



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:58 AM UTC

PDB ID : 6SVL / pdb_00006svl
Title : human Myeloid-derived growth factor (MYDGF) in complex with neutralizing Fab
Authors : Ebenhoch, R.; Nar, H.
Deposited on : 2019-09-18
Resolution : 1.58 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

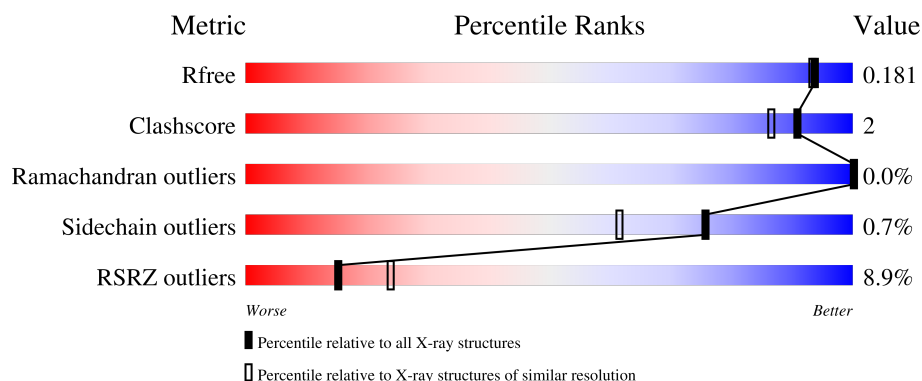
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	244	12% 80% 5% 13%
1	D	244	3% 83% 13%
1	G	244	2% 85% 12%
1	H	244	10% 84% 13%
1	K	244	2% 83% 13%

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Mol	Chain	Length	Quality of chain
1	O	244	
2	B	234	
2	E	234	
2	I	234	
2	L	234	
2	M	234	
2	P	234	
3	C	142	
3	F	142	
3	J	142	
3	N	142	
3	Q	142	
3	R	142	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27628 atoms, of which 24 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 Fab_heavy_chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	4	0
			1645	1036	274	329	6			
1	D	213	Total	C	N	O	S	0	2	0
			1636	1031	273	324	8			
1	G	215	Total	C	N	O	S	0	1	0
			1640	1033	274	326	7			
1	H	213	Total	C	N	O	S	0	1	0
			1630	1028	272	323	7			
1	K	213	Total	C	N	O	S	0	0	0
			1622	1023	271	322	6			
1	O	213	Total	C	N	O	S	0	1	0
			1630	1028	272	323	7			

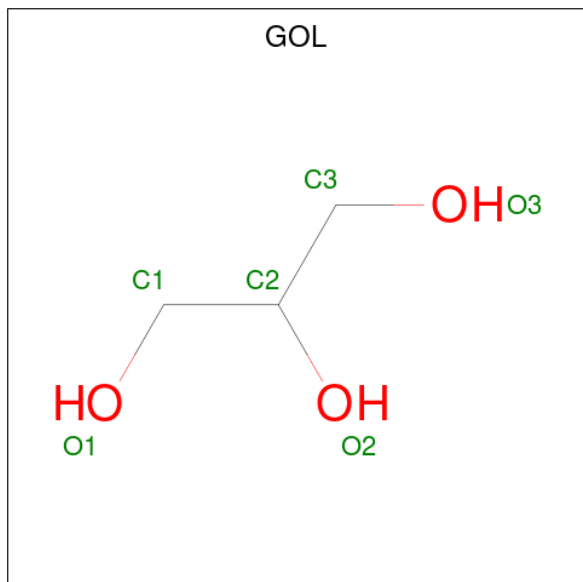
- Molecule 2 is a protein called Fab_light_chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	1	0
			1628	1023	271	329	5			
2	E	212	Total	C	N	O	S	0	0	0
			1638	1028	275	330	5			
2	I	212	Total	C	N	O	S	0	0	0
			1638	1028	275	330	5			
2	L	212	Total	C	N	O	S	0	0	0
			1638	1028	275	330	5			
2	M	212	Total	C	N	O	S	0	0	0
			1638	1028	275	330	5			
2	P	191	Total	C	N	O	S	0	0	0
			1458	914	242	297	5			

- Molecule 3 is a protein called Myeloid-derived growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	95	Total	C	N	O	S	0	0	0
			747	484	124	134	5			
3	F	116	Total	C	N	O	S	0	0	0
			903	579	151	168	5			
3	J	126	Total	C	N	O	S	0	0	0
			995	633	169	188	5			
3	N	123	Total	C	N	O	S	0	1	0
			981	630	164	182	5			
3	Q	123	Total	C	N	O	S	0	0	0
			972	624	163	180	5			
3	R	120	Total	C	N	O	S	0	0	0
			943	606	158	174	5			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	M	1	Total	C	H	O	0	0
			14	3	8	3		
4	R	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is water.

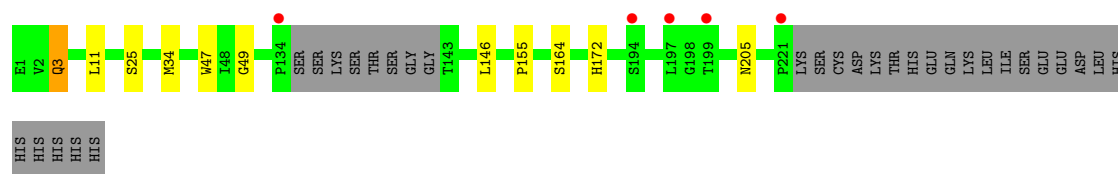
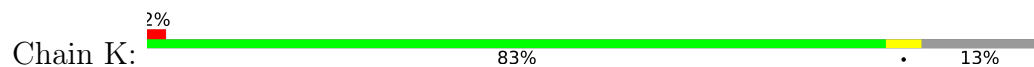
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	156	Total	O	0	0
			156	156		

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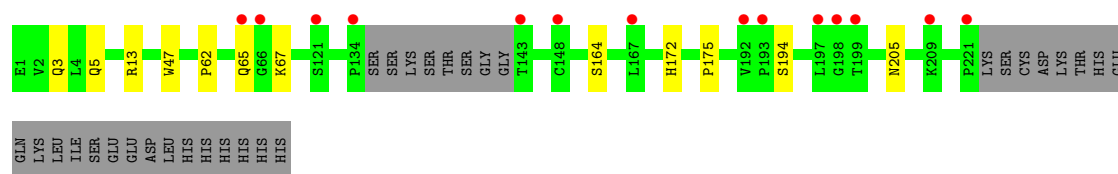
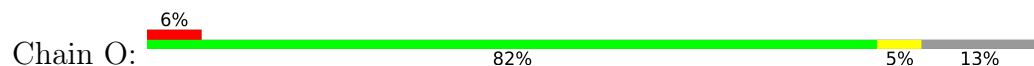
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	116	Total 116	O 116	0	0
5	C	26	Total 26	O 26	0	0
5	D	216	Total 216	O 216	0	0
5	E	172	Total 172	O 172	0	0
5	F	44	Total 44	O 44	0	0
5	G	204	Total 204	O 204	0	0
5	H	181	Total 181	O 181	0	0
5	I	237	Total 237	O 237	0	0
5	J	92	Total 92	O 92	0	0
5	K	196	Total 196	O 196	0	0
5	L	163	Total 163	O 163	0	0
5	M	227	Total 227	O 227	0	0
5	N	53	Total 53	O 53	0	0
5	O	191	Total 191	O 191	0	0
5	P	173	Total 173	O 173	0	0
5	Q	87	Total 87	O 87	0	0
5	R	70	Total 70	O 70	0	0

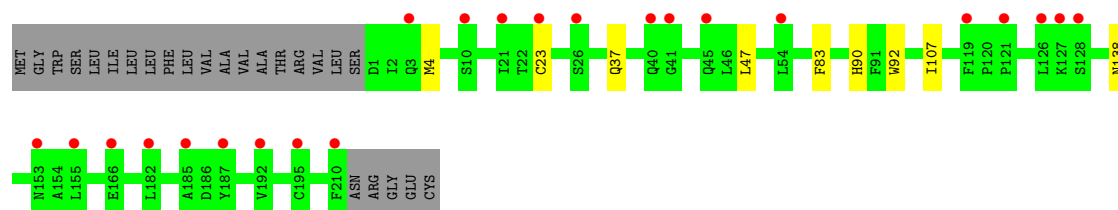
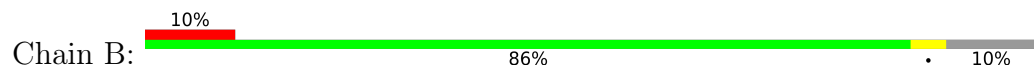
- Molecule 1: Fab_heavy_chain



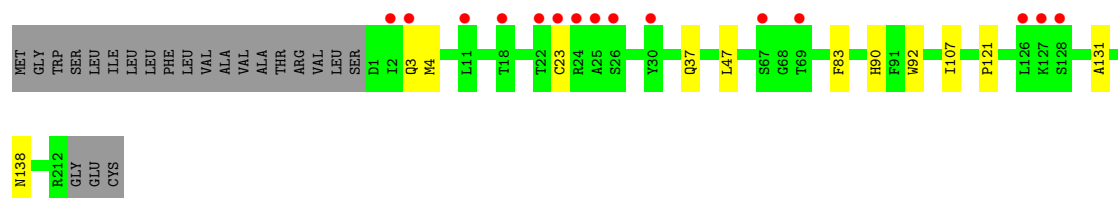
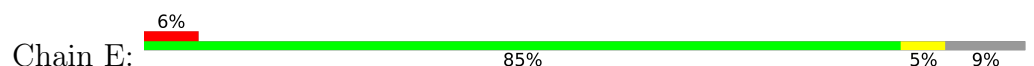
- Molecule 1: Fab_heavy_chain



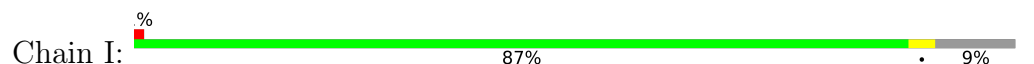
- Molecule 2: Fab_light_chain



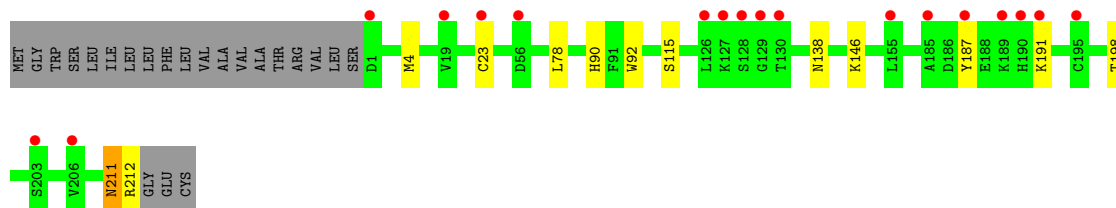
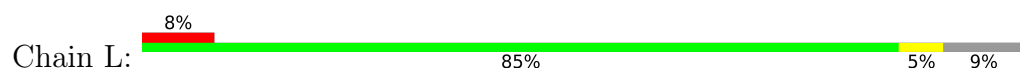
- Molecule 2: Fab_light_chain



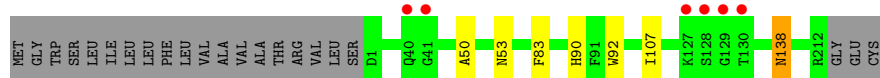
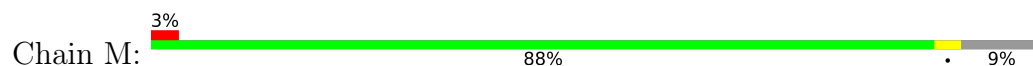
- Molecule 2: Fab_light_chain



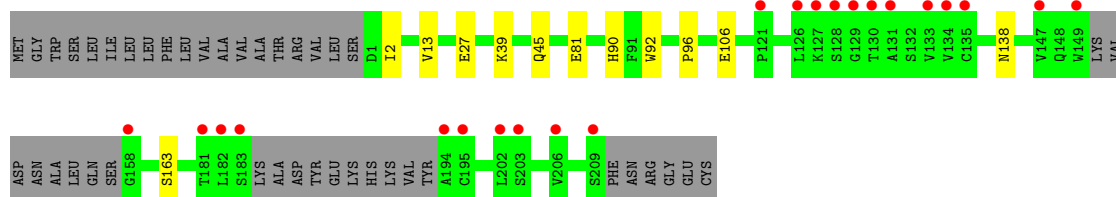
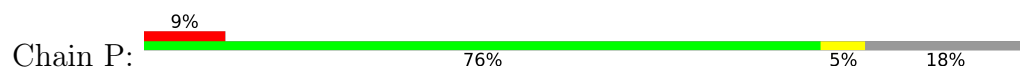
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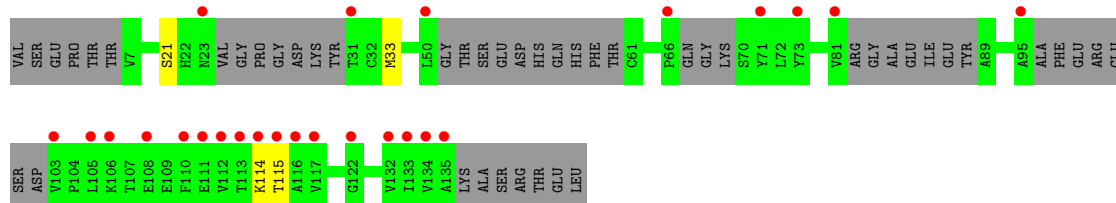
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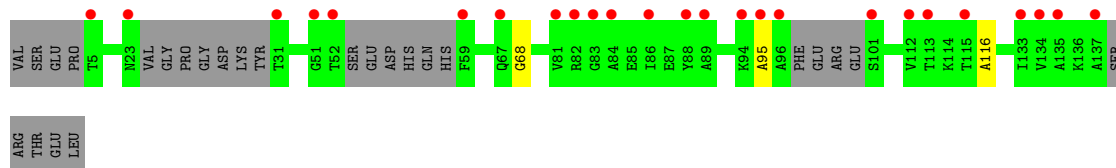
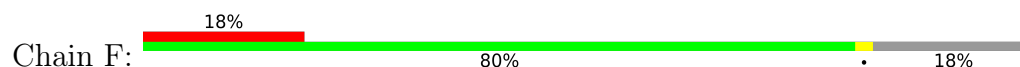
- Molecule 2: Fab_light_chain



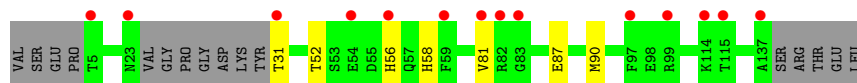
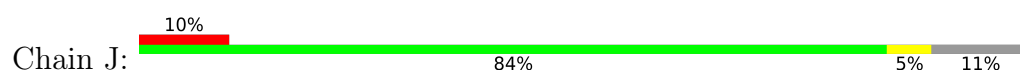
- Molecule 3: Myeloid-derived growth factor



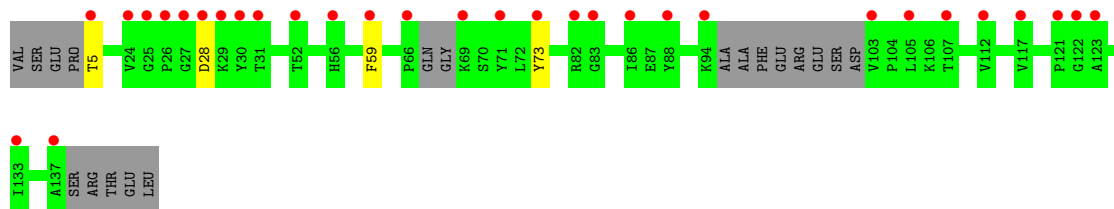
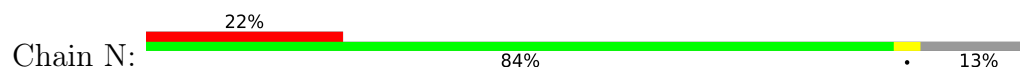
- Molecule 3: Myeloid-derived growth factor



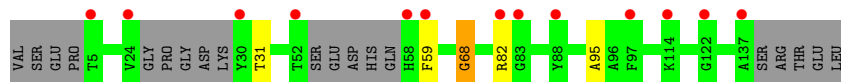
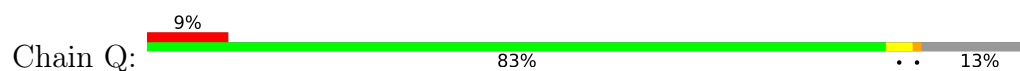
- Molecule 3: Myeloid-derived growth factor



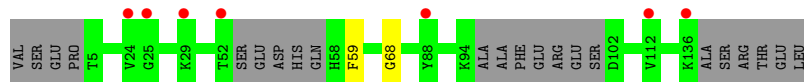
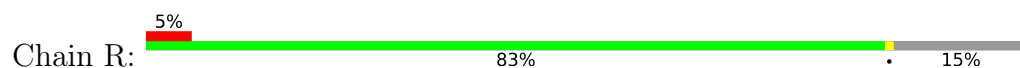
- Molecule 3: Myeloid-derived growth factor



- Molecule 3: Myeloid-derived growth factor



- Molecule 3: Myeloid-derived growth factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	89.52Å 107.43Å 109.37Å 71.54° 86.25° 73.38°	Depositor
Resolution (Å)	97.82 – 1.58 97.82 – 1.58	Depositor EDS
% Data completeness (in resolution range)	62.6 (97.82-1.58) 63.1 (97.82-1.58)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.58Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.181 , 0.206 0.183 , 0.181	Depositor DCC
R_{free} test set	16198 reflections (3.17%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27628	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.35% 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: GOL

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	0.73	0/1685	0.97	2/2298 (0.1%)
1	D	0.76	0/1676	0.97	1/2285 (0.0%)
1	G	0.79	0/1680	0.97	2/2290 (0.1%)
1	H	0.79	0/1670	0.99	3/2277 (0.1%)
1	K	0.80	1/1662 (0.1%)	0.96	0/2267
1	O	0.82	0/1670	0.99	1/2277 (0.0%)
2	B	0.73	0/1666	0.97	0/2265
2	E	0.80	0/1676	0.96	0/2278
2	I	0.82	0/1676	0.95	0/2278
2	L	0.79	0/1676	0.98	1/2278 (0.0%)
2	M	0.82	0/1676	0.98	0/2278
2	P	0.82	0/1490	0.99	1/2026 (0.0%)
3	C	0.67	0/763	1.06	2/1027 (0.2%)
3	F	0.65	0/923	1.03	1/1245 (0.1%)
3	J	0.78	1/1020 (0.1%)	1.03	0/1378
3	N	0.70	0/1007	1.06	3/1361 (0.2%)
3	Q	0.72	0/996	1.06	2/1345 (0.1%)
3	R	0.75	0/967	1.08	2/1306 (0.2%)
All	All	0.77	2/25579 (0.0%)	0.99	21/34759 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	90	MET	SD-CE	-5.67	1.65	1.79
1	K	34	MET	SD-CE	5.07	1.92	1.79

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	PHE	CA-CB-CG	-7.25	106.55	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	64	PHE	CA-CB-CG	-7.15	106.65	113.80
3	Q	68	GLY	N-CA-C	6.56	122.88	115.08
3	C	114	LYS	CA-C-N	6.00	133.00	121.54
3	C	114	LYS	C-N-CA	6.00	133.00	121.54
3	N	59	PHE	CA-CB-CG	5.79	119.59	113.80
1	O	67	LYS	N-CA-C	-5.76	106.29	113.55
3	R	59	PHE	CA-CB-CG	5.75	119.55	113.80
3	R	68	GLY	N-CA-C	5.74	122.97	115.40
1	A	89	GLU	CB-CG-CD	5.59	122.10	112.60
3	Q	59	PHE	CA-CB-CG	5.53	119.33	113.80
1	H	163	ASN	CA-C-N	5.51	131.91	123.47
1	H	163	ASN	C-N-CA	5.51	131.91	123.47
2	L	115	SER	N-CA-C	-5.39	100.52	109.46
3	N	28	ASP	CA-C-N	5.29	127.37	120.28
3	N	28	ASP	C-N-CA	5.29	127.37	120.28
1	G	61	ASP	N-CA-C	-5.23	101.81	109.50
2	P	45	GLN	CB-CG-CD	5.08	121.24	112.60
3	F	116	ALA	N-CA-C	5.04	116.85	109.24
1	G	109	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	64	PHE	CA-CB-CG	-5.02	108.78	113.80

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	1645	0	1582	12	0
1	D	1636	0	1580	6	0
1	G	1640	0	1585	6	0
1	H	1630	0	1577	7	0
1	K	1622	0	1569	7	0
1	O	1630	0	1577	9	0
2	B	1628	0	1567	7	0
2	E	1638	0	1579	7	0
2	I	1638	0	1579	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1638	0	1579	8	0
2	M	1638	0	1579	6	0
2	P	1458	0	1400	7	0
3	C	747	0	726	1	0
3	F	903	0	877	1	0
3	J	995	0	950	2	0
3	N	981	0	941	1	0
3	Q	972	0	937	2	0
3	R	943	0	913	0	0
4	E	6	8	8	0	0
4	M	6	8	8	0	0
4	R	6	8	8	0	0
5	A	156	0	0	0	0
5	B	116	0	0	0	0
5	C	26	0	0	0	0
5	D	216	0	0	0	0
5	E	172	0	0	0	0
5	F	44	0	0	0	0
5	G	204	0	0	0	0
5	H	181	0	0	0	0
5	I	237	0	0	0	0
5	J	92	0	0	0	0
5	K	196	0	0	0	0
5	L	163	0	0	0	0
5	M	227	0	0	0	0
5	N	53	0	0	0	0
5	O	191	0	0	0	0
5	P	173	0	0	0	0
5	Q	87	0	0	0	0
5	R	70	0	0	0	0
All	All	27604	24	24121	82	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 2.

All (82) 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:18[B]:VAL:HG23	1:A:86:LEU:HD11	1.57	0.85
2:L:90:HIS:HD2	2:L:92:TRP:H	1.30	0.79
2:M:90:HIS:HD2	2:M:92:TRP:H	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:SER:H	1:D:205:ASN:HD21	1.34	0.75
2:P:90:HIS:HD2	2:P:92:TRP:H	1.35	0.75
2:I:90:HIS:HD2	2:I:92:TRP:H	1.34	0.75
2:E:90:HIS:HD2	2:E:92:TRP:H	1.32	0.74
1:O:164:SER:H	1:O:205:ASN:HD21	1.36	0.74
1:A:172:HIS:CD2	2:B:138:ASN:HD21	2.07	0.73
1:H:164:SER:H	1:H:205:ASN:HD21	1.39	0.71
1:K:164:SER:H	1:K:205:ASN:HD21	1.38	0.70
1:G:164:SER:H	1:G:205:ASN:HD21	1.36	0.70
1:A:172:HIS:HD2	2:B:138:ASN:HD21	1.39	0.70
2:B:90:HIS:HD2	2:B:92:TRP:H	1.38	0.70
1:A:150:VAL:HG11	1:A:158:VAL:HG11	1.75	0.68
1:A:164:SER:H	1:A:205:ASN:HD21	1.45	0.63
1:H:172:HIS:HD2	2:L:138:ASN:HD21	1.51	0.58
2:L:187:TYR:CZ	2:L:212:ARG:HD2	2.38	0.58
2:M:90:HIS:CD2	2:M:92:TRP:H	2.19	0.57
3:C:21:SER:HB3	3:C:33:MET:HG3	1.86	0.57
1:H:172:HIS:CD2	2:L:138:ASN:HD21	2.21	0.57
1:G:12:VAL:HG11	1:G:18:VAL:HG13	1.86	0.57
2:L:90:HIS:CD2	2:L:92:TRP:H	2.18	0.57
1:G:12:VAL:HG11	1:G:18:VAL:CG1	2.34	0.56
1:A:38:LYS:HB3	1:A:46[B]:GLU:HG3	1.86	0.56
3:F:68:GLY:HA2	3:F:95:ALA:HB3	1.87	0.56
1:G:172:HIS:CD2	2:I:138:ASN:HD21	2.24	0.55
2:E:90:HIS:CD2	2:E:92:TRP:H	2.19	0.54
2:B:90:HIS:CD2	2:B:92:TRP:H	2.23	0.54
1:K:3:GLN:HG2	1:K:25:SER:HB2	1.89	0.54
1:K:172:HIS:CD2	2:M:138:ASN:HD21	2.26	0.54
2:I:90:HIS:CD2	2:I:92:TRP:H	2.21	0.53
1:A:12:VAL:HG21	1:A:18[B]:VAL:CG2	2.40	0.52
1:G:172:HIS:HD2	2:I:138:ASN:HD21	1.58	0.52
2:P:39:LYS:HE2	2:P:81:GLU:O	2.09	0.52
1:A:131:PRO:HD3	1:A:217:LYS:HE3	1.90	0.51
1:H:164:SER:H	1:H:205:ASN:ND2	2.08	0.51
3:Q:31:THR:HB	3:Q:82:ARG:HB2	1.93	0.51
2:E:4:MET:HE3	2:E:23:CYS:SG	2.50	0.51
1:D:64:PHE:O	1:D:67:LYS:HB2	2.11	0.51
3:J:58:HIS:HD2	3:J:87:GLU:OE1	1.94	0.50
2:L:4:MET:HE3	2:L:23:CYS:SG	2.52	0.49
2:M:50:ALA:HB3	2:M:53:ASN:HD22	1.76	0.49
1:D:164:SER:H	1:D:205:ASN:ND2	2.07	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:PHE:HB3	2:B:107:ILE:HG12	1.95	0.49
1:H:3:GLN:HE21	1:H:5:GLN:HG2	1.78	0.49
2:L:191:LYS:HE2	2:L:211:ASN:HD21	1.77	0.48
2:I:4:MET:HE3	2:I:23:CYS:SG	2.52	0.48
1:O:62:PRO:HA	1:O:65:GLN:HG2	1.95	0.48
1:A:12:VAL:HG11	1:A:18[A]:VAL:CG1	2.44	0.47
1:O:164:SER:H	1:O:205:ASN:ND2	2.08	0.47
1:D:38:LYS:HB2	1:D:48:ILE:HD11	1.95	0.46
1:K:164:SER:H	1:K:205:ASN:ND2	2.11	0.46
1:K:11:LEU:HB2	1:K:155:PRO:HG3	1.96	0.46
1:H:5:GLN:HA	1:O:3:GLN:HE22	1.81	0.46
1:O:172:HIS:HD2	2:P:138:ASN:HD21	1.64	0.45
3:Q:68:GLY:HA2	3:Q:95:ALA:HB3	1.98	0.45
1:O:3:GLN:HE21	1:O:5:GLN:HG2	1.81	0.45
2:B:4:MET:HE3	2:B:23:CYS:SG	2.58	0.44
2:M:83:PHE:HB3	2:M:107:ILE:HG12	2.00	0.44
2:E:83:PHE:HB3	2:E:107:ILE:HG12	1.99	0.43
3:J:52:THR:HG22	3:J:56:HIS:HA	2.01	0.43
1:A:12:VAL:HG21	1:A:18[B]:VAL:HG21	2.01	0.42
2:B:37:GLN:HB2	2:B:47:LEU:HD11	2.00	0.42
1:A:18[B]:VAL:HG23	1:A:86:LEU:CD1	2.39	0.42
2:I:83:PHE:HB3	2:I:107:ILE:HG12	2.02	0.42
2:E:37:GLN:HB2	2:E:47:LEU:HD11	2.00	0.42
1:G:164:SER:H	1:G:205:ASN:ND2	2.12	0.41
1:O:47:TRP:CZ3	2:P:96:PRO:HA	2.55	0.41
1:H:3:GLN:NE2	1:H:5:GLN:HG2	2.35	0.41
2:I:83:PHE:HE2	2:I:166:GLU:CD	2.28	0.41
1:D:172:HIS:CD2	2:E:138:ASN:HD21	2.39	0.41
2:L:146:LYS:HB3	2:L:198:THR:HB	2.03	0.41
1:K:47:TRP:CH2	1:K:49:GLY:HA2	2.56	0.41
3:N:73[A]:TYR:HE1	1:O:13:ARG:HH21	1.68	0.41
2:P:90:HIS:CD2	2:P:92:TRP:H	2.26	0.41
1:O:175:PRO:HD2	2:P:163:SER:OG	2.21	0.40
1:D:47:TRP:CH2	1:D:49:GLY:HA2	2.56	0.40
1:A:64:PHE:O	1:A:67:LYS:HB2	2.21	0.40
2:E:121:PRO:HG3	2:E:131:ALA:HB1	2.04	0.40
1:K:172:HIS:HD2	2:M:138:ASN:HD21	1.70	0.40
2:P:2:ILE:HG12	2:P:27:GLU:HG2	2.04	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	212/244 (87%)	210 (99%)	2 (1%)	0	100	100
1	D	211/244 (86%)	209 (99%)	2 (1%)	0	100	100
1	G	212/244 (87%)	210 (99%)	2 (1%)	0	100	100
1	H	210/244 (86%)	210 (100%)	0	0	100	100
1	K	209/244 (86%)	208 (100%)	1 (0%)	0	100	100
1	O	210/244 (86%)	208 (99%)	2 (1%)	0	100	100
2	B	209/234 (89%)	205 (98%)	4 (2%)	0	100	100
2	E	210/234 (90%)	206 (98%)	4 (2%)	0	100	100
2	I	210/234 (90%)	207 (99%)	3 (1%)	0	100	100
2	L	210/234 (90%)	207 (99%)	3 (1%)	0	100	100
2	M	210/234 (90%)	207 (99%)	3 (1%)	0	100	100
2	P	185/234 (79%)	182 (98%)	3 (2%)	0	100	100
3	C	83/142 (58%)	81 (98%)	1 (1%)	1 (1%)	10	1
3	F	108/142 (76%)	107 (99%)	1 (1%)	0	100	100
3	J	122/142 (86%)	118 (97%)	4 (3%)	0	100	100
3	N	118/142 (83%)	116 (98%)	2 (2%)	0	100	100
3	Q	117/142 (82%)	114 (97%)	3 (3%)	0	100	100
3	R	114/142 (80%)	111 (97%)	3 (3%)	0	100	100
All	All	3160/3720 (85%)	3116 (99%)	43 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	115	THR

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	185/211 (88%)	182 (98%)	3 (2%)	55	28
1	D	184/211 (87%)	183 (100%)	1 (0%)	81	70
1	G	184/211 (87%)	183 (100%)	1 (0%)	81	70
1	H	183/211 (87%)	180 (98%)	3 (2%)	55	28
1	K	182/211 (86%)	180 (99%)	2 (1%)	65	43
1	O	183/211 (87%)	182 (100%)	1 (0%)	81	70
2	B	184/203 (91%)	184 (100%)	0	100	100
2	E	185/203 (91%)	184 (100%)	1 (0%)	81	70
2	I	185/203 (91%)	185 (100%)	0	100	100
2	L	185/203 (91%)	183 (99%)	2 (1%)	65	43
2	M	185/203 (91%)	184 (100%)	1 (0%)	81	70
2	P	166/203 (82%)	164 (99%)	2 (1%)	63	40
3	C	79/118 (67%)	79 (100%)	0	100	100
3	F	94/118 (80%)	94 (100%)	0	100	100
3	J	104/118 (88%)	102 (98%)	2 (2%)	50	21
3	N	103/118 (87%)	102 (99%)	1 (1%)	68	49
3	Q	101/118 (86%)	101 (100%)	0	100	100
3	R	99/118 (84%)	99 (100%)	0	100	100
All	All	2771/3192 (87%)	2751 (99%)	20 (1%)	76	61

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	43	GLN
1	A	158	VAL
1	D	65	GLN
2	E	3	GLN
1	G	12	VAL

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Mol	Chain	Res	Type
1	H	12	VAL
1	H	164	SER
1	H	187	SER
3	J	31	THR
3	J	81	VAL
1	K	3	GLN
1	K	146	LEU
2	L	78	LEU
2	L	211	ASN
2	M	138	ASN
3	N	5	THR
1	O	194	SER
2	P	13	VAL
2	P	106	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	207	ASN
2	B	79	GLN
2	B	85	ASN
2	B	90	HIS
2	B	138	ASN
2	B	153	ASN
3	C	39	GLN
1	D	205	ASN
1	D	207	ASN
2	E	37	GLN
2	E	40	GLN
2	E	53	ASN
2	E	79	GLN
2	E	85	ASN
2	E	90	HIS
2	E	138	ASN
2	E	139	ASN
2	E	161	GLN
1	G	205	ASN
1	G	207	ASN
1	H	3	GLN
1	H	5	GLN
1	H	205	ASN

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Mol	Chain	Res	Type
1	H	207	ASN
2	I	32	ASN
2	I	37	GLN
2	I	40	GLN
2	I	53	ASN
2	I	79	GLN
2	I	85	ASN
2	I	90	HIS
2	I	138	ASN
2	I	153	ASN
2	I	161	GLN
3	J	58	HIS
1	K	82	GLN
1	K	205	ASN
1	K	207	ASN
2	L	37	GLN
2	L	85	ASN
2	L	90	HIS
2	L	138	ASN
2	L	211	ASN
2	M	37	GLN
2	M	40	GLN
2	M	53	ASN
2	M	85	ASN
2	M	90	HIS
2	M	138	ASN
3	N	39	GLN
3	N	58	HIS
1	O	3	GLN
1	O	5	GLN
1	O	58	ASN
1	O	205	ASN
1	O	207	ASN
2	P	53	ASN
2	P	70	GLN
2	P	85	ASN
2	P	90	HIS
2	P	138	ASN
2	P	161	GLN
3	Q	58	HIS
3	Q	67	GLN
3	R	39	GLN

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Mol	Chain	Res	Type
3	R	47	GLN
3	R	58	HIS

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](#)

3 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	$\# Z > 2$
4	GOL	R	201	-	5,5,5	0.28	0	5,5,5	0.60	0
4	GOL	M	301	-	5,5,5	0.29	0	5,5,5	0.35	0
4	GOL	E	301	-	5,5,5	0.20	0	5,5,5	0.49	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
4	GOL	R	201	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	M	301	-	-	0/4/4/4	-
4	GOL	E	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	212/244 (86%)	0.71	30 (14%) 6 10	10, 32, 63, 74	4 (1%)
1	D	213/244 (87%)	0.10	8 (3%) 44 55	9, 24, 45, 60	2 (0%)
1	G	215/244 (88%)	0.16	5 (2%) 61 72	9, 24, 47, 58	1 (0%)
1	H	213/244 (87%)	0.43	24 (11%) 10 15	7, 29, 62, 83	1 (0%)
1	K	213/244 (87%)	0.21	5 (2%) 61 72	13, 23, 55, 61	0
1	O	213/244 (87%)	0.33	14 (6%) 24 33	7, 28, 60, 76	1 (0%)
2	B	210/234 (89%)	0.87	23 (10%) 10 17	16, 37, 72, 88	1 (0%)
2	E	212/234 (90%)	0.45	15 (7%) 22 31	15, 31, 58, 72	0
2	I	212/234 (90%)	-0.02	2 (0%) 81 86	14, 22, 41, 65	0
2	L	212/234 (90%)	0.58	18 (8%) 16 25	14, 32, 62, 84	0
2	M	212/234 (90%)	0.04	6 (2%) 55 67	13, 22, 48, 69	0
2	P	191/234 (81%)	0.51	22 (11%) 9 15	13, 26, 59, 80	0
3	C	95/142 (66%)	1.48	25 (26%) 1 2	25, 52, 80, 107	0
3	F	116/142 (81%)	1.33	25 (21%) 2 4	24, 46, 82, 107	0
3	J	126/142 (88%)	0.59	14 (11%) 10 16	17, 28, 63, 77	0
3	N	123/142 (86%)	1.20	31 (25%) 1 2	15, 45, 79, 87	1 (0%)
3	Q	123/142 (86%)	0.60	13 (10%) 11 18	15, 28, 55, 78	0
3	R	120/142 (84%)	0.47	7 (5%) 29 39	14, 28, 62, 70	0
All	All	3231/3720 (86%)	0.48	287 (8%) 15 24	7, 29, 64, 107	11 (0%)

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	24	VAL	8.8
3	F	96	ALA	7.5
3	C	135	ALA	7.3

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Mol	Chain	Res	Type	RSRZ
1	G	198	GLY	7.2
3	F	95	ALA	6.3
2	P	183	SER	6.2
3	N	137	ALA	6.1
3	F	59	PHE	6.0
3	C	95	ALA	5.8
3	Q	137	ALA	5.8
3	C	81	VAL	5.6
3	F	52	THR	5.5
3	J	137	ALA	5.5
3	Q	30	TYR	5.3
3	C	50	LEU	4.9
3	F	88	TYR	4.9
1	G	199	THR	4.9
2	P	209	SER	4.7
3	F	137	ALA	4.7
3	J	81	VAL	4.4
1	A	201	THR	4.4
1	H	197	LEU	4.4
2	E	23	CYS	4.4
2	P	126	LEU	4.3
1	A	197	LEU	4.2
2	B	210	PHE	4.2
3	Q	59	PHE	4.2
3	J	23	ASN	4.1
3	F	5	THR	4.1
3	C	103	VAL	4.0
2	P	149	TRP	4.0
1	O	221	PRO	4.0
2	B	185	ALA	4.0
3	F	31	THR	4.0
1	A	134	PRO	3.9
3	Q	52	THR	3.8
3	J	5	THR	3.8
3	C	133	ILE	3.8
3	Q	88	TYR	3.8
3	Q	97	PHE	3.7
1	H	221	PRO	3.7
3	J	83	GLY	3.7
3	F	89	ALA	3.7
1	A	144	ALA	3.6
3	N	5	THR	3.6

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Mol	Chain	Res	Type	RSRZ
3	J	97	PHE	3.6
2	P	181	THR	3.6
3	C	31	THR	3.6
2	B	155	LEU	3.6
1	A	219	VAL	3.6
3	N	59	PHE	3.6
2	P	147	VAL	3.5
3	J	59	PHE	3.5
3	C	115	THR	3.5
2	P	195	CYS	3.5
2	P	194	ALA	3.5
3	C	134	VAL	3.5
3	N	24	VAL	3.5
1	H	196	SER	3.4
1	O	197	LEU	3.4
3	J	31	THR	3.4
2	E	3	GLN	3.4
1	A	148	CYS	3.4
3	R	52	THR	3.4
1	K	134	PRO	3.4
3	N	105	LEU	3.4
2	M	127	LYS	3.3
3	C	23	ASN	3.3
3	C	73	TYR	3.3
2	P	158	GLY	3.3
3	C	105	LEU	3.3
3	N	112	VAL	3.3
1	A	221	PRO	3.3
1	K	221	PRO	3.3
3	C	66	PRO	3.3
3	N	121	PRO	3.3
1	D	221	PRO	3.2
2	P	131	ALA	3.2
3	F	84	ALA	3.2
3	F	83	GLY	3.2
3	F	86	ILE	3.2
3	N	86	ILE	3.2
3	N	66	PRO	3.2
1	O	65	GLN	3.1
3	R	24	VAL	3.1
3	N	71	TYR	3.1
1	O	66	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
3	N	27	GLY	3.1
3	N	82	ARG	3.1
2	P	129	GLY	3.1
3	N	94	LYS	3.1
3	C	113	THR	3.0
3	F	23	ASN	3.0
1	A	199	THR	3.0
2	B	128	SER	3.0
2	B	192	VAL	3.0
1	H	193	PRO	3.0
3	N	25	GLY	3.0
1	A	167	LEU	3.0
2	L	155	LEU	3.0
3	C	112	VAL	3.0
3	F	112	VAL	3.0
3	N	88	TYR	3.0
3	R	29	LYS	3.0
1	H	166	ALA	2.9
2	L	185	ALA	2.9
3	C	116	ALA	2.9
3	C	114	LYS	2.9
3	N	122	GLY	2.9
2	M	128	SER	2.9
1	H	203	ILE	2.9
3	N	73[A]	TYR	2.9
3	N	133	ILE	2.8
3	F	101	SER	2.8
2	B	182	LEU	2.8
1	A	194	SER	2.8
1	A	196	SER	2.8
1	O	143	THR	2.8
3	F	115	THR	2.8
3	N	52	THR	2.8
2	B	126	LEU	2.8
2	P	202	LEU	2.8
2	B	45[A]	GLN	2.8
1	H	134	PRO	2.8
3	N	29	LYS	2.8
1	G	135	SER	2.8
1	H	165	GLY	2.8
3	C	122	GLY	2.8
2	L	127	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	221	PRO	2.7
1	O	134	PRO	2.7
1	K	197	LEU	2.7
2	L	126	LEU	2.7
2	L	206	VAL	2.7
2	L	129	GLY	2.7
1	H	143	THR	2.7
2	P	130	THR	2.7
3	J	82	ARG	2.7
3	J	114	LYS	2.7
1	O	209	LYS	2.6
3	J	54	GLU	2.6
1	A	122	ALA	2.6
2	P	182	LEU	2.6
2	L	203	SER	2.6
1	A	158	VAL	2.6
1	O	192	VAL	2.6
1	H	214	LYS	2.6
2	M	129	GLY	2.6
3	F	135	ALA	2.6
3	J	99	ARG	2.6
3	C	110	PHE	2.6
1	H	219	VAL	2.6
1	D	134	PRO	2.6
1	A	204	CYS	2.5
2	L	195	CYS	2.5
3	N	107	THR	2.5
1	A	64	PHE	2.5
3	Q	82	ARG	2.5
1	A	198	GLY	2.5
3	F	134	VAL	2.5
1	A	162	TRP	2.5
2	I	41	GLY	2.5
2	I	128	SER	2.5
2	B	127	LYS	2.5
3	F	81	VAL	2.5
2	B	195	CYS	2.5
2	B	54	LEU	2.5
2	P	203	SER	2.4
1	A	203	ILE	2.4
2	E	2	ILE	2.4
1	G	212	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
3	R	88	TYR	2.4
1	O	199	THR	2.4
1	A	215	VAL	2.4
3	N	83	GLY	2.4
3	N	56	HIS	2.4
3	Q	58	HIS	2.4
2	E	30	TYR	2.4
2	E	69	THR	2.4
1	H	67	LYS	2.4
2	L	191	LYS	2.4
1	H	198	GLY	2.4
2	P	134	VAL	2.4
3	C	132	VAL	2.4
2	B	40	GLN	2.4
1	A	146	LEU	2.4
2	E	126	LEU	2.4
1	A	195	SER	2.4
1	H	201	THR	2.4
1	A	171	VAL	2.3
1	A	206	VAL	2.3
1	H	65	GLN	2.3
3	N	26	PRO	2.3
2	P	127	LYS	2.3
2	E	67	SER	2.3
2	M	130	THR	2.3
1	O	167	LEU	2.3
1	H	202	TYR	2.3
3	F	51	GLY	2.3
3	N	123	ALA	2.3
3	N	117	VAL	2.3
1	O	198	GLY	2.3
2	B	41	GLY	2.3
1	H	167	LEU	2.3
3	R	136	LYS	2.3
2	B	26	SER	2.3
3	C	111	GLU	2.3
1	O	193	PRO	2.3
3	Q	83	GLY	2.3
3	F	133	ILE	2.3
2	B	23	CYS	2.2
3	F	67	GLN	2.2
1	A	130	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	168	THR	2.2
2	B	119	PHE	2.2
2	L	130	THR	2.2
2	M	41	GLY	2.2
3	N	103	VAL	2.2
3	R	112	VAL	2.2
2	B	21	ILE	2.2
3	C	71	TYR	2.2
2	E	25	ALA	2.2
1	H	199	THR	2.2
1	K	199	THR	2.2
3	F	94	LYS	2.2
3	J	115	THR	2.2
1	H	64	PHE	2.2
2	L	128	SER	2.2
3	F	82	ARG	2.2
1	A	131	PRO	2.2
2	B	121	PRO	2.2
1	O	148	CYS	2.2
2	L	23	CYS	2.2
1	D	143	THR	2.2
2	E	22	THR	2.2
1	H	212	ASN	2.2
1	D	64	PHE	2.2
2	L	1	ASP	2.2
1	D	42	GLU	2.2
3	C	117	VAL	2.2
3	N	69	LYS	2.2
3	Q	122	GLY	2.1
1	A	202	TYR	2.1
2	B	187	TYR	2.1
1	H	164	SER	2.1
2	M	40	GLN	2.1
2	B	153	ASN	2.1
2	L	19	VAL	2.1
2	P	133	VAL	2.1
2	P	206	VAL	2.1
2	E	26	SER	2.1
2	P	128	SER	2.1
2	E	18	THR	2.1
3	Q	5	THR	2.1
2	L	56	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	63	LYS	2.1
2	E	127	LYS	2.1
2	B	166	GLU	2.1
3	R	25	GLY	2.1
1	D	212	ASN	2.1
3	N	31	THR	2.1
2	L	189	LYS	2.1
3	Q	114	LYS	2.1
1	D	220	GLU	2.1
1	K	194	SER	2.1
1	O	121	SER	2.1
3	N	28	ASP	2.1
2	P	121	PRO	2.1
3	C	106	LYS	2.0
3	F	113	THR	2.0
1	A	129	VAL	2.0
2	E	24	ARG	2.0
1	D	197	LEU	2.0
2	E	11	LEU	2.0
2	L	190	HIS	2.0
1	H	148	CYS	2.0
2	B	10	SER	2.0
2	E	128	SER	2.0
1	H	63	LYS	2.0
1	H	218	ARG	2.0
3	J	56	HIS	2.0
2	B	3	GLN	2.0
3	C	108	GLU	2.0
1	A	132	LEU	2.0
2	P	135	CYS	2.0
2	L	187	TYR	2.0
3	N	30	TYR	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(Å ²)	Q<0.9
4	GOL	E	301	6/6	0.92	0.08	20,22,27,27	0
4	GOL	M	301	6/6	0.95	0.07	20,25,27,28	0
4	GOL	R	201	6/6	0.95	0.07	17,23,27,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.