



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:22 AM UTC

PDB ID : 4I18 / pdb_00004i18
Title : Crystal structure of human prolactin receptor complexed with Fab fragment
Authors : Duguid, E.M.; Mukherjee, S.; Kouadio, J.L.
Deposited on : 2012-11-20
Resolution : 3.24 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:

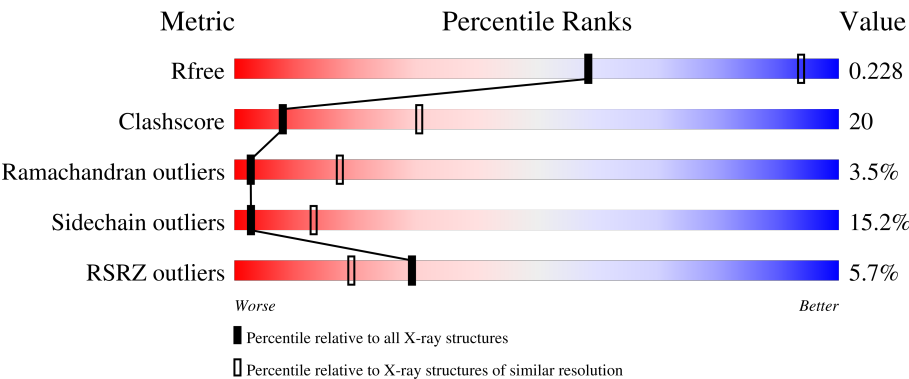
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.24 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	B	217	11% 71% 24% • •
1	L	217	69% 26% •
2	A	236	% 67% 19% 7% • 7%
2	H	236	% 66% 22% 7% • •
3	C	211	10% 34% 30% 20% 5% 11%

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Mol	Chain	Length	Quality of chain
3	R	211	

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
6	ACT	R	301	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9903 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 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1673	1052	276	340	5			
1	B	215	Total	C	N	O	S	0	0	0
			1664	1047	275	337	5			

- Molecule 2 is a protein called antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	0	0
			1686	1065	278	336	7			
2	A	220	Total	C	N	O	S	0	0	1
			1641	1039	270	325	7			

- Molecule 3 is a protein called Prolactin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	205	Total	C	N	O	S	0	0	0
			1677	1086	273	307	11			
3	C	188	Total	C	N	O	S	0	0	0
			1532	999	246	278	9			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

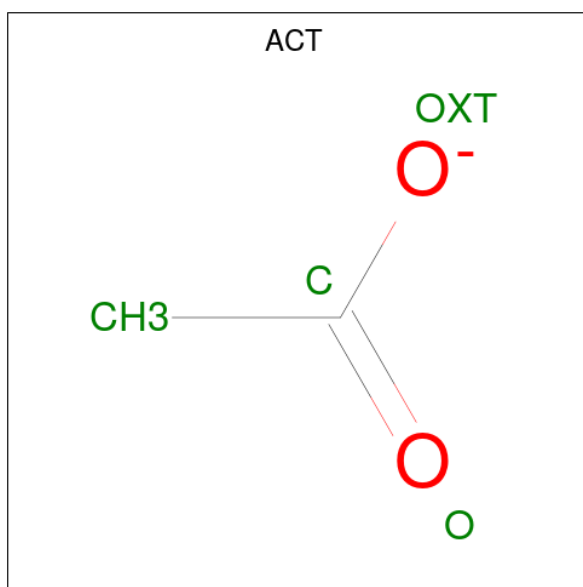


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).

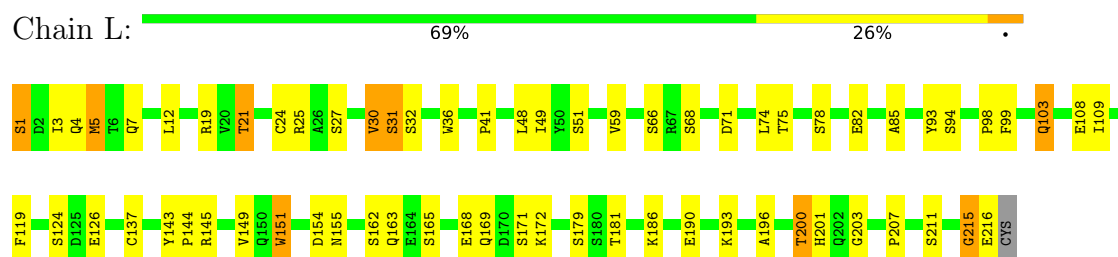


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	R	1	Total	C	O	0	0
			4	2	2		

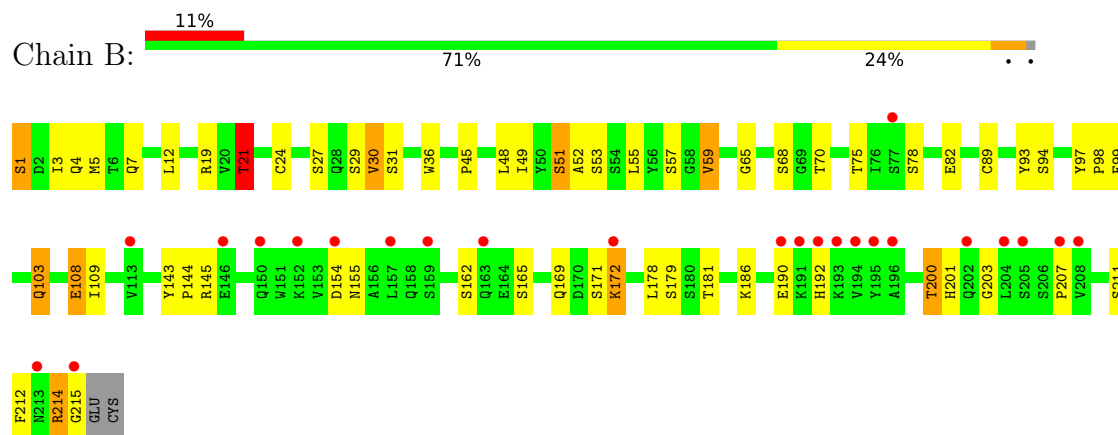
3 Residue-property plots

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.

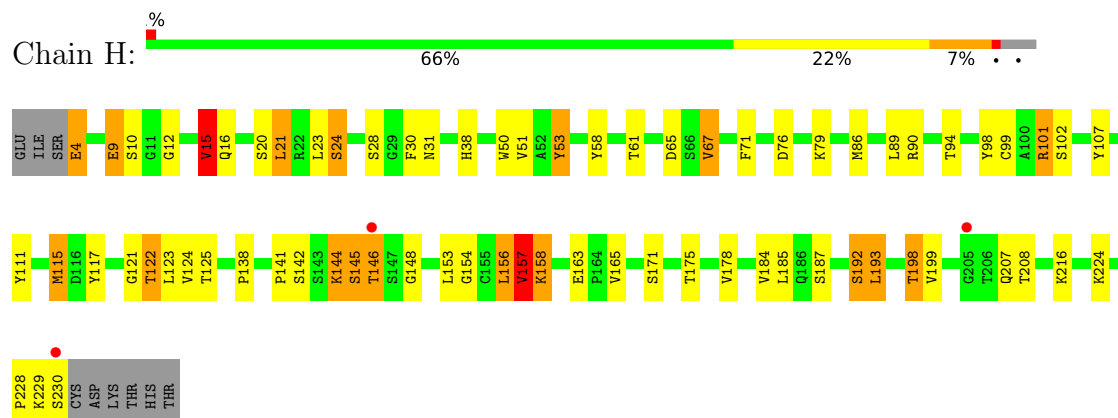
- Molecule 1: antibody light chain



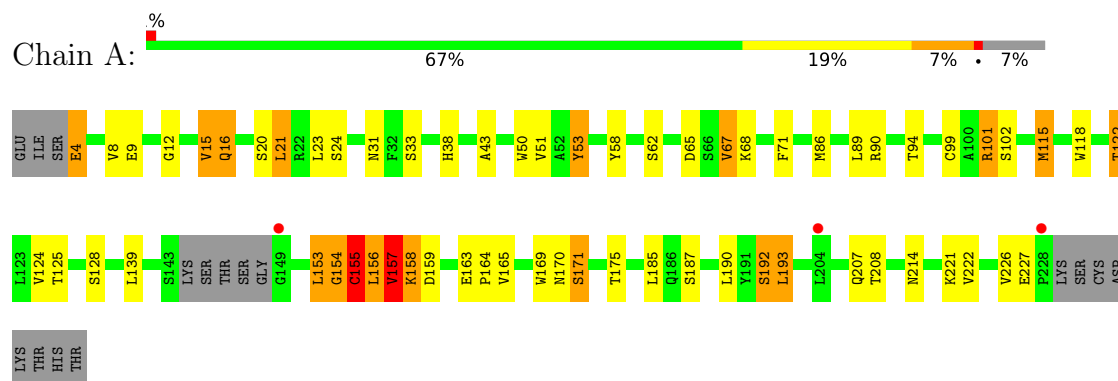
- Molecule 1: antibody light chain



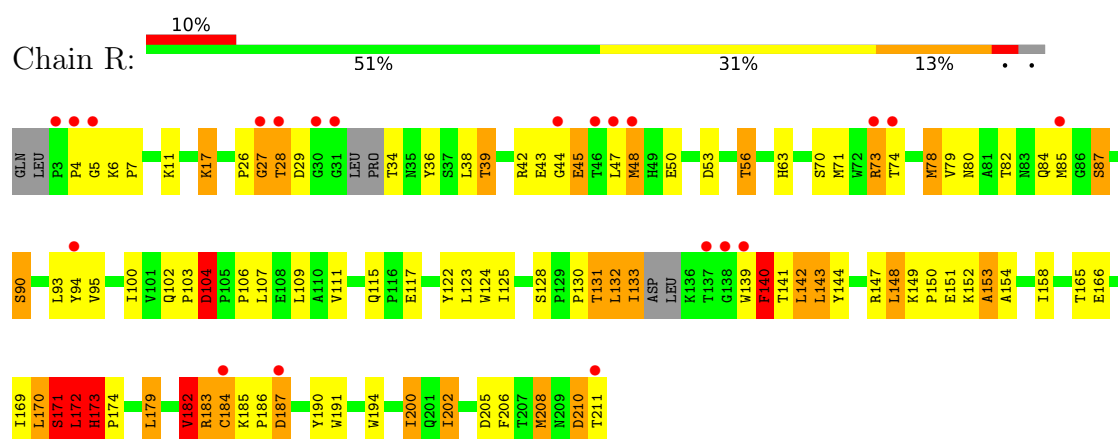
- Molecule 2: antibody heavy chain



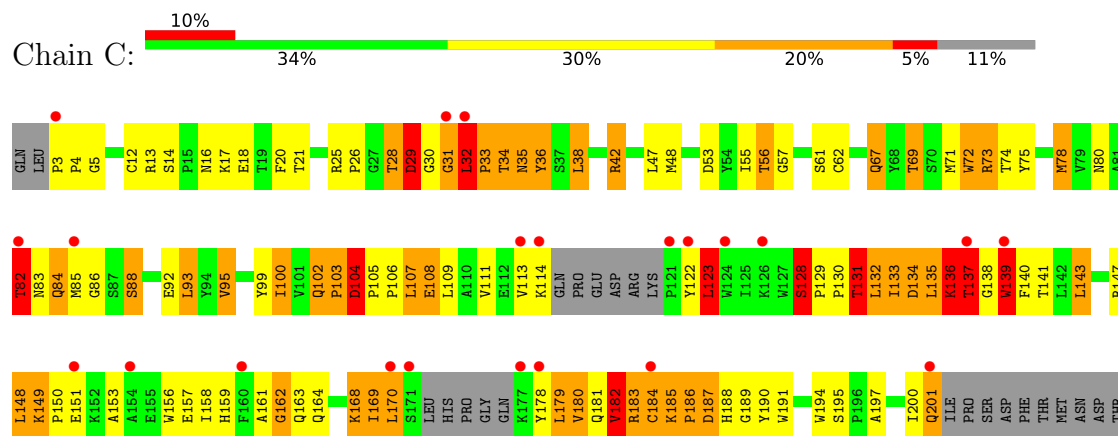
- Molecule 2: antibody heavy chain



- Molecule 3: Prolactin receptor



- Molecule 3: Prolactin receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	285.83Å 285.83Å 62.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.51 – 3.24 49.51 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.51-3.24) 99.3 (49.51-3.24)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.25Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.246 (Not available) , 0.228	Depositor DCC
R_{free} test set	2365 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9903	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: ACT, CA, 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	B	0.90	0/1703	1.14	5/2313 (0.2%)
1	L	1.02	1/1712 (0.1%)	1.24	7/2325 (0.3%)
2	A	1.16	0/1685	1.36	11/2301 (0.5%)
2	H	1.19	0/1731	1.41	16/2363 (0.7%)
3	C	1.16	2/1588 (0.1%)	1.42	22/2168 (1.0%)
3	R	1.23	2/1737 (0.1%)	1.45	17/2368 (0.7%)
All	All	1.12	5/10156 (0.0%)	1.34	78/13838 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2
2	H	0	1
3	C	0	3
3	R	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	210	ASP	N-CA	6.22	1.54	1.46
3	C	178	TYR	N-CA	5.41	1.52	1.45
1	L	151	TRP	CA-C	-5.29	1.46	1.52
3	C	122	TYR	N-CA	5.22	1.52	1.46
3	R	6	LYS	CA-C	5.02	1.59	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	156	LEU	N-CA-C	-9.99	92.55	109.24
2	H	156	LEU	CA-C-N	9.89	139.51	121.70
2	H	156	LEU	C-N-CA	9.89	139.51	121.70
2	A	156	LEU	CA-C-N	9.84	139.41	121.70
2	A	156	LEU	C-N-CA	9.84	139.41	121.70
3	C	123	LEU	N-CA-C	9.00	123.08	108.41
2	H	51	VAL	CB-CA-C	-8.65	103.22	111.44
3	R	153	ALA	N-CA-C	8.54	123.53	109.95
3	R	182	VAL	CB-CA-C	-8.04	99.69	111.19
3	C	178	TYR	N-CA-C	7.93	121.94	109.81
3	R	210	ASP	N-CA-C	7.86	127.55	110.80
2	A	155	CYS	N-CA-C	7.77	122.46	110.42
3	R	149	LYS	N-CA-C	-7.63	99.39	108.25
3	C	88	SER	N-CA-C	7.60	120.86	108.55
3	C	131	THR	N-CA-C	-7.36	101.36	110.41
3	R	45	GLU	N-CA-C	-7.35	95.15	110.80
1	B	172	LYS	N-CA-C	-7.26	101.87	111.24
3	R	131	THR	N-CA-C	-7.15	101.09	110.53
3	R	140	PHE	N-CA-C	7.11	125.94	110.80
1	L	59	VAL	CA-C-N	7.08	127.13	119.90
1	L	59	VAL	C-N-CA	7.08	127.13	119.90
3	C	102	GLN	CA-C-N	-7.07	111.00	119.84
3	C	102	GLN	C-N-CA	-7.07	111.00	119.84
3	R	172	LEU	N-CA-C	-6.96	95.98	110.80
3	R	173	HIS	CA-C-N	6.84	126.80	120.03
3	R	173	HIS	C-N-CA	6.84	126.80	120.03
3	C	139	TRP	N-CA-C	-6.59	105.98	112.97
3	R	63	HIS	N-CA-C	6.55	119.62	109.07
3	C	128	SER	CA-C-N	-6.48	113.71	120.38
3	C	128	SER	C-N-CA	-6.48	113.71	120.38
2	H	61	THR	N-CA-C	6.41	118.91	109.24
2	H	28	SER	N-CA-C	6.40	118.58	108.79
3	C	187	ASP	N-CA-C	-6.34	101.30	110.24
3	C	134	ASP	N-CA-C	6.32	117.96	111.14
3	C	136	LYS	N-CA-C	-6.26	97.47	110.80
3	R	122	TYR	N-CA-C	6.02	117.39	108.60
3	R	184	CYS	N-CA-C	6.01	118.21	109.07
2	H	24	SER	CA-CB-OG	-5.97	99.16	111.10
1	L	85	ALA	N-CA-C	5.96	115.72	107.73
2	H	15	VAL	CB-CA-C	-5.94	100.07	110.71
1	B	211	SER	N-CA-C	5.93	117.26	108.60
3	C	104	ASP	N-CA-CB	-5.92	99.84	110.37
2	H	229	LYS	N-CA-C	5.87	119.20	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	156	LEU	N-CA-C	-5.83	99.90	109.40
2	A	157	VAL	N-CA-CB	5.76	121.29	111.50
3	C	195	SER	CA-C-N	-5.74	113.85	119.76
3	C	195	SER	C-N-CA	-5.74	113.85	119.76
3	R	90	SER	N-CA-C	-5.71	101.54	110.17
1	L	5	MET	CA-C-N	-5.68	114.88	122.72
1	L	5	MET	C-N-CA	-5.68	114.88	122.72
2	H	157	VAL	N-CA-CB	5.67	121.14	111.50
2	A	156	LEU	CA-C-O	-5.67	114.58	120.70
2	A	51	VAL	CB-CA-C	-5.67	106.06	111.44
2	H	10	SER	N-CA-C	5.62	115.96	108.38
2	H	178	VAL	CB-CA-C	-5.61	103.96	110.91
1	B	21	THR	N-CA-C	5.52	117.35	107.80
2	A	169	TRP	N-CA-C	5.46	117.80	108.90
2	A	43	ALA	N-CA-C	-5.42	102.94	109.83
2	A	153	LEU	CA-C-N	5.40	126.35	121.82
2	A	153	LEU	C-N-CA	5.40	126.35	121.82
3	C	55	ILE	N-CA-C	5.34	116.82	111.00
3	C	122	TYR	N-CA-C	5.29	116.32	108.60
3	C	180	VAL	N-CA-C	5.29	115.73	108.12
3	R	27	GLY	CA-C-N	5.25	131.15	121.70
3	R	27	GLY	C-N-CA	5.25	131.15	121.70
3	C	182	VAL	CB-CA-C	-5.25	102.57	110.55
1	B	59	VAL	CA-C-N	5.15	125.16	119.90
1	B	59	VAL	C-N-CA	5.15	125.16	119.90
2	H	144	LYS	CA-C-N	5.14	130.95	121.70
2	H	144	LYS	C-N-CA	5.14	130.95	121.70
3	C	95	VAL	CB-CA-C	-5.12	103.51	110.42
3	C	82	THR	CB-CA-C	5.11	118.93	109.54
1	L	149	VAL	CA-C-N	-5.08	115.83	122.99
1	L	149	VAL	C-N-CA	-5.08	115.83	122.99
2	H	51	VAL	N-CA-C	5.07	115.92	111.56
3	R	104	ASP	N-CA-CB	-5.06	101.36	110.37
2	H	148	GLY	N-CA-C	-5.04	103.10	112.37
3	C	72	TRP	N-CA-C	5.04	117.00	109.59

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	154	GLY	Peptide
2	A	155	CYS	Peptide

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Mol	Chain	Res	Type	Group
3	C	103	PRO	Peptide
3	C	136	LYS	Peptide
3	C	35	ASN	Peptide
2	H	154	GLY	Peptide
3	R	103	PRO	Peptide

5.2 Too-close contacts [i](#)

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	B	1664	0	1610	43	0
1	L	1673	0	1616	46	0
2	A	1641	0	1567	56	0
2	H	1686	0	1605	65	0
3	C	1532	0	1446	112	0
3	R	1677	0	1586	88	0
4	A	6	0	8	0	0
4	C	6	0	8	0	0
4	H	6	0	8	3	0
4	L	6	0	8	0	0
5	B	1	0	0	0	0
5	H	1	0	0	0	0
6	R	4	0	3	2	0
All	All	9903	0	9465	380	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 20.

All (380) 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)
3:R:172:LEU:CA	3:R:173:HIS:HB2	1.69	1.20
3:C:30:GLY:HA2	3:C:31:GLY:O	1.43	1.17
1:L:119:PHE:CD1	2:H:145:SER:HA	1.81	1.16
3:R:170:LEU:O	3:R:171:SER:HB2	1.43	1.15
3:R:172:LEU:O	3:R:172:LEU:HD12	1.50	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:16:GLN:HA	2:A:16:GLN:HE21	1.09	1.09
1:L:119:PHE:HD1	2:H:145:SER:HA	1.04	1.07
3:R:82:THR:HA	3:R:87:SER:HB3	1.31	1.07
3:R:172:LEU:HA	3:R:173:HIS:CB	1.86	1.06
3:R:53:ASP:OD2	3:R:56:THR:HG23	1.63	0.99
3:R:11:LYS:CE	6:R:301:ACT:H2	1.93	0.98
3:R:111:VAL:HG12	3:R:200:ILE:HD13	1.47	0.95
1:B:190:GLU:HA	1:B:214:ARG:HD2	1.45	0.95
3:C:26:PRO:HB3	3:C:36:TYR:OH	1.65	0.94
2:A:16:GLN:HA	2:A:16:GLN:NE2	1.81	0.94
3:R:172:LEU:HA	3:R:173:HIS:HB2	0.93	0.93
3:R:104:ASP:HB3	3:R:130:PRO:HB3	1.51	0.91
3:C:35:ASN:HA	3:C:36:TYR:HB2	1.54	0.90
3:R:172:LEU:HD13	3:R:202:ILE:HD12	1.56	0.87
3:C:103:PRO:HB3	3:C:133:ILE:HD12	1.56	0.87
2:H:4:GLU:OE2	2:H:4:GLU:HA	1.73	0.87
3:R:171:SER:O	3:R:172:LEU:HG	1.75	0.87
3:C:32:LEU:HB3	3:C:33:PRO:HD2	1.57	0.86
3:R:172:LEU:HD12	3:R:172:LEU:C	2.03	0.82
2:H:15:VAL:CG2	2:H:21:LEU:HD13	2.09	0.82
1:L:163:GLN:HG2	2:H:184:VAL:HG11	1.61	0.81
3:C:28:THR:HG22	3:C:28:THR:O	1.80	0.81
3:R:53:ASP:OD2	3:R:56:THR:CG2	2.28	0.81
3:R:47:LEU:O	3:R:48:MET:HB2	1.80	0.81
3:R:171:SER:O	3:R:172:LEU:CG	2.29	0.81
3:C:169:ILE:C	3:C:170:LEU:HG	2.06	0.80
3:R:53:ASP:CG	3:R:56:THR:HG23	2.06	0.80
2:H:15:VAL:HG21	2:H:21:LEU:HD13	1.64	0.80
3:R:5:GLY:HA2	3:R:28:THR:HB	1.63	0.80
3:C:4:PRO:HD3	3:C:83:ASN:HD22	1.46	0.80
3:R:148:LEU:HD21	3:R:169:ILE:HD13	1.64	0.79
1:L:109:ILE:HB	1:L:169:GLN:HE22	1.48	0.79
1:L:201:HIS:CD2	1:L:203:GLY:H	2.01	0.79
3:R:171:SER:O	3:R:172:LEU:CB	2.31	0.78
3:C:30:GLY:HA2	3:C:31:GLY:C	2.08	0.77
3:R:172:LEU:O	3:R:172:LEU:CD1	2.30	0.77
2:A:16:GLN:HE21	2:A:16:GLN:CA	1.92	0.76
1:B:214:ARG:HG2	1:B:215:GLY:N	1.98	0.76
3:R:171:SER:C	3:R:172:LEU:HG	2.11	0.75
3:R:170:LEU:O	3:R:171:SER:CB	2.29	0.74
3:C:32:LEU:HD13	3:C:84:GLN:HG2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:207:GLN:HE21	2:H:208:THR:N	1.85	0.73
2:H:31:ASN:H	3:C:56:THR:HG21	1.53	0.73
3:C:53:ASP:OD1	3:C:56:THR:HG23	1.88	0.73
2:A:101:ARG:HD3	2:A:101:ARG:C	2.14	0.72
3:R:17:LYS:HD3	3:R:71:MET:HE2	1.72	0.71
1:L:7:GLN:H	1:L:103:GLN:HE22	1.39	0.71
1:L:21:THR:O	1:L:21:THR:HG22	1.91	0.71
3:C:34:THR:CG2	3:C:83:ASN:HB2	2.20	0.71
1:B:109:ILE:HB	1:B:169:GLN:HE22	1.56	0.70
3:C:32:LEU:HB3	3:C:33:PRO:CD	2.21	0.69
1:L:108:GLU:HG2	1:L:169:GLN:OE1	1.92	0.69
3:C:28:THR:O	3:C:28:THR:CG2	2.41	0.68
1:B:192:HIS:O	1:B:214:ARG:HD3	1.94	0.68
3:C:201:GLN:C	3:C:201:GLN:NE2	2.52	0.68
3:R:143:LEU:O	3:R:184:CYS:HB2	1.93	0.68
2:A:207:GLN:HE21	2:A:208:THR:N	1.92	0.67
2:A:4:GLU:OE2	2:A:4:GLU:HA	1.94	0.67
3:C:143:LEU:HA	3:C:162:GLY:O	1.94	0.67
3:C:53:ASP:CG	3:C:56:THR:HG23	2.20	0.66
3:R:132:LEU:O	3:R:133:ILE:HB	1.95	0.66
3:C:35:ASN:HA	3:C:36:TYR:CB	2.25	0.66
3:C:4:PRO:HD3	3:C:83:ASN:ND2	2.11	0.66
1:B:201:HIS:CD2	1:B:203:GLY:H	2.13	0.65
2:H:15:VAL:HG22	2:H:21:LEU:CD1	2.26	0.65
3:R:171:SER:O	3:R:172:LEU:HB3	1.94	0.65
3:C:131:THR:O	3:C:132:LEU:HB2	1.95	0.65
3:C:183:ARG:HG3	3:C:191:TRP:CE3	2.31	0.65
3:C:3:PRO:HA	3:C:86:GLY:HA3	1.78	0.65
2:H:38:HIS:CD2	2:H:53:TYR:HB3	2.31	0.65
3:C:148:LEU:CD1	3:C:157:GLU:HB3	2.27	0.65
3:C:48:MET:HE2	3:C:78:MET:HE2	1.77	0.65
3:C:42:ARG:HH21	3:C:74:THR:H	1.44	0.65
1:L:30:VAL:HG22	1:L:93:TYR:HB3	1.79	0.65
2:H:101:ARG:HD3	2:H:101:ARG:C	2.22	0.64
1:B:214:ARG:CG	1:B:215:GLY:N	2.59	0.64
2:A:38:HIS:CD2	2:A:50:TRP:HE1	2.16	0.64
3:C:35:ASN:HA	3:C:36:TYR:CD2	2.32	0.64
1:L:5:MET:HE3	1:L:24:CYS:SG	2.37	0.64
1:B:200:THR:HG23	1:B:207:PRO:HG3	1.80	0.64
2:A:58:TYR:CE1	3:R:132:LEU:HA	2.32	0.64
1:L:119:PHE:HD1	2:H:145:SER:CA	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:THR:HG22	1:B:21:THR:O	1.97	0.64
2:H:38:HIS:CD2	2:H:50:TRP:HE1	2.15	0.64
2:H:23:LEU:HG	2:H:86:MET:HE2	1.78	0.63
2:H:144:LYS:HA	2:H:146:THR:H	1.62	0.63
2:H:9:GLU:OE2	2:H:99:CYS:N	2.29	0.63
3:C:35:ASN:HA	3:C:36:TYR:HD2	1.63	0.63
1:B:45:PRO:HG2	2:A:118:TRP:CZ3	2.33	0.63
3:C:102:GLN:HB2	3:C:190:TYR:HB2	1.82	0.62
1:B:30:VAL:HG22	1:B:93:TYR:HB3	1.82	0.62
1:L:200:THR:HG23	1:L:207:PRO:HG3	1.82	0.62
3:C:169:ILE:HG23	3:C:170:LEU:N	2.15	0.61
2:A:94:THR:HG23	2:A:125:THR:HA	1.81	0.61
2:A:38:HIS:HD2	2:A:50:TRP:HE1	1.47	0.61
3:C:53:ASP:OD2	3:C:56:THR:HG23	2.00	0.61
2:H:15:VAL:CG2	2:H:21:LEU:CD1	2.78	0.61
3:C:18:GLU:HA	3:C:69:THR:HG21	1.81	0.61
2:H:31:ASN:H	3:C:56:THR:CG2	2.13	0.61
3:C:35:ASN:CA	3:C:36:TYR:HB2	2.30	0.60
1:L:7:GLN:H	1:L:103:GLN:NE2	1.99	0.60
2:H:193:LEU:C	2:H:193:LEU:HD12	2.26	0.60
3:C:42:ARG:NH2	3:C:74:THR:H	1.98	0.60
3:C:106:PRO:HG2	3:C:182:VAL:HB	1.84	0.60
3:C:35:ASN:CA	3:C:36:TYR:HD2	2.14	0.60
1:L:186:LYS:HE2	1:L:190:GLU:OE2	2.02	0.60
2:H:38:HIS:HD2	2:H:50:TRP:HE1	1.49	0.60
1:L:154:ASP:O	1:L:155:ASN:HB2	2.02	0.59
2:A:214:ASN:HD21	2:A:221:LYS:HE2	1.67	0.59
3:C:78:MET:HG3	3:C:92:GLU:HG2	1.84	0.59
3:R:172:LEU:CA	3:R:173:HIS:CB	2.57	0.59
3:R:142:LEU:HD12	3:R:186:PRO:HA	1.84	0.58
3:C:99:TYR:HD2	3:C:188:HIS:HB2	1.68	0.58
3:C:34:THR:HG22	3:C:83:ASN:HB2	1.84	0.58
3:C:148:LEU:HA	3:C:179:LEU:O	2.02	0.58
3:C:168:LYS:H	3:C:168:LYS:HD3	1.68	0.58
1:B:143:TYR:CD1	1:B:144:PRO:HA	2.39	0.58
2:A:15:VAL:HG21	2:A:21:LEU:HD13	1.85	0.58
2:H:9:GLU:OE2	2:H:98:TYR:HA	2.03	0.58
1:B:98:PRO:HB2	1:B:99:PHE:CD2	2.38	0.58
2:H:107:TYR:O	4:H:302:GOL:H32	2.03	0.58
1:L:124:SER:CB	2:H:138:PRO:HD2	2.34	0.58
3:C:169:ILE:O	3:C:170:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:CYS:HA	3:C:191:TRP:HZ3	1.68	0.58
3:R:139:TRP:CG	3:R:140:PHE:H	2.22	0.57
2:H:16:GLN:HA	2:H:16:GLN:NE2	2.19	0.57
1:B:5:MET:HE3	1:B:24:CYS:SG	2.44	0.57
3:C:74:THR:C	3:C:75:TYR:CD2	2.83	0.57
3:C:168:LYS:HD3	3:C:168:LYS:N	2.20	0.57
3:R:183:ARG:HD2	3:R:194:TRP:CZ3	2.40	0.57
3:C:113:VAL:HG23	3:C:200:ILE:HD11	1.86	0.57
3:R:169:ILE:HG21	3:R:172:LEU:HD23	1.87	0.57
2:A:38:HIS:CD2	2:A:53:TYR:HB3	2.40	0.57
3:C:99:TYR:CD2	3:C:188:HIS:HB2	2.39	0.57
1:L:215:GLY:O	1:L:216:GLU:HG3	2.04	0.56
2:H:38:HIS:HE1	2:H:102:SER:HB3	1.70	0.56
2:H:76:ASP:OD2	2:H:79:LYS:HD2	2.05	0.56
2:A:139:LEU:HD12	2:A:154:GLY:HA3	1.87	0.56
3:C:128:SER:HB2	3:C:129:PRO:HD2	1.86	0.56
2:H:144:LYS:HA	2:H:146:THR:N	2.20	0.56
3:C:169:ILE:CG2	3:C:170:LEU:N	2.69	0.56
3:R:94:TYR:N	3:R:94:TYR:CD1	2.74	0.56
3:R:124:TRP:CH2	3:R:166:GLU:OE1	2.58	0.56
3:C:83:ASN:O	3:C:84:GLN:HB2	2.04	0.56
1:L:4:GLN:HB2	1:L:27:SER:HB3	1.88	0.56
1:B:99:PHE:CD1	2:A:115:MET:HE3	2.40	0.56
2:A:9:GLU:HA	2:A:24:SER:O	2.06	0.56
2:A:31:ASN:H	3:R:56:THR:CG2	2.18	0.56
2:A:16:GLN:HE22	2:A:128:SER:HA	1.69	0.56
2:A:38:HIS:CD2	2:A:115:MET:CE	2.90	0.55
3:C:134:ASP:O	3:C:135:LEU:HD12	2.06	0.55
1:L:201:HIS:HD2	1:L:203:GLY:H	1.53	0.55
3:R:104:ASP:HB3	3:R:130:PRO:CB	2.32	0.55
3:C:57:GLY:HA3	3:C:61:SER:OG	2.06	0.55
3:C:28:THR:O	3:C:29:ASP:C	2.50	0.55
2:A:38:HIS:CD2	2:A:115:MET:HE2	2.41	0.55
3:R:111:VAL:CG1	3:R:200:ILE:HD13	2.29	0.55
3:C:201:GLN:C	3:C:201:GLN:HE21	2.14	0.55
1:L:31:SER:OG	1:L:32:SER:N	2.25	0.55
3:C:93:LEU:HD23	3:C:95:VAL:HG22	1.89	0.54
2:A:50:TRP:HE1	2:A:115:MET:HE1	1.72	0.54
3:C:4:PRO:HB3	3:C:5:GLY:HA3	1.90	0.54
1:B:53:SER:HB2	1:B:65:GLY:O	2.07	0.54
2:A:101:ARG:NH2	3:R:56:THR:O	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:SER:HB3	2:H:138:PRO:HD2	1.89	0.54
3:C:16:ASN:ND2	3:C:18:GLU:HB2	2.22	0.54
2:A:16:GLN:NE2	2:A:16:GLN:CA	2.58	0.54
1:L:163:GLN:CG	2:H:184:VAL:HG11	2.35	0.54
2:H:101:ARG:HD2	2:H:117:TYR:HD2	1.73	0.54
3:R:111:VAL:HG12	3:R:200:ILE:CD1	2.32	0.54
3:R:172:LEU:CD1	3:R:202:ILE:HD12	2.34	0.54
3:R:94:TYR:N	3:R:94:TYR:HD1	2.05	0.54
2:H:58:TYR:CE2	3:C:132:LEU:CD2	2.92	0.53
3:C:33:PRO:O	3:C:34:THR:HG23	2.07	0.53
3:C:179:LEU:HD23	3:C:197:ALA:HB1	1.89	0.53
3:R:131:THR:O	3:R:132:LEU:HG	2.09	0.53
2:H:141:PRO:HG2	2:H:228:PRO:HB3	1.89	0.53
1:B:99:PHE:CG	2:A:115:MET:HE3	2.43	0.53
2:A:15:VAL:CG2	2:A:21:LEU:HD13	2.38	0.53
2:A:207:GLN:HE21	2:A:208:THR:H	1.54	0.53
3:C:107:LEU:HD13	3:C:108:GLU:H	1.74	0.53
3:C:186:PRO:O	3:C:187:ASP:C	2.52	0.53
3:R:183:ARG:HD2	3:R:194:TRP:CH2	2.44	0.52
1:L:99:PHE:CD1	2:H:115:MET:HE3	2.43	0.52
1:B:214:ARG:CG	1:B:215:GLY:H	2.22	0.52
3:R:53:ASP:OD1	3:R:56:THR:HG23	2.09	0.52
3:C:16:ASN:HD21	3:C:18:GLU:HB2	1.75	0.52
3:C:137:THR:HA	3:C:138:GLY:C	2.35	0.52
3:R:172:LEU:C	3:R:172:LEU:CD1	2.73	0.52
1:B:3:ILE:HD12	1:B:94:SER:HB2	1.91	0.52
2:A:38:HIS:HE1	2:A:102:SER:HB3	1.74	0.52
3:C:103:PRO:HB3	3:C:133:ILE:CD1	2.32	0.52
3:C:184:CYS:HA	3:C:191:TRP:CZ3	2.44	0.52
3:C:150:PRO:HB2	3:C:153:ALA:HB2	1.91	0.52
3:R:115:GLN:NE2	3:R:208:MET:HE3	2.24	0.52
2:H:30:PHE:CZ	2:H:101:ARG:HG2	2.45	0.51
3:R:147:ARG:HD3	3:R:194:TRP:CZ2	2.45	0.51
2:A:139:LEU:HB2	2:A:154:GLY:HA3	1.91	0.51
1:L:25:ARG:HG3	1:L:71:ASP:OD1	2.11	0.51
2:H:58:TYR:CE2	3:C:132:LEU:HD22	2.45	0.51
2:A:50:TRP:NE1	2:A:115:MET:HE1	2.25	0.51
3:C:148:LEU:HD12	3:C:157:GLU:HB3	1.92	0.51
3:R:107:LEU:HD11	3:R:131:THR:CG2	2.41	0.51
3:R:115:GLN:HE22	3:R:208:MET:CE	2.24	0.51
3:R:172:LEU:O	3:R:172:LEU:CG	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1:SER:HB2	1:L:4:GLN:HE22	1.75	0.51
2:A:163:GLU:HB3	2:A:164:PRO:HA	1.93	0.51
3:C:109:LEU:HD13	3:C:182:VAL:HG22	1.92	0.51
2:A:31:ASN:H	3:R:56:THR:HG21	1.75	0.50
3:R:179:LEU:H	3:R:179:LEU:HD12	1.75	0.50
1:L:21:THR:O	1:L:21:THR:CG2	2.55	0.50
2:A:4:GLU:OE2	2:A:4:GLU:CA	2.60	0.50
3:R:169:ILE:CG2	3:R:172:LEU:HD23	2.42	0.50
3:R:5:GLY:CA	3:R:28:THR:HB	2.39	0.50
3:C:104:ASP:O	3:C:130:PRO:HB3	2.12	0.50
1:L:99:PHE:CG	2:H:115:MET:HE3	2.46	0.50
3:C:123:LEU:HD21	3:C:200:ILE:HD13	1.93	0.50
1:B:154:ASP:O	1:B:155:ASN:HB2	2.12	0.50
2:A:86:MET:HB3	2:A:89:LEU:HD21	1.94	0.50
1:L:196:ALA:HB2	1:L:211:SER:HB3	1.94	0.50
1:B:7:GLN:H	1:B:103:GLN:NE2	2.09	0.50
3:R:39:THR:HG22	3:R:50:GLU:HA	1.93	0.49
2:A:31:ASN:HB2	3:R:56:THR:HG21	1.95	0.49
3:C:169:ILE:HG23	3:C:170:LEU:H	1.76	0.49
1:B:55:LEU:HD11	1:B:59:VAL:CG1	2.43	0.49
1:B:186:LYS:HE2	1:B:190:GLU:OE2	2.13	0.49
2:A:67:VAL:HG13	2:A:71:PHE:HB2	1.94	0.49
3:C:73:ARG:HB3	3:C:73:ARG:CZ	2.43	0.49
3:C:38:LEU:HD12	3:C:38:LEU:C	2.38	0.49
2:A:31:ASN:CB	3:R:56:THR:HG21	2.43	0.49
2:H:86:MET:HE1	2:H:124:VAL:HG21	1.95	0.49
2:A:65:ASP:C	2:A:67:VAL:H	2.21	0.49
2:H:21:LEU:HB3	2:H:86:MET:HE3	1.95	0.49
1:L:82:GLU:HA	1:L:171:SER:HB2	1.95	0.48
2:H:65:ASP:C	2:H:67:VAL:H	2.21	0.48
2:H:38:HIS:O	2:H:99:CYS:HA	2.13	0.48
3:C:14:SER:HB2	3:C:20:PHE:HB3	1.96	0.48
1:L:143:TYR:CD1	1:L:144:PRO:HA	2.49	0.48
3:C:159:HIS:CD2	3:C:169:ILE:HD11	2.48	0.48
3:C:107:LEU:O	3:C:108:GLU:C	2.57	0.48
2:H:207:GLN:NE2	2:H:208:THR:N	2.59	0.48
3:C:71:MET:HG3	3:C:72:TRP:H	1.78	0.48
2:A:50:TRP:CD1	2:A:115:MET:HE1	2.49	0.48
2:A:193:LEU:C	2:A:193:LEU:HD12	2.39	0.48
2:H:16:GLN:HA	2:H:16:GLN:HE21	1.79	0.48
1:B:82:GLU:HA	1:B:171:SER:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLU:HG2	1:B:169:GLN:OE1	2.14	0.48
2:A:38:HIS:NE2	2:A:115:MET:HE2	2.29	0.47
3:C:104:ASP:OD2	3:C:131:THR:O	2.32	0.47
1:B:55:LEU:HD11	1:B:59:VAL:HG12	1.96	0.47
2:H:94:THR:HG23	2:H:125:THR:HA	1.95	0.47
3:C:161:ALA:O	3:C:163:GLN:N	2.48	0.47
1:B:212:PHE:CD1	1:B:212:PHE:C	2.92	0.47
3:C:111:VAL:HG12	3:C:200:ILE:HD12	1.97	0.47
1:B:97:TYR:N	1:B:98:PRO:CD	2.78	0.47
1:L:143:TYR:CG	1:L:144:PRO:HA	2.50	0.47
1:B:36:TRP:CH2	1:B:89:CYS:HB3	2.50	0.47
3:C:107:LEU:HD22	3:C:107:LEU:HA	1.62	0.47
2:H:158:LYS:HG2	2:H:192:SER:OG	2.16	0.46
2:A:139:LEU:HB2	2:A:154:GLY:CA	2.44	0.46
3:R:173:HIS:H	3:R:174:PRO:HD3	1.80	0.46
3:R:174:PRO:HA	3:R:202:ILE:HG22	1.96	0.46
3:C:42:ARG:NH2	3:C:73:ARG:H	2.13	0.46
1:B:178:LEU:C	1:B:178:LEU:HD23	2.40	0.46
3:C:113:VAL:CG2	3:C:200:ILE:HD11	2.44	0.46
3:C:21:THR:HG23	3:C:62:CYS:O	2.15	0.46
3:C:32:LEU:HD22	3:C:84:GLN:OE1	2.15	0.46
3:C:32:LEU:HD13	3:C:84:GLN:CG	2.41	0.46
3:C:4:PRO:CB	3:C:5:GLY:HA3	2.46	0.46
3:R:150:PRO:HG2	3:R:153:ALA:HB2	1.97	0.46
3:R:173:HIS:H	3:R:174:PRO:CD	2.27	0.46
3:C:106:PRO:CG	3:C:182:VAL:HB	2.45	0.46
2:H:9:GLU:OE1	2:H:121:GLY:N	2.37	0.46
3:C:151:GLU:HA	3:C:179:LEU:HD12	1.98	0.46
1:L:30:VAL:HG22	1:L:93:TYR:CB	2.46	0.45
1:B:51:SER:O	1:B:52:ALA:HB3	2.16	0.45
3:R:34:THR:HG22	3:R:36:TYR:CE2	2.51	0.45
3:C:35:ASN:CA	3:C:36:TYR:CD2	2.95	0.45
3:C:53:ASP:OD2	3:C:56:THR:CG2	2.63	0.45
1:B:143:TYR:CG	1:B:144:PRO:HA	2.51	0.45
2:A:170:ASN:O	2:A:171:SER:C	2.59	0.45
3:R:115:GLN:HE22	3:R:208:MET:HE3	1.81	0.45
3:C:137:THR:CG2	3:C:139:TRP:CE3	2.99	0.45
1:B:7:GLN:H	1:B:103:GLN:HE22	1.65	0.45
2:A:12:GLY:HA3	2:A:122:THR:HB	1.99	0.45
2:A:158:LYS:HD3	2:A:159:ASP:OD1	2.17	0.45
3:R:107:LEU:HD11	3:R:131:THR:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:SER:CB	1:B:65:GLY:O	2.65	0.45
2:H:38:HIS:CD2	2:H:115:MET:CE	2.99	0.45
2:H:50:TRP:HE1	2:H:115:MET:HE1	1.82	0.45
3:R:186:PRO:O	3:R:187:ASP:C	2.59	0.44
3:R:7:PRO:HG2	3:R:90:SER:HB3	1.98	0.44
3:R:139:TRP:CG	3:R:140:PHE:N	2.84	0.44
3:C:183:ARG:HD2	3:C:194:TRP:CE2	2.52	0.44
2:A:58:TYR:CE2	3:R:132:LEU:HD22	2.53	0.44
3:C:67:GLN:HE21	3:C:67:GLN:HB3	1.64	0.44
1:L:99:PHE:HB3	2:H:115:MET:HE3	1.98	0.44
2:A:158:LYS:HA	2:A:192:SER:OG	2.18	0.44
2:H:12:GLY:HA3	2:H:122:THR:HB	2.00	0.44
3:R:102:GLN:HB2	3:R:190:TYR:HB2	1.99	0.44
2:H:123:LEU:HD21	2:H:163:GLU:HB2	2.00	0.43
2:H:198:THR:C	2:H:199:VAL:HG13	2.43	0.43
3:R:185:LYS:HB3	3:R:191:TRP:HA	2.00	0.43
1:L:119:PHE:HE1	2:H:146:THR:N	2.15	0.43
1:L:137:CYS:HB2	1:L:151:TRP:CH2	2.54	0.43
2:A:214:ASN:ND2	2:A:221:LYS:HG3	2.33	0.43
3:C:67:GLN:HG2	3:C:67:GLN:O	2.19	0.43
1:L:144:PRO:O	1:L:201:HIS:HE1	2.00	0.43
2:A:207:GLN:NE2	2:A:208:THR:H	2.16	0.43
1:L:215:GLY:O	1:L:216:GLU:CG	2.66	0.43
2:H:207:GLN:HE21	2:H:208:THR:H	1.65	0.43
2:A:86:MET:HE1	2:A:124:VAL:HG21	2.00	0.43
2:H:4:GLU:OE2	2:H:4:GLU:CA	2.57	0.43
2:H:31:ASN:N	3:C:56:THR:HG21	2.27	0.43
2:H:67:VAL:HG13	2:H:71:PHE:HB2	1.99	0.43
3:C:12:CYS:HB3	3:C:100:ILE:HD12	2.01	0.43
3:C:35:ASN:CA	3:C:36:TYR:CB	2.96	0.43
1:L:98:PRO:HB2	1:L:99:PHE:CD2	2.53	0.43
3:R:132:LEU:O	3:R:133:ILE:CB	2.66	0.43
3:C:38:LEU:C	3:C:38:LEU:CD1	2.92	0.43
3:C:34:THR:HG22	3:C:82:THR:O	2.19	0.43
1:L:36:TRP:CD2	1:L:74:LEU:HB2	2.53	0.42
1:B:45:PRO:HG2	2:A:118:TRP:CH2	2.54	0.42
2:A:38:HIS:CD2	2:A:115:MET:HE1	2.53	0.42
2:A:38:HIS:O	2:A:99:CYS:HA	2.18	0.42
3:R:11:LYS:CE	6:R:301:ACT:CH3	2.82	0.42
1:B:1:SER:HA	1:B:97:TYR:CG	2.54	0.42
2:A:38:HIS:CE1	2:A:102:SER:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:25:ARG:NH1	1:L:25:ARG:HB2	2.35	0.42
3:R:106:PRO:HG2	3:R:182:VAL:HB	2.00	0.42
2:H:38:HIS:CD2	2:H:115:MET:HE1	2.54	0.42
3:R:93:LEU:HD23	3:R:95:VAL:CG2	2.49	0.42
4:H:302:GOL:H12	3:C:105:PRO:HD3	2.01	0.42
1:B:4:GLN:HB2	1:B:27:SER:HB3	2.01	0.42
1:B:29:SER:HA	1:B:70:THR:HG22	2.01	0.42
3:R:125:ILE:O	3:R:166:GLU:HA	2.20	0.42
2:A:23:LEU:HG	2:A:86:MET:HE2	2.01	0.42
2:A:159:ASP:HB3	2:A:190:LEU:CD1	2.49	0.42
3:R:183:ARG:HB3	3:R:194:TRP:CE3	2.55	0.42
1:B:162:SER:HA	1:B:181:THR:O	2.19	0.41
3:R:38:LEU:HD12	3:R:79:VAL:HG22	2.02	0.41
3:R:78:MET:HE3	3:R:78:MET:HB3	1.47	0.41
1:L:126:GLU:OE1	2:H:224:LYS:NZ	2.54	0.41
2:H:86:MET:HB3	2:H:89:LEU:HD21	2.02	0.41
1:L:3:ILE:HD12	1:L:94:SER:HB2	2.02	0.41
1:L:41:PRO:CG	1:L:168:GLU:HG3	2.50	0.41
3:R:111:VAL:HG11	3:R:200:ILE:HG21	2.01	0.41
3:R:205:ASP:O	3:R:208:MET:HB3	2.20	0.41
3:R:93:LEU:HD23	3:R:95:VAL:HG22	2.01	0.41
3:C:147:ARG:HB2	3:C:156:TRP:CE3	2.56	0.41
2:H:50:TRP:NE1	2:H:115:MET:HE1	2.36	0.41
1:B:36:TRP:CZ3	1:B:89:CYS:HB3	2.55	0.41
1:B:103:GLN:CD	1:B:103:GLN:H	2.27	0.41
2:H:38:HIS:NE2	2:H:115:MET:HE2	2.35	0.41
2:H:111:TYR:OH	3:C:102:GLN:OE1	2.22	0.41
2:H:107:TYR:C	4:H:302:GOL:H32	2.45	0.41
3:R:144:TYR:CD1	3:R:184:CYS:HB3	2.56	0.41
1:L:119:PHE:CE1	2:H:145:SER:HA	2.46	0.41
1:B:30:VAL:O	1:B:30:VAL:HG13	2.21	0.41
1:B:48:LEU:O	1:B:49:ILE:HG13	2.21	0.41
3:C:71:MET:CG	3:C:72:TRP:H	2.33	0.41
3:C:78:MET:HB3	3:C:78:MET:HE3	1.51	0.41
3:C:137:THR:HG21	3:C:139:TRP:CE3	2.56	0.41
3:C:185:LYS:HD2	3:C:189:GLY:O	2.21	0.41
3:R:109:LEU:HD13	3:R:182:VAL:HG22	2.02	0.41
2:H:142:SER:O	2:H:145:SER:O	2.39	0.40
3:R:150:PRO:O	3:R:152:LYS:N	2.53	0.40
3:R:42:ARG:NH2	3:R:73:ARG:HG3	2.37	0.40
3:C:181:GLN:HG2	3:C:197:ALA:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:LEU:O	1:L:49:ILE:HG13	2.21	0.40
3:R:26:PRO:HB3	3:R:36:TYR:CE1	2.56	0.40
3:C:17:LYS:NZ	3:C:139:TRP:O	2.54	0.40
1:L:162:SER:HA	1:L:181:THR:O	2.21	0.40
1:B:30:VAL:HG22	1:B:93:TYR:CB	2.49	0.40
3:R:125:ILE:CD1	3:R:169:ILE:HD12	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	213/217 (98%)	201 (94%)	10 (5%)	2 (1%)	14	44
1	L	214/217 (99%)	201 (94%)	11 (5%)	2 (1%)	14	44
2	A	216/236 (92%)	199 (92%)	15 (7%)	2 (1%)	14	44
2	H	225/236 (95%)	207 (92%)	14 (6%)	4 (2%)	6	31
3	C	182/211 (86%)	148 (81%)	18 (10%)	16 (9%)	0	3
3	R	199/211 (94%)	159 (80%)	22 (11%)	18 (9%)	0	3
All	All	1249/1328 (94%)	1115 (89%)	90 (7%)	44 (4%)	3	17

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	145	SER
1	B	214	ARG
3	R	27	GLY
3	R	29	ASP
3	R	45	GLU
3	R	104	ASP

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Mol	Chain	Res	Type
3	R	117	GLU
3	R	151	GLU
3	R	154	ALA
3	R	171	SER
3	R	173	HIS
3	C	29	ASP
3	C	31	GLY
3	C	32	LEU
3	C	84	GLN
1	B	31	SER
2	A	171	SER
3	R	43	GLU
3	R	44	GLY
3	R	48	MET
3	R	140	PHE
3	R	172	LEU
3	R	187	ASP
3	R	210	ASP
3	C	85	MET
3	C	136	LYS
3	C	149	LYS
3	C	162	GLY
2	H	171	SER
3	R	4	PRO
3	R	206	PHE
3	C	28	THR
3	C	33	PRO
3	C	108	GLU
3	C	137	THR
2	H	146	THR
3	C	36	TYR
3	C	69	THR
3	C	186	PRO
1	L	31	SER
1	L	215	GLY
2	H	157	VAL
3	C	104	ASP
2	A	157	VAL

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	B	190/192 (99%)	173 (91%)	17 (9%)	9	32
1	L	191/192 (100%)	174 (91%)	17 (9%)	9	32
2	A	181/197 (92%)	152 (84%)	29 (16%)	2	11
2	H	185/197 (94%)	160 (86%)	25 (14%)	4	17
3	C	165/191 (86%)	121 (73%)	44 (27%)	0	2
3	R	183/191 (96%)	149 (81%)	34 (19%)	1	8
All	All	1095/1160 (94%)	929 (85%)	166 (15%)	3	13

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	SER
1	L	12	LEU
1	L	19	ARG
1	L	21	THR
1	L	30	VAL
1	L	51	SER
1	L	66	SER
1	L	68	SER
1	L	75	THR
1	L	78	SER
1	L	103	GLN
1	L	145	ARG
1	L	165	SER
1	L	172	LYS
1	L	179	SER
1	L	193	LYS
1	L	200	THR
2	H	4	GLU
2	H	9	GLU
2	H	15	VAL
2	H	20	SER
2	H	21	LEU

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Mol	Chain	Res	Type
2	H	24	SER
2	H	53	TYR
2	H	67	VAL
2	H	90	ARG
2	H	101	ARG
2	H	115	MET
2	H	122	THR
2	H	153	LEU
2	H	156	LEU
2	H	157	VAL
2	H	158	LYS
2	H	165	VAL
2	H	175	THR
2	H	185	LEU
2	H	187	SER
2	H	192	SER
2	H	193	LEU
2	H	198	THR
2	H	216	LYS
2	H	230	SER
1	B	1	SER
1	B	12	LEU
1	B	19	ARG
1	B	21	THR
1	B	30	VAL
1	B	51	SER
1	B	57	SER
1	B	68	SER
1	B	75	THR
1	B	78	SER
1	B	103	GLN
1	B	108	GLU
1	B	145	ARG
1	B	165	SER
1	B	172	LYS
1	B	179	SER
1	B	200	THR
2	A	4	GLU
2	A	8	VAL
2	A	15	VAL
2	A	16	GLN
2	A	20	SER

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Mol	Chain	Res	Type
2	A	21	LEU
2	A	33	SER
2	A	53	TYR
2	A	62	SER
2	A	67	VAL
2	A	68	LYS
2	A	90	ARG
2	A	101	ARG
2	A	115	MET
2	A	122	THR
2	A	153	LEU
2	A	155	CYS
2	A	156	LEU
2	A	157	VAL
2	A	158	LYS
2	A	165	VAL
2	A	175	THR
2	A	185	LEU
2	A	187	SER
2	A	192	SER
2	A	193	LEU
2	A	222	VAL
2	A	226	VAL
2	A	227	GLU
3	R	17	LYS
3	R	28	THR
3	R	39	THR
3	R	56	THR
3	R	70	SER
3	R	73	ARG
3	R	74	THR
3	R	78	MET
3	R	80	ASN
3	R	84	GLN
3	R	85	MET
3	R	87	SER
3	R	100	ILE
3	R	123	LEU
3	R	128	SER
3	R	132	LEU
3	R	133	ILE
3	R	140	PHE

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Mol	Chain	Res	Type
3	R	141	THR
3	R	142	LEU
3	R	143	LEU
3	R	148	LEU
3	R	158	ILE
3	R	165	THR
3	R	170	LEU
3	R	171	SER
3	R	173	HIS
3	R	179	LEU
3	R	182	VAL
3	R	183	ARG
3	R	200	ILE
3	R	202	ILE
3	R	208	MET
3	R	211	THR
3	C	13	ARG
3	C	25	ARG
3	C	29	ASP
3	C	32	LEU
3	C	34	THR
3	C	38	LEU
3	C	42	ARG
3	C	47	LEU
3	C	56	THR
3	C	67	GLN
3	C	73	ARG
3	C	78	MET
3	C	80	ASN
3	C	82	THR
3	C	88	SER
3	C	93	LEU
3	C	100	ILE
3	C	107	LEU
3	C	114	LYS
3	C	123	LEU
3	C	128	SER
3	C	131	THR
3	C	132	LEU
3	C	133	ILE
3	C	135	LEU
3	C	137	THR

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Mol	Chain	Res	Type
3	C	139	TRP
3	C	140	PHE
3	C	141	THR
3	C	143	LEU
3	C	148	LEU
3	C	149	LYS
3	C	158	ILE
3	C	164	GLN
3	C	168	LYS
3	C	169	ILE
3	C	170	LEU
3	C	179	LEU
3	C	180	VAL
3	C	182	VAL
3	C	183	ARG
3	C	184	CYS
3	C	185	LYS
3	C	201	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	4	GLN
1	L	103	GLN
1	L	141	ASN
1	L	192	HIS
1	L	201	HIS
1	L	202	GLN
1	L	213	ASN
2	H	16	GLN
2	H	38	HIS
2	H	207	GLN
1	B	103	GLN
1	B	192	HIS
1	B	201	HIS
1	B	202	GLN
2	A	16	GLN
2	A	38	HIS
2	A	109	ASN
2	A	120	GLN
2	A	179	HIS
2	A	207	GLN

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Mol	Chain	Res	Type
2	A	214	ASN
2	A	219	ASN
3	R	41	HIS
3	R	49	HIS
3	R	80	ASN
3	R	83	ASN
3	R	115	GLN
3	R	209	ASN
3	C	67	GLN
3	C	83	ASN
3	C	159	HIS
3	C	201	GLN

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](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ACT	R	301	-	3,3,3	1.45	0	3,3,3	0.75	0
4	GOL	H	302	-	5,5,5	1.29	0	5,5,5	1.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	L	301	-	5,5,5	0.41	0	5,5,5	0.32	0
4	GOL	C	301	-	5,5,5	0.52	0	5,5,5	0.55	0
4	GOL	A	301	-	5,5,5	0.35	0	5,5,5	0.85	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	A	301	-	-	0/4/4/4	-
4	GOL	C	301	-	-	2/4/4/4	-
4	GOL	H	302	-	-	1/4/4/4	-
4	GOL	L	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	301	GOL	C1-C2-C3-O3
4	L	301	GOL	O2-C2-C3-O3
4	C	301	GOL	O1-C1-C2-C3
4	C	301	GOL	O1-C1-C2-O2
4	H	302	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	301	ACT	2	0
4	H	302	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	B	215/217 (99%)	0.63	24 (11%) 10 7	34, 76, 121, 134	0
1	L	216/217 (99%)	-0.10	0 100 100	35, 51, 70, 89	0
2	A	220/236 (93%)	-0.21	3 (1%) 73 54	28, 42, 94, 116	0
2	H	227/236 (96%)	-0.17	3 (1%) 75 56	28, 42, 88, 105	0
3	C	188/211 (89%)	0.64	22 (11%) 9 7	37, 71, 119, 144	0
3	R	205/211 (97%)	0.47	21 (10%) 12 8	30, 53, 109, 159	0
All	All	1271/1328 (95%)	0.19	73 (5%) 29 19	28, 52, 108, 159	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	139	TRP	6.4
3	C	85	MET	6.3
3	C	121	PRO	5.9
3	R	3	PRO	5.9
1	B	215	GLY	5.9
3	R	31	GLY	5.7
3	R	211	THR	5.6
3	C	177	LYS	5.3
3	C	32	LEU	5.1
3	C	3	PRO	5.0
3	C	113	VAL	4.5
3	R	4	PRO	4.4
3	C	114	LYS	4.4
1	B	191	LYS	3.9
1	B	207	PRO	3.8
3	C	178	TYR	3.8
3	R	137	THR	3.8
3	R	30	GLY	3.7
2	H	146	THR	3.7

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Mol	Chain	Res	Type	RSRZ
3	R	46	THR	3.5
1	B	193	LYS	3.4
1	B	202	GLN	3.3
1	B	77	SER	3.3
2	A	149	GLY	3.2
3	C	31	GLY	3.2
3	R	27	GLY	3.1
3	C	122	TYR	3.1
3	R	44	GLY	3.0
1	B	157	LEU	3.0
2	H	205	GLY	2.9
1	B	205	SER	2.9
3	C	170	LEU	2.9
1	B	194	VAL	2.9
2	H	230	SER	2.8
3	C	171	SER	2.8
3	R	5	GLY	2.7
3	R	73	ARG	2.7
3	R	28	THR	2.7
1	B	154	ASP	2.7
3	C	139	TRP	2.7
2	A	228	PRO	2.7
3	C	160	PHE	2.7
2	A	204	LEU	2.7
3	R	85	MET	2.6
1	B	150	GLN	2.6
1	B	159	SER	2.6
1	B	172	LYS	2.6
3	C	201	GLN	2.5
3	C	154	ALA	2.4
3	R	47	LEU	2.4
3	C	124	TRP	2.4
1	B	146	GLU	2.4
3	R	94	TYR	2.4
1	B	152	LYS	2.4
1	B	208	VAL	2.4
1	B	192	HIS	2.3
1	B	195	TYR	2.3
3	C	82	THR	2.3
1	B	113	VAL	2.2
3	R	138	GLY	2.2
3	R	74	THR	2.2

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Mol	Chain	Res	Type	RSRZ
3	R	187	ASP	2.2
3	C	137	THR	2.1
3	C	126	LYS	2.1
1	B	213	ASN	2.1
3	C	184	CYS	2.1
3	R	48	MET	2.1
1	B	196	ALA	2.1
3	C	151	GLU	2.1
1	B	190	GLU	2.1
3	R	184	CYS	2.1
1	B	204	LEU	2.0
1	B	163	GLN	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	H	302	6/6	0.89	0.18	37,53,61,62	0
6	ACT	R	301	4/4	0.92	0.25	43,47,50,51	0
4	GOL	L	301	6/6	0.94	0.11	46,55,66,75	0
5	CA	B	301	1/1	0.95	0.07	53,53,53,53	0
4	GOL	C	301	6/6	0.96	0.14	46,53,56,59	0
5	CA	H	301	1/1	0.97	0.06	52,52,52,52	0
4	GOL	A	301	6/6	0.98	0.06	32,34,37,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.