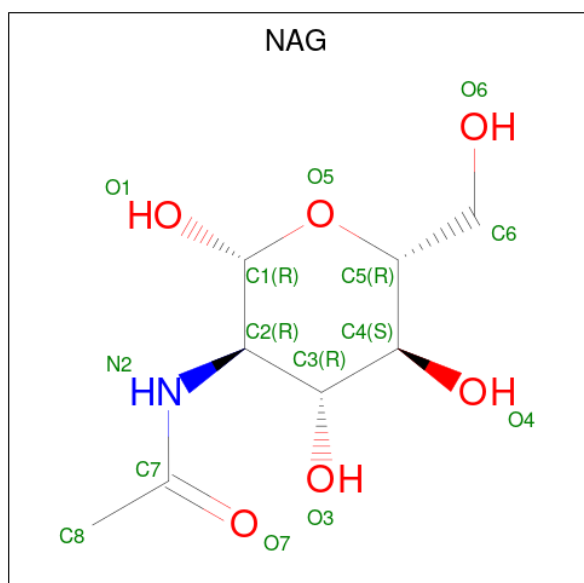
- Molecule 5 is a protein called Omi-18 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	215	Total	C	N	O	S	0	0	0
			1580	997	265	311	7			
5	J	215	Total	C	N	O	S	0	0	0
			1580	997	265	311	7			

- Molecule 6 is a protein called Omi-18 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	208	Total	C	N	O	S	0	0	0
			1566	973	268	321	4			
6	K	207	Total	C	N	O	S	0	0	0
			1557	968	267	318	4			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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: Nanobody C1

Chain M: 



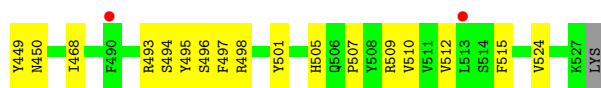
- Molecule 1: Nanobody C1

Chain N: 



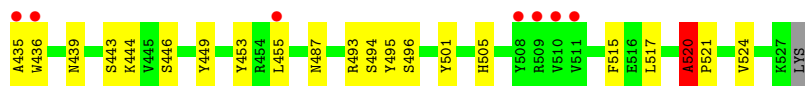
- Molecule 2: Spike protein S1

Chain E: 

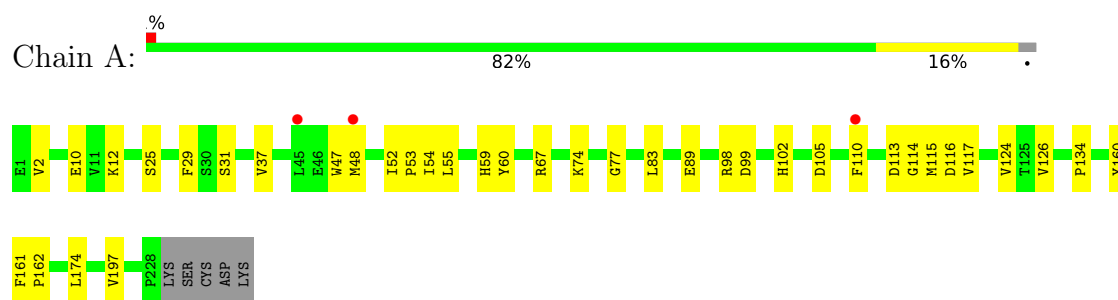


- Molecule 2: Spike protein S1

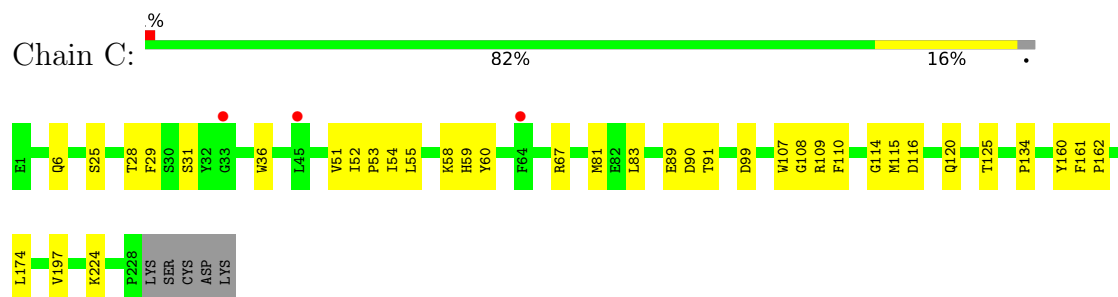
Chain F: 



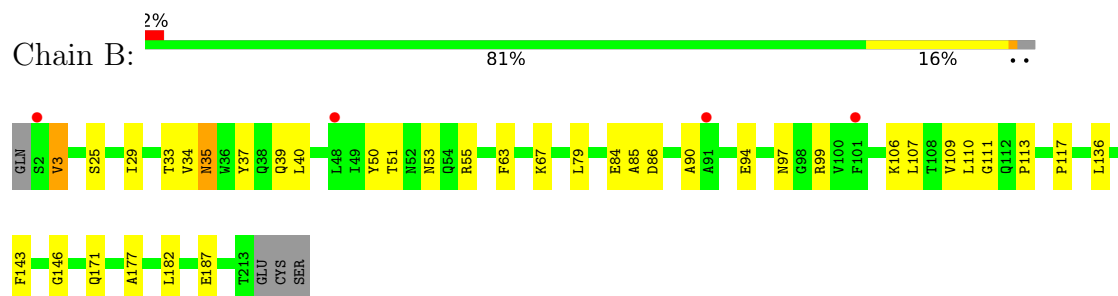
- Molecule 3: Omi-31 heavy chain



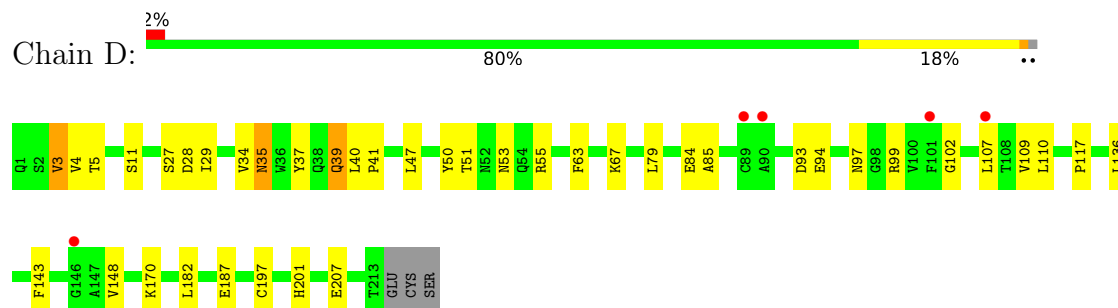
• Molecule 3: Omi-31 heavy chain



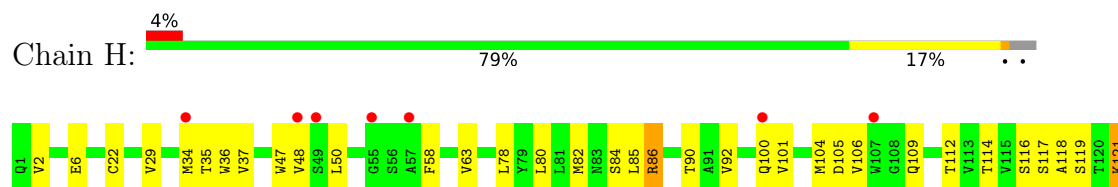
• Molecule 4: Omi-31 light chain



• Molecule 4: Omi-31 light chain

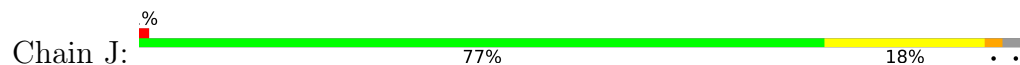


• Molecule 5: Omi-18 heavy chain

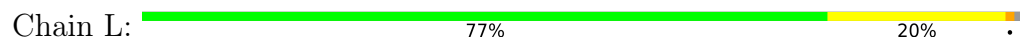




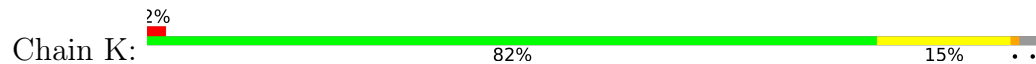
- Molecule 5: Omi-18 heavy chain



- Molecule 6: Omi-18 light chain



- Molecule 6: Omi-18 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.19Å 135.09Å 112.24Å 90.00° 101.66° 90.00°	Depositor
Resolution (Å)	70.56 – 3.08 70.56 – 3.08	Depositor EDS
% Data completeness (in resolution range)	89.0 (70.56-3.08) 83.9 (70.56-3.08)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.261 , 0.308 0.251 , 0.296	Depositor DCC
R_{free} test set	3047 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	110.9	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 153.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.067 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17936	wwPDB-VP
Average B, all atoms (Å ²)	176.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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

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	M	0.15	0/998	0.34	0/1358
1	N	0.13	0/1004	0.31	0/1366
2	E	0.23	0/1609	0.40	0/2190
2	F	0.29	1/1609 (0.1%)	0.45	0/2190
3	A	0.15	0/1746	0.33	0/2378
3	C	0.18	0/1746	0.33	0/2378
4	B	0.20	0/1613	0.40	1/2205 (0.0%)
4	D	0.22	0/1618	0.40	0/2212
5	H	0.18	0/1614	0.39	0/2202
5	J	0.17	0/1614	0.38	0/2202
6	K	0.16	0/1596	0.35	0/2185
6	L	0.20	0/1605	0.35	0/2197
All	All	0.20	1/18372 (0.0%)	0.37	1/25063 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	520	ALA	C-N	5.45	1.39	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	111	GLY	N-CA-C	5.53	126.28	113.18

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	M	967	0	917	14	0
1	N	973	0	922	14	0
2	E	1563	0	1488	44	0
2	F	1563	0	1488	57	0
3	A	1704	0	1671	26	0
3	C	1704	0	1671	24	0
4	B	1573	0	1524	23	0
4	D	1578	0	1529	33	0
5	H	1580	0	1552	26	0
5	J	1580	0	1552	27	1
6	K	1557	0	1494	28	0
6	L	1566	0	1500	33	1
7	E	14	0	13	0	0
7	F	14	0	13	1	0
All	All	17936	0	17334	288	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (288) 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)
5:H:100:GLN:HB3	6:L:90:TRP:HE1	1.34	0.91
1:N:105:ASP:HB2	2:F:378:LYS:HE3	1.59	0.85
5:H:173:VAL:HG12	6:L:163:THR:HG23	1.64	0.80
5:H:84:SER:O	5:H:86:ARG:NH2	2.13	0.79
2:E:446:SER:HB2	3:A:60:TYR:HD2	1.49	0.78
1:N:76:ASN:ND2	1:N:80:TYR:OH	2.17	0.77
6:L:33:HIS:HE1	6:L:90:TRP:HB2	1.50	0.76
5:H:29:VAL:HG13	5:H:34:MET:HG3	1.69	0.74
6:K:33:HIS:HE1	6:K:90:TRP:HB2	1.53	0.72
6:K:163:THR:HG23	5:J:173:VAL:HG12	1.71	0.72
3:C:60:TYR:HD2	2:F:446:SER:HB2	1.56	0.71
2:F:375:PHE:HB3	2:F:436:TRP:HB3	1.73	0.70
6:K:11:SER:HB3	6:K:107:LEU:HD21	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:116:SER:OG	5:H:178:GLY:HA3	1.92	0.69
2:E:359:SER:HA	2:E:524:VAL:HG22	1.75	0.69
2:E:375:PHE:HB3	2:E:436:TRP:HB3	1.73	0.69
2:E:450:ASN:ND2	4:B:94:GLU:OE2	2.25	0.68
6:L:111:LYS:HZ1	6:L:199:GLU:HB2	1.58	0.68
5:H:82:MET:HB3	5:H:85:LEU:HD21	1.76	0.67
1:N:105:ASP:OD2	2:F:378:LYS:NZ	2.28	0.66
5:H:123:PRO:HB3	5:H:149:TYR:HB3	1.78	0.66
1:N:104:ARG:NH1	2:F:375:PHE:O	2.29	0.66
2:E:410:ILE:HD13	2:E:510:VAL:HG11	1.78	0.65
2:E:367:VAL:O	2:E:371:LEU:HB2	1.97	0.65
2:E:446:SER:HB2	3:A:60:TYR:CD2	2.31	0.64
3:C:109:ARG:HH12	2:F:346:ARG:CZ	2.11	0.64
2:F:393:THR:HG23	2:F:517:LEU:HD12	1.81	0.63
2:E:365:TYR:HA	2:E:368:LEU:HD22	1.80	0.63
2:F:367:VAL:O	2:F:371:LEU:HB2	1.98	0.63
6:K:33:HIS:NE2	5:J:101:VAL:O	2.27	0.63
6:L:4:LEU:HD11	6:L:89:VAL:HG13	1.80	0.62
2:F:359:SER:HA	2:F:524:VAL:HG22	1.80	0.62
2:E:375:PHE:HD2	2:E:436:TRP:HB3	1.64	0.62
3:A:113:ASP:OD1	4:B:33:THR:OG1	2.14	0.62
4:B:40:LEU:HD23	4:B:85:ALA:HB2	1.82	0.61
4:D:97:ASN:HB2	2:F:444:LYS:NZ	2.16	0.61
5:H:121:LYS:HD2	5:H:149:TYR:HA	1.82	0.61
2:E:468:ILE:HD12	3:A:105:ASP:HB2	1.83	0.60
3:C:134:PRO:HB3	3:C:160:TYR:HB3	1.84	0.60
1:M:73:HIS:HE2	4:D:27:SER:HG	1.44	0.60
5:J:100:GLN:HG3	2:F:455:LEU:HD11	1.83	0.60
2:F:375:PHE:HD2	2:F:436:TRP:HB3	1.66	0.60
6:L:17:THR:HG22	6:L:75:THR:HA	1.82	0.60
1:M:73:HIS:ND1	4:D:3:VAL:HG21	2.16	0.60
4:D:94:GLU:HG2	2:F:346:ARG:NH2	2.17	0.60
3:C:67:ARG:NH2	3:C:90:ASP:OD2	2.35	0.59
2:F:365:TYR:HA	2:F:368:LEU:HD22	1.84	0.59
4:D:41:PRO:HG2	4:D:170:LYS:HD3	1.83	0.59
6:L:11:SER:OG	6:L:199:GLU:OE2	2.13	0.59
3:A:134:PRO:HB3	3:A:160:TYR:HB3	1.84	0.59
5:J:82:MET:HB3	5:J:85:LEU:HD21	1.85	0.58
3:A:2:VAL:HB	3:A:25:SER:HB2	1.84	0.58
5:H:6:GLU:H	5:H:109:GLN:HE22	1.51	0.58
3:C:109:ARG:HH12	2:F:346:ARG:NH2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:379:CYS:SG	2:E:384:PRO:HG3	2.44	0.58
4:D:94:GLU:HG2	2:F:346:ARG:CZ	2.33	0.57
6:K:94:ARG:HH22	2:F:408:ARG:HD3	1.67	0.57
2:E:449:TYR:HA	2:E:495:TYR:O	2.05	0.57
1:N:73:HIS:HB3	1:N:76:ASN:OD1	2.05	0.57
5:H:100:GLN:CB	6:L:90:TRP:HE1	2.12	0.57
6:K:54:PRO:HG2	6:K:57:ILE:HD12	1.87	0.57
3:C:52:ILE:HG22	3:C:55:LEU:H	1.69	0.57
4:D:94:GLU:HG2	2:F:346:ARG:NH1	2.19	0.57
5:H:104:MET:HE1	6:L:98:PHE:HZ	1.69	0.56
2:F:439:ASN:O	2:F:443:SER:OG	2.23	0.56
2:E:375:PHE:CD2	2:E:436:TRP:HB3	2.41	0.56
6:L:16:GLN:HG2	6:L:17:THR:H	1.70	0.56
4:D:97:ASN:HB2	2:F:444:LYS:HZ2	1.70	0.56
6:L:139:ASP:OD1	6:L:168:GLN:NE2	2.37	0.55
3:C:114:GLY:H	4:D:99:ARG:HH22	1.53	0.55
5:J:29:VAL:HG13	5:J:34:MET:HG3	1.88	0.55
5:J:12:ILE:HG23	5:J:115:VAL:HG22	1.88	0.55
6:L:33:HIS:CE1	6:L:90:TRP:HB2	2.36	0.54
4:D:40:LEU:HD23	4:D:85:ALA:HB2	1.89	0.54
6:L:34:TRP:HB2	6:L:47:VAL:HB	1.89	0.54
5:J:34:MET:HB3	5:J:78:LEU:HD22	1.89	0.54
2:E:444:LYS:NZ	4:B:97:ASN:HB2	2.23	0.54
5:J:92:VAL:HG22	5:J:112:THR:HG22	1.91	0.53
6:K:94:ARG:HD3	5:J:58:PHE:CE1	2.44	0.53
4:B:29:ILE:HG22	4:B:67:LYS:HE3	1.90	0.53
1:N:105:ASP:OD1	1:N:106:THR:N	2.42	0.53
5:J:22:CYS:C	5:J:77:THR:HG23	2.33	0.53
5:J:56:SER:OG	2:F:420:ASP:OD2	2.22	0.53
2:F:375:PHE:CD2	2:F:436:TRP:HB3	2.42	0.53
4:D:51:THR:O	4:D:53:ASN:N	2.39	0.53
2:E:409:GLN:HG2	6:L:94:ARG:HH21	1.73	0.52
4:D:84:GLU:HB2	4:D:109:VAL:HG23	1.91	0.52
5:J:123:PRO:HB3	5:J:149:TYR:HB3	1.91	0.52
4:D:35:ASN:HB3	4:D:50:TYR:HA	1.90	0.52
3:A:174:LEU:HD21	3:A:197:VAL:HG21	1.91	0.52
2:F:379:CYS:SG	2:F:384:PRO:HG3	2.50	0.52
5:H:48:VAL:HG13	5:H:63:VAL:HG21	1.91	0.52
1:M:82:GLN:HG2	4:D:5:THR:HG21	1.92	0.52
4:D:47:LEU:HD21	4:D:50:TYR:HB3	1.91	0.52
6:K:12:VAL:HG21	6:K:18:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:GLY:HA2	4:D:37:TYR:OH	2.10	0.52
2:E:375:PHE:HB3	2:E:436:TRP:CB	2.39	0.51
3:C:91:THR:HG23	3:C:125:THR:HA	1.90	0.51
3:A:29:PHE:HE2	3:A:74:LYS:HA	1.74	0.51
6:K:16:GLN:HG2	6:K:17:THR:H	1.75	0.51
3:A:29:PHE:CE2	3:A:77:GLY:HA2	2.46	0.51
4:D:136:LEU:HD12	4:D:182:LEU:HD23	1.93	0.51
2:E:378:LYS:HD3	2:E:380:TYR:OH	2.10	0.51
4:B:84:GLU:HB2	4:B:109:VAL:HG23	1.93	0.51
5:H:50:LEU:HD11	5:H:58:PHE:HD2	1.76	0.51
6:L:4:LEU:HB2	6:L:99:GLY:HA2	1.93	0.51
6:K:114:PRO:HB3	6:K:140:PHE:HB3	1.92	0.51
6:K:91:ASP:OD2	2:F:505:HIS:NE2	2.43	0.50
5:J:6:GLU:H	5:J:109:GLN:HE22	1.58	0.50
5:J:35:THR:HG22	5:J:50:LEU:HB3	1.94	0.50
5:J:120:THR:HG22	5:J:207:SER:HB3	1.93	0.50
6:K:34:TRP:HB2	6:K:47:VAL:HB	1.93	0.50
2:F:375:PHE:HB3	2:F:436:TRP:CB	2.40	0.50
3:C:6:GLN:H	3:C:120:GLN:HE22	1.59	0.50
1:N:109:SER:HB2	2:F:408:ARG:NE	2.27	0.50
2:E:431:GLY:HA2	2:E:515:PHE:HD2	1.76	0.50
3:A:52:ILE:HG22	3:A:55:LEU:H	1.76	0.50
2:F:342:PHE:HB2	7:F:601:NAG:H82	1.93	0.50
2:F:367:VAL:HG23	2:F:371:LEU:HD22	1.93	0.50
6:L:133:LEU:HD12	6:L:179:LEU:HD23	1.93	0.50
4:B:84:GLU:HG3	4:B:107:LEU:O	2.12	0.50
4:D:11:SER:HB2	4:D:110:LEU:HD11	1.94	0.50
1:N:67:ARG:HB3	1:N:84:ASN:O	2.12	0.49
6:L:54:PRO:HG2	6:L:57:ILE:HD12	1.93	0.49
5:J:86:ARG:HD2	5:J:89:ASP:OD2	2.11	0.49
5:J:101:VAL:HB	2:F:493:ARG:NH2	2.27	0.49
2:F:449:TYR:HA	2:F:495:TYR:O	2.12	0.49
4:B:35:ASN:HB3	4:B:50:TYR:HA	1.94	0.49
2:F:496:SER:O	2:F:501:TYR:HE2	1.94	0.49
1:N:110:SER:HB3	2:F:378:LYS:HZ3	1.77	0.49
2:E:375:PHE:HB2	2:E:435:ALA:O	2.12	0.49
3:A:37:VAL:HG22	3:A:47:TRP:HA	1.95	0.49
2:F:378:LYS:HD3	2:F:380:TYR:OH	2.13	0.48
3:C:51:VAL:HG23	3:C:58:LYS:HB3	1.96	0.48
3:A:98:ARG:HG2	3:A:117:VAL:HB	1.94	0.48
5:H:22:CYS:HB3	5:H:78:LEU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:431:GLY:HA2	2:F:515:PHE:CD2	2.48	0.48
2:E:431:GLY:HA2	2:E:515:PHE:CD2	2.49	0.48
2:F:431:GLY:HA2	2:F:515:PHE:HD2	1.78	0.48
2:E:334:ASN:O	2:E:362:VAL:HG23	2.14	0.48
6:L:151:ALA:O	6:L:153:SER:N	2.46	0.48
4:D:136:LEU:HB2	4:D:182:LEU:HB3	1.94	0.48
6:K:4:LEU:HD11	6:K:89:VAL:HG13	1.94	0.48
3:A:114:GLY:H	4:B:99:ARG:HH22	1.62	0.48
2:F:334:ASN:O	2:F:334:ASN:ND2	2.36	0.48
3:C:36:TRP:CE2	3:C:81:MET:HB2	2.49	0.47
3:C:108:GLY:O	3:C:109:ARG:HD3	2.14	0.47
1:N:50:TRP:NE1	1:N:105:ASP:O	2.46	0.47
2:F:334:ASN:HA	2:F:362:VAL:HB	1.95	0.47
1:M:110:SER:HB3	2:E:378:LYS:NZ	2.29	0.47
2:F:453:TYR:OH	2:F:493:ARG:HD2	2.15	0.47
1:M:73:HIS:CE1	4:D:27:SER:HG	2.30	0.47
1:M:105:ASP:OD1	1:M:106:THR:N	2.47	0.47
2:E:367:VAL:HG23	2:E:371:LEU:HD22	1.95	0.47
6:K:90:TRP:HH2	2:F:453:TYR:OH	1.97	0.47
1:M:17[B]:SER:OG	1:M:82:GLN:NE2	2.48	0.47
4:D:4:VAL:HG13	4:D:102:GLY:HA2	1.97	0.47
2:F:375:PHE:HB2	2:F:435:ALA:O	2.14	0.47
3:A:67:ARG:O	3:A:83:LEU:HD12	2.14	0.47
4:D:187:GLU:OE1	4:D:187:GLU:N	2.48	0.47
2:E:449:TYR:OH	2:E:498:ARG:NH2	2.48	0.47
6:L:12:VAL:HG21	6:L:18:ALA:HB2	1.97	0.47
4:D:94:GLU:CD	2:F:346:ARG:HH22	2.23	0.47
3:A:47:TRP:CG	4:B:99:ARG:HB3	2.49	0.47
2:F:493:ARG:HG2	2:F:494:SER:N	2.30	0.47
3:A:89:GLU:OE1	3:A:89:GLU:N	2.48	0.46
4:B:86:ASP:OD1	4:B:106:LYS:HG2	2.15	0.46
1:N:32:TYR:CE2	1:N:53:VAL:HG21	2.51	0.46
5:H:92:VAL:HG22	5:H:112:THR:HG22	1.98	0.46
3:A:116:ASP:OD1	3:A:116:ASP:N	2.49	0.46
5:H:100:GLN:C	6:L:90:TRP:CD1	2.94	0.46
2:E:493:ARG:HG2	2:E:494:SER:N	2.31	0.46
2:E:497:PHE:CD2	2:E:507:PRO:HB3	2.51	0.46
6:L:92:SER:OG	6:L:95:ASP:O	2.33	0.46
1:M:32:TYR:CE2	1:M:53:VAL:HG21	2.52	0.46
2:F:365:TYR:O	2:F:366:SER:C	2.59	0.46
2:F:520:ALA:HB1	2:F:521:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:18:ALA:HB2	6:L:77:ILE:HD11	1.99	0.45
4:D:55:ARG:HD3	4:D:63:PHE:O	2.16	0.45
5:H:90:THR:HG23	5:H:114:THR:HA	1.98	0.45
6:K:151:ALA:O	6:K:153:SER:N	2.49	0.45
2:E:444:LYS:HZ3	4:B:97:ASN:HB2	1.82	0.45
2:E:493:ARG:HD2	5:H:101:VAL:HG21	1.99	0.45
5:J:100:GLN:OE1	5:J:100:GLN:HA	2.17	0.45
1:M:105:ASP:HB2	2:E:378:LYS:HE3	1.99	0.45
1:N:5:VAL:HB	1:N:23:ALA:HB3	1.99	0.45
1:N:99:GLY:HA3	1:N:101:PHE:CE2	2.52	0.45
4:B:3:VAL:HG11	4:B:25:SER:OG	2.17	0.45
4:B:79:LEU:HD23	4:B:79:LEU:HA	1.79	0.45
5:H:105:ASP:OD1	5:H:105:ASP:N	2.49	0.45
6:L:109:GLN:HB2	6:L:110:PRO:HD2	1.99	0.45
3:A:115:MET:HG2	4:B:37:TYR:OH	2.17	0.45
6:K:30:LYS:HD2	6:K:89:VAL:HB	1.99	0.45
3:A:12:LYS:O	3:A:126:VAL:HA	2.17	0.44
5:H:37:VAL:HG22	5:H:47:TRP:HA	1.99	0.44
2:F:374:PHE:HB3	2:F:375:PHE:CD2	2.52	0.44
6:L:60:ARG:HH22	6:L:78:GLU:CD	2.21	0.44
1:M:82:GLN:CD	4:D:5:THR:HG21	2.42	0.44
2:E:496:SER:O	2:E:501:TYR:HE2	2.00	0.44
2:E:399:SER:HA	2:E:510:VAL:O	2.18	0.44
3:C:29:PHE:HB3	3:C:53:PRO:HB2	2.00	0.44
3:C:99:ASP:OD1	3:C:115:MET:HB3	2.17	0.44
2:F:339:ASP:O	2:F:343:ASN:HB2	2.18	0.44
3:C:107:TRP:CE2	2:F:346:ARG:HG2	2.53	0.44
5:J:163:LEU:HD21	5:J:186:VAL:HG21	2.00	0.44
2:E:365:TYR:O	2:E:366:SER:C	2.61	0.44
4:B:35:ASN:HD21	4:B:90:ALA:HB3	1.82	0.44
5:J:120:THR:HG21	5:J:206:PRO:C	2.43	0.44
1:M:18:LEU:HD12	1:M:18:LEU:HA	1.85	0.43
6:K:18:ALA:HB2	6:K:77:ILE:HD11	2.00	0.43
2:E:505:HIS:HE1	6:L:91:ASP:OD1	2.00	0.43
3:C:116:ASP:OD1	3:C:116:ASP:N	2.38	0.43
6:K:53:ARG:HD3	6:K:61:PHE:O	2.17	0.43
6:K:94:ARG:NH2	2:F:408:ARG:HH11	2.17	0.43
1:M:104:ARG:NH1	2:E:375:PHE:O	2.52	0.43
4:D:29:ILE:HG22	4:D:67:LYS:HE3	2.00	0.43
6:K:33:HIS:HE2	5:J:101:VAL:C	2.22	0.43
3:A:102:HIS:HB2	3:A:113:ASP:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:2:VAL:HG11	5:H:106:VAL:HG21	2.01	0.43
3:C:67:ARG:O	3:C:83:LEU:HD12	2.18	0.43
6:K:133:LEU:HD12	6:K:179:LEU:HD23	2.01	0.43
6:L:20:ILE:HD12	6:L:72:LEU:HD23	2.01	0.43
3:C:31:SER:H	3:C:54:ILE:HG21	1.84	0.43
6:K:120:PRO:HA	6:K:133:LEU:HD23	1.99	0.43
3:A:10:GLU:O	3:A:124:VAL:HA	2.19	0.43
3:A:31:SER:H	3:A:54:ILE:HG21	1.84	0.43
3:C:25:SER:O	3:C:28:THR:OG1	2.33	0.43
3:C:89:GLU:OE1	3:C:89:GLU:N	2.47	0.43
5:J:36:TRP:CG	5:J:80:LEU:HD22	2.54	0.43
4:B:187:GLU:OE1	4:B:187:GLU:N	2.52	0.43
4:D:84:GLU:HG3	4:D:107:LEU:O	2.18	0.43
6:K:94:ARG:CZ	2:F:408:ARG:HH11	2.32	0.43
3:A:99:ASP:OD2	3:A:115:MET:HE2	2.17	0.43
3:C:161:PHE:HA	3:C:162:PRO:HA	1.79	0.42
4:B:171:GLN:OE1	4:B:177:ALA:HB2	2.19	0.42
1:M:25:SER:O	1:M:27:PHE:N	2.47	0.42
6:L:53:ARG:HD3	6:L:61:PHE:O	2.19	0.42
2:E:398:ASP:HB2	2:E:512:VAL:HB	2.01	0.42
2:E:401:VAL:HG22	2:E:509:ARG:HG2	2.00	0.42
3:A:53:PRO:HB3	3:A:74:LYS:HE2	2.02	0.42
2:F:392:PHE:HA	2:F:517:LEU:HD13	2.01	0.42
6:L:60:ARG:HB2	6:L:75:THR:O	2.19	0.42
3:C:174:LEU:HD21	3:C:197:VAL:HG21	2.01	0.42
6:K:29:ALA:HB2	2:F:501:TYR:CD2	2.53	0.42
1:M:55:ASP:OD1	2:E:383:SER:HB3	2.20	0.42
4:B:136:LEU:HD12	4:B:182:LEU:HD23	2.02	0.42
2:E:415:THR:O	6:L:94:ARG:NH2	2.53	0.42
4:B:55:ARG:HD3	4:B:63:PHE:O	2.20	0.41
6:K:33:HIS:CE1	6:K:90:TRP:HB2	2.42	0.41
5:H:104:MET:HE1	6:L:98:PHE:CZ	2.53	0.41
5:H:158:TRP:CH2	5:H:200:CYS:HB3	2.55	0.41
6:K:12:VAL:HG12	6:K:16:GLN:HB3	2.01	0.41
5:J:36:TRP:NE1	5:J:80:LEU:HB2	2.35	0.41
2:E:374:PHE:HB3	2:E:375:PHE:CD2	2.56	0.41
2:F:334:ASN:HD22	2:F:334:ASN:C	2.23	0.41
1:N:104:ARG:N	2:F:377:PHE:O	2.41	0.41
4:B:51:THR:O	4:B:53:ASN:N	2.47	0.41
4:D:28:ASP:HB3	4:D:93:ASP:HB2	2.02	0.41
6:L:109:GLN:HG2	6:L:141:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:365:TYR:CE2	2:E:385:THR:HA	2.56	0.41
3:C:224:LYS:HD2	3:C:224:LYS:HA	1.83	0.41
4:D:39:GLN:O	4:D:85:ALA:HB1	2.21	0.41
3:A:161:PHE:HA	3:A:162:PRO:HA	1.85	0.41
4:B:143:PHE:CE2	4:B:146:GLY:HA2	2.56	0.41
5:H:34:MET:HB3	5:H:78:LEU:HD22	2.03	0.41
5:J:27:ILE:HG12	2:F:487:ASN:HD21	1.86	0.41
5:J:48:VAL:HG13	5:J:63:VAL:HG21	2.03	0.41
2:F:339:ASP:N	2:F:339:ASP:OD1	2.53	0.41
2:E:333:THR:HG22	2:E:362:VAL:HG21	2.02	0.41
5:H:36:TRP:CE2	5:H:80:LEU:HB2	2.56	0.41
4:D:148:VAL:HG12	4:D:201:HIS:HB2	2.02	0.41
6:K:4:LEU:HB2	6:K:99:GLY:HA2	2.02	0.41
6:K:92:SER:HB3	6:K:95:ASP:O	2.21	0.41
2:E:347:PHE:CE1	2:E:509:ARG:HD3	2.55	0.40
2:E:350:VAL:HG22	2:E:422:ASN:HB3	2.03	0.40
4:D:117:PRO:HB3	4:D:143:PHE:HB3	2.03	0.40
5:J:32:ASN:OD1	5:J:97:ARG:HD3	2.21	0.40
5:J:204:HIS:HB3	5:J:209:THR:HB	2.02	0.40
4:B:117:PRO:HB3	4:B:143:PHE:HB3	2.02	0.40
5:H:35:THR:HG22	5:H:50:LEU:HB3	2.03	0.40
6:L:78:GLU:O	6:L:106:VAL:HG21	2.21	0.40
2:F:366:SER:O	2:F:370:ASN:HB2	2.20	0.40
2:F:370:ASN:O	2:F:371:LEU:C	2.64	0.40
3:A:48:MET:HE2	3:A:48:MET:HB3	2.00	0.40
4:D:79:LEU:HD23	4:D:79:LEU:HA	1.84	0.40
4:D:197:CYS:O	4:D:207:GLU:HA	2.22	0.40
2:E:370:ASN:O	2:E:371:LEU:C	2.64	0.40
6:L:11:SER:HB3	6:L:107:LEU:HD21	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:127:GLN:NE2	5:J:118:ALA:O[2_656]	2.15	0.05

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	M	123/131 (94%)	118 (96%)	5 (4%)	0	100	100
1	N	124/131 (95%)	118 (95%)	5 (4%)	1 (1%)	16	44
2	E	193/202 (96%)	176 (91%)	16 (8%)	1 (0%)	24	54
2	F	193/202 (96%)	173 (90%)	18 (9%)	2 (1%)	12	39
3	A	226/233 (97%)	216 (96%)	10 (4%)	0	100	100
3	C	226/233 (97%)	216 (96%)	10 (4%)	0	100	100
4	B	211/216 (98%)	192 (91%)	18 (8%)	1 (0%)	24	54
4	D	212/216 (98%)	199 (94%)	13 (6%)	0	100	100
5	H	211/222 (95%)	198 (94%)	11 (5%)	2 (1%)	14	41
5	J	211/222 (95%)	199 (94%)	8 (4%)	4 (2%)	6	24
6	K	205/213 (96%)	191 (93%)	13 (6%)	1 (0%)	24	54
6	L	206/213 (97%)	193 (94%)	12 (6%)	1 (0%)	24	54
All	All	2341/2434 (96%)	2189 (94%)	139 (6%)	13 (1%)	21	49

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	371	LEU
2	F	371	LEU
6	L	152	ASP
6	K	152	ASP
5	J	119	SER
2	F	520	ALA
4	B	113	PRO
5	H	117	SER
5	H	118	ALA
5	J	116	SER
5	J	2	VAL
5	J	41	PRO

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Mol	Chain	Res	Type
1	N	26	GLY

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	M	104/110 (94%)	103 (99%)	1 (1%)	68	77
1	N	105/110 (96%)	104 (99%)	1 (1%)	68	77
2	E	169/177 (96%)	163 (96%)	6 (4%)	31	58
2	F	169/177 (96%)	163 (96%)	6 (4%)	31	58
3	A	190/195 (97%)	188 (99%)	2 (1%)	65	76
3	C	190/195 (97%)	188 (99%)	2 (1%)	65	76
4	B	179/182 (98%)	174 (97%)	5 (3%)	38	63
4	D	179/182 (98%)	175 (98%)	4 (2%)	45	68
5	H	176/185 (95%)	173 (98%)	3 (2%)	53	71
5	J	176/185 (95%)	171 (97%)	5 (3%)	38	63
6	K	175/181 (97%)	173 (99%)	2 (1%)	65	76
6	L	176/181 (97%)	172 (98%)	4 (2%)	44	67
All	All	1988/2060 (96%)	1947 (98%)	41 (2%)	47	68

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	62	ASP
1	N	62	ASP
2	E	359	SER
2	E	362	VAL
2	E	367	VAL
2	E	368	LEU
2	E	371	LEU
2	E	375	PHE
3	A	59	HIS

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Mol	Chain	Res	Type
3	A	110	PHE
4	B	3	VAL
4	B	34	VAL
4	B	35	ASN
4	B	39	GLN
4	B	110	LEU
5	H	86	ARG
5	H	119	SER
5	H	121	LYS
6	L	3	GLU
6	L	92	SER
6	L	93	SER
6	L	163	THR
3	C	59	HIS
3	C	110	PHE
4	D	3	VAL
4	D	34	VAL
4	D	35	ASN
4	D	39	GLN
6	K	89	VAL
6	K	163	THR
5	J	12	ILE
5	J	86	ARG
5	J	100	GLN
5	J	102	TYR
5	J	119	SER
2	F	334	ASN
2	F	362	VAL
2	F	367	VAL
2	F	368	LEU
2	F	371	LEU
2	F	375	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	39	GLN
1	M	82	GLN
1	N	39	GLN
2	E	505	HIS
4	B	38	GLN
5	H	175	GLN

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Mol	Chain	Res	Type
3	C	62	GLN
4	D	112	GLN
4	D	132	ASN
6	K	171	ASN
2	F	354	ASN

5.3.3 RNA [i](#)

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](#)

2 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	$\# Z > 2$
7	NAG	F	601	2	14,14,15	0.25	0	17,19,21	0.47	0
7	NAG	E	601	2	14,14,15	0.75	1 (7%)	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
7	NAG	F	601	2	-	0/6/23/26	0/1/1/1
7	NAG	E	601	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	601	NAG	C1-C2	2.43	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	601	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	M	123/131 (93%)	-0.23	0 100 100	119, 162, 210, 244	2 (1%)
1	N	124/131 (94%)	-0.16	2 (1%) 70 47	168, 266, 334, 387	2 (1%)
2	E	195/202 (96%)	-0.05	6 (3%) 51 29	105, 143, 240, 297	0
2	F	195/202 (96%)	0.26	18 (9%) 14 8	104, 176, 294, 332	0
3	A	228/233 (97%)	-0.18	3 (1%) 75 53	103, 182, 255, 331	0
3	C	228/233 (97%)	-0.30	3 (1%) 75 53	110, 157, 264, 342	0
4	B	212/216 (98%)	-0.15	4 (1%) 66 44	92, 170, 257, 330	1 (0%)
4	D	213/216 (98%)	-0.23	5 (2%) 61 38	96, 143, 204, 296	1 (0%)
5	H	215/222 (96%)	-0.08	8 (3%) 45 25	112, 173, 229, 293	0
5	J	215/222 (96%)	-0.29	2 (0%) 81 61	104, 156, 208, 243	0
6	K	207/213 (97%)	-0.12	4 (1%) 66 44	122, 180, 238, 355	0
6	L	208/213 (97%)	-0.29	0 100 100	126, 180, 256, 313	0
All	All	2363/2434 (97%)	-0.15	55 (2%) 61 38	92, 169, 270, 387	6 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	410	ILE	7.9
3	A	110	PHE	6.0
2	E	435	ALA	5.6
2	F	402	ILE	4.6
3	A	45	LEU	4.3
2	F	407	VAL	4.3
2	F	347	PHE	3.8
2	F	342	PHE	3.7
2	F	341	VAL	3.7
5	H	48	VAL	3.6
2	E	513	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	F	400	PHE	3.4
2	F	433	VAL	3.3
2	F	511	VAL	3.3
2	E	417	ASN	3.3
2	F	436	TRP	3.3
3	C	33	GLY	3.2
2	E	410	ILE	3.1
4	B	48	LEU	3.1
6	K	134	VAL	3.1
2	F	510	VAL	3.1
4	D	90	ALA	3.0
5	J	123	PRO	3.0
2	F	423	TYR	3.0
4	B	101	PHE	2.9
2	F	434	ILE	2.9
2	F	508	TYR	2.8
5	J	183	SER	2.8
2	F	435	ALA	2.8
2	E	434	ILE	2.8
2	F	401	VAL	2.8
4	D	101	PHE	2.7
4	D	89	CYS	2.6
5	H	55	GLY	2.6
4	B	2	SER	2.5
4	D	146	GLY	2.5
2	F	509	ARG	2.4
1	N	70	ILE	2.4
5	H	49	SER	2.4
3	A	48	MET	2.3
5	H	145	LEU	2.3
1	N	71	SER	2.3
3	C	64	PHE	2.3
5	H	100	GLN	2.3
4	B	91	ALA	2.2
3	C	45	LEU	2.2
2	E	490	PHE	2.2
6	K	98	PHE	2.2
5	H	34	MET	2.1
6	K	149	TRP	2.1
4	D	107	LEU	2.1
5	H	107	TRP	2.0
5	H	57	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
6	K	110	PRO	2.0
2	F	455	LEU	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
7	NAG	E	601	14/15	0.49	0.14	170,252,277,310	0
7	NAG	F	601	14/15	0.67	0.07	183,222,238,245	0

6.5 Other polymers [i](#)

There are no such residues in this entry.