



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:35 AM UTC

PDB ID : 6M2M / pdb_00006m2m
Title : A role for histone chaperone OsChz1 in histone recognition and deposition
Authors : Luo, Q.; Wang, B.
Deposited on : 2020-02-28
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

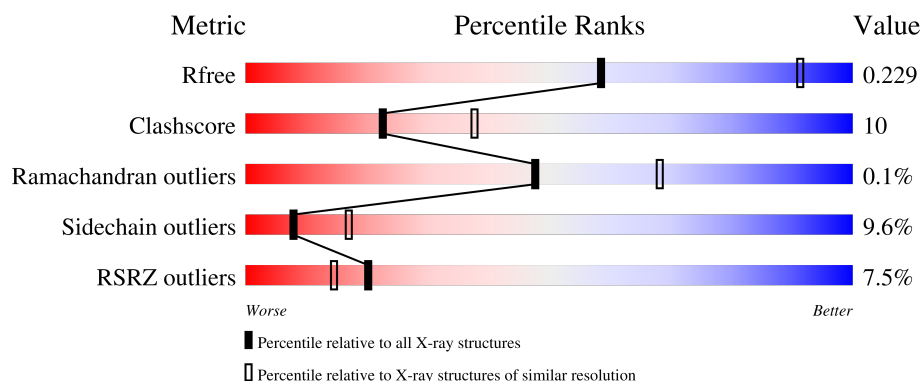
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	93	75% 18% • 5%
1	C	93	75% 16% • 5%
1	E	93	72% 22% • 5%
1	G	93	14% 57% 23% 5% 15%
1	I	93	12% 58% 25% • 14%

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Mol	Chain	Length	Quality of chain
1	K	93	18%69%12%6%13%
2	B	98	2%72%14%•12%
2	D	98	6%64%24%•10%
2	F	98	%62%20%••12%
2	H	98	2%67%21%•10%
2	J	98	11%64%23%•9%
2	L	98	6%76%14%•9%
3	M	105	%8%•90%
3	N	105	5%13%•86%
3	O	105	2%9%••88%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8020 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 Probable histone H2A.3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	E	88	Total	C	N	O	0	0	0
			666	421	124	121			
1	A	88	Total	C	N	O	0	0	0
			666	421	124	121			
1	C	88	Total	C	N	O	0	0	0
			666	421	124	121			
1	G	79	Total	C	N	O	0	0	0
			575	369	103	103			
1	I	80	Total	C	N	O	0	0	0
			582	372	102	108			
1	K	81	Total	C	N	O	0	0	0
			552	358	97	97			

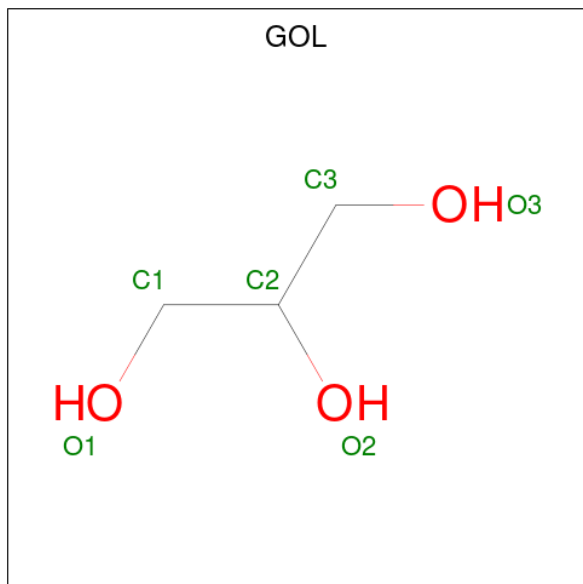
- Molecule 2 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	88	Total	C	N	O	S	0	0	0
			676	435	114	125	2			
2	F	86	Total	C	N	O	S	0	0	0
			655	421	110	122	2			
2	J	89	Total	C	N	O	S	0	0	0
			649	412	112	123	2			
2	H	88	Total	C	N	O	S	0	0	0
			666	427	112	125	2			
2	L	89	Total	C	N	O	S	0	0	0
			669	425	115	127	2			
2	B	86	Total	C	N	O	S	0	0	0
			664	426	114	122	2			

- Molecule 3 is a protein called Expressed protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	10	Total	C	N	O	0	0	0
			81	43	11	27			
3	N	15	Total	C	N	O	0	0	0
			121	67	17	37			
3	O	13	Total	C	N	O	0	0	0
			100	54	15	31			

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	2	Total	O	0	0
			2	2		
5	A	3	Total	O	0	0
			3	3		
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	O 1	0	0
5	I	1	Total 1	O 1	0	0
5	F	3	Total 3	O 3	0	0
5	H	1	Total 1	O 1	0	0
5	B	1	Total 1	O 1	0	0

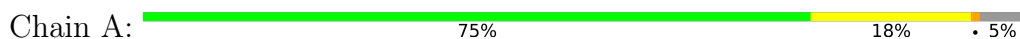
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

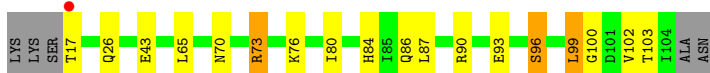
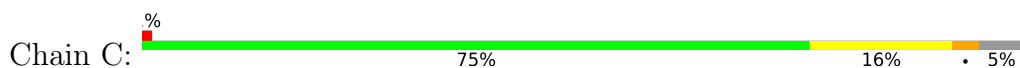
- Molecule 1: Probable histone H2A.3



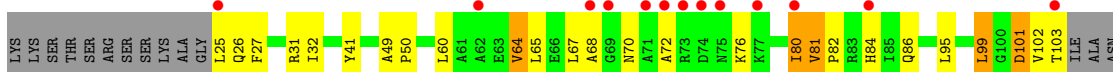
- Molecule 1: Probable histone H2A.3



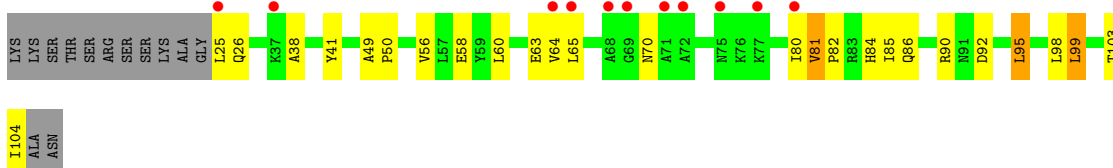
- Molecule 1: Probable histone H2A.3



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- Molecule 1: Probable histone H2A.3



- Molecule 1: Probable histone H2A.3



- Molecule 2: Histone H2B.1



- Molecule 2: Histone H2B.1



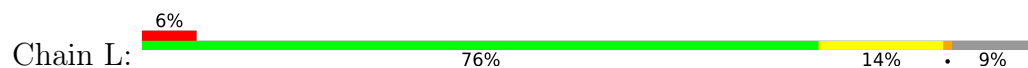
- Molecule 2: Histone H2B.1



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- Molecule 2: Histone H2B.1

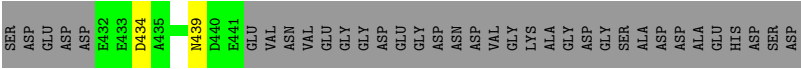
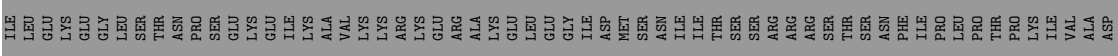


- Molecule 2: Histone H2B.1

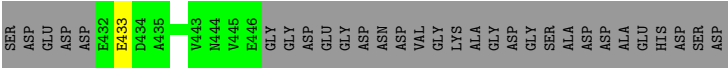
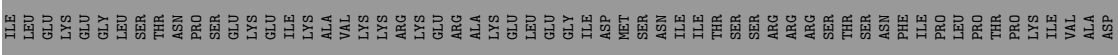




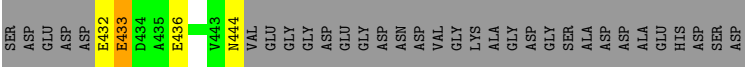
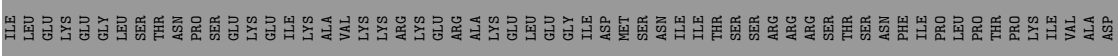
● Molecule 3: Expressed protein



● Molecule 3: Expressed protein



● Molecule 3: Expressed protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.36Å 116.34Å 101.90Å 90.00° 114.98° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85 30.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.85) 94.5 (30.00-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.194 , 0.253 (Not available) , 0.229	Depositor DCC
R_{free} test set	1890 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.447 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.450 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8020	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: 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	1.28	0/674	1.11	4/910 (0.4%)
1	C	1.15	0/674	1.23	3/910 (0.3%)
1	E	1.24	1/674 (0.1%)	1.22	3/910 (0.3%)
1	G	1.02	0/583	1.23	1/793 (0.1%)
1	I	1.04	0/590	1.32	6/805 (0.7%)
1	K	0.98	0/560	1.23	2/766 (0.3%)
2	B	1.05	0/674	1.17	0/908
2	D	1.04	0/687	1.20	2/927 (0.2%)
2	F	1.24	0/665	1.14	4/898 (0.4%)
2	H	1.20	0/676	1.21	3/914 (0.3%)
2	J	1.28	3/659 (0.5%)	1.32	5/893 (0.6%)
2	L	1.03	0/679	1.26	3/917 (0.3%)
3	M	0.80	0/80	0.79	0/107
3	N	1.07	0/120	0.98	0/162
3	O	1.05	0/99	1.06	0/133
All	All	1.13	4/8094 (0.0%)	1.21	36/10953 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	82	ALA	N-CA	5.72	1.53	1.46
2	J	122	VAL	C-O	-5.51	1.17	1.24
1	E	87	LEU	CA-C	-5.14	1.46	1.52
2	J	143	THR	C-O	-5.04	1.18	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	72	VAL	N-CA-C	10.24	120.16	110.53
2	J	108	ASN	N-CA-C	9.53	121.26	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	41	TYR	N-CA-C	-8.32	102.15	111.14
2	L	108	ASN	N-CA-C	8.05	120.05	111.28
2	L	61	TYR	N-CA-C	-8.03	101.38	112.30
1	I	98	LEU	N-CA-C	7.28	119.00	111.14
2	F	143	THR	N-CA-C	7.23	118.95	111.14
1	G	101	ASP	N-CA-C	-7.08	96.97	108.52
2	F	124	LEU	N-CA-C	7.02	119.01	111.36
1	E	94	GLU	N-CA-C	6.82	118.80	111.36
2	F	63	ILE	CB-CA-C	-6.82	103.25	111.97
2	D	109	LYS	N-CA-C	6.78	120.88	112.47
2	J	89	PHE	N-CA-C	6.77	121.37	113.18
1	I	95	LEU	N-CA-C	6.73	118.69	111.36
1	C	73	ARG	CB-CA-C	-6.68	100.40	110.88
2	J	109	LYS	N-CA-C	6.50	120.38	111.54
2	H	143	THR	N-CA-C	-6.40	99.58	109.76
2	F	62	LYS	N-CA-C	6.40	118.25	111.28
1	C	99	LEU	N-CA-C	6.14	120.88	112.04
1	A	100	GLY	N-CA-C	-6.10	103.00	112.45
2	H	128	GLY	N-CA-C	6.02	122.39	110.77
1	K	71	ALA	N-CA-C	-5.99	104.75	111.28
1	C	76	LYS	N-CA-C	5.69	119.27	111.54
2	D	108	ASN	N-CA-C	5.68	118.40	111.82
1	I	38	ALA	N-CA-C	5.63	117.41	111.28
2	L	109	LYS	N-CA-C	5.51	119.04	111.54
1	K	41	TYR	N-CA-C	-5.50	104.80	112.45
1	I	92	ASP	N-CA-C	5.47	117.66	108.96
1	A	76	LYS	N-CA-C	5.39	119.02	111.90
1	E	76	LYS	N-CA-C	5.36	118.97	111.90
2	J	130	LEU	N-CA-C	-5.32	105.48	111.28
1	A	94	GLU	N-CA-C	5.18	117.01	111.36
1	A	95	LEU	N-CA-C	5.14	116.89	111.28
1	I	85	ILE	N-CA-C	-5.07	105.56	110.42
1	E	20	SER	N-CA-C	-5.02	105.28	111.40
2	J	89	PHE	N-CA-CB	5.01	118.83	110.41

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	666	0	694	11	0
1	C	666	0	694	10	0
1	E	666	0	694	19	0
1	G	575	0	575	31	0
1	I	582	0	570	28	0
1	K	552	0	528	19	0
2	B	664	0	691	8	0
2	D	676	0	695	20	0
2	F	655	0	671	25	0
2	H	666	0	678	16	0
2	J	649	0	626	19	0
2	L	669	0	673	8	0
3	M	81	0	50	2	0
3	N	121	0	86	0	0
3	O	100	0	66	6	0
4	A	6	0	8	1	0
4	C	6	0	8	0	0
4	F	6	0	8	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
5	F	3	0	0	2	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
All	All	8020	0	8015	168	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 10.

All (168) 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:I:64:VAL:CG1	2:J:86:MET:HE1	1.35	1.56
1:E:99:LEU:HD21	2:F:89:PHE:CE1	1.62	1.34
1:I:81:VAL:HG22	1:I:82:PRO:CD	1.69	1.22
1:E:99:LEU:HD21	2:F:89:PHE:CD1	1.74	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:64:VAL:CG1	2:J:86:MET:CE	2.28	1.11
1:I:81:VAL:HG22	1:I:82:PRO:HD2	1.26	1.10
1:I:64:VAL:HG11	2:J:86:MET:HE1	1.20	1.10
1:I:64:VAL:HG12	2:J:86:MET:HE1	1.11	1.07
1:K:95:LEU:O	1:K:99:LEU:HD12	1.62	0.99
1:E:99:LEU:CD2	2:F:89:PHE:CD1	2.48	0.96
1:I:64:VAL:HG12	2:J:86:MET:CE	1.92	0.93
1:I:81:VAL:HG22	1:I:82:PRO:HD3	1.47	0.93
1:K:99:LEU:HD12	1:K:99:LEU:H	1.34	0.91
2:F:63:ILE:HG12	5:F:302:HOH:O	1.69	0.90
2:D:64:TYR:O	2:D:68:VAL:HG23	1.76	0.85
1:G:68:ALA:CB	1:G:80:ILE:HD13	2.07	0.84
1:I:64:VAL:HG11	2:J:86:MET:CE	2.02	0.84
1:I:81:VAL:CG2	1:I:82:PRO:CD	2.55	0.83
1:G:68:ALA:HB1	1:G:80:ILE:CD1	2.10	0.81
1:G:68:ALA:HB1	1:G:80:ILE:HD13	1.62	0.80
1:C:73:ARG:HH11	2:H:73:HIS:HD2	1.28	0.79
1:K:104:ILE:HD12	1:K:104:ILE:O	1.80	0.79
1:E:99:LEU:CD2	2:F:89:PHE:CE1	2.58	0.79
1:A:41:TYR:O	2:B:102:SER:HB2	1.83	0.79
1:I:81:VAL:CG2	1:I:82:PRO:HD2	2.12	0.79
2:F:116:ARG:HD3	3:O:432:GLU:HA	1.65	0.79
1:C:99:LEU:HD11	2:H:89:PHE:CE1	2.18	0.79
1:E:19:ARG:H	1:E:19:ARG:HD3	1.49	0.78
1:G:68:ALA:CB	1:G:80:ILE:CD1	2.62	0.78
1:C:43:GLU:HG2	2:D:110:LYS:HD2	1.64	0.78
1:E:19:ARG:H	1:E:19:ARG:CD	1.96	0.78
1:K:25:LEU:HD23	1:K:25:LEU:N	2.01	0.76
2:D:60:THR:HG22	2:D:62:LYS:H	1.53	0.73
1:K:99:LEU:HD12	1:K:99:LEU:N	2.02	0.72
2:L:102:SER:O	2:L:106:ARG:HG3	1.89	0.71
1:I:81:VAL:CG2	1:I:82:PRO:HD3	2.20	0.69
1:K:70:ASN:HD22	1:K:70:ASN:N	1.89	0.68
2:B:140:LYS:HG3	3:M:439:ASN:HD22	1.57	0.68
1:K:40:LYS:HD3	1:K:40:LYS:C	2.21	0.66
1:G:70:ASN:HD22	1:G:70:ASN:N	1.92	0.66
1:I:95:LEU:O	1:I:99:LEU:HD12	1.94	0.66
2:D:65:ILE:CG2	1:G:65:LEU:HD11	2.26	0.65
1:K:95:LEU:O	1:K:99:LEU:CD1	2.42	0.65
2:J:102:SER:O	2:J:106:ARG:HG3	1.97	0.64
1:E:75:ASN:HD22	1:E:84:HIS:HE1	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:104:ILE:HD12	1:K:104:ILE:C	2.20	0.64
1:K:81:VAL:HG23	1:K:84:HIS:CD2	2.33	0.63
2:F:123:ARG:NH1	2:F:135:VAL:HG11	2.13	0.62
1:G:103:THR:HG22	1:G:103:THR:O	1.98	0.61
1:G:68:ALA:HB3	1:G:80:ILE:HD13	1.82	0.61
1:I:81:VAL:HG23	2:J:79:SER:CB	2.30	0.61
2:D:73:HIS:HB3	2:D:76:ILE:HG13	1.82	0.61
1:C:73:ARG:NH1	2:L:116:ARG:HD3	2.17	0.60
2:D:65:ILE:HG22	1:G:65:LEU:HD11	1.83	0.60
2:F:60:THR:OG1	2:F:62:LYS:HG3	2.02	0.60
2:F:62:LYS:HD3	2:F:83:MET:HG3	1.82	0.60
1:K:60:LEU:HD21	2:B:126:LEU:HD21	1.84	0.59
2:L:64:TYR:O	2:L:68:VAL:HG23	2.02	0.59
1:K:44:ARG:HG2	1:K:44:ARG:HH11	1.68	0.58
1:G:49:ALA:HB3	1:G:50:PRO:HD3	1.85	0.58
2:H:145:PHE:C	2:H:146:THR:HG23	2.29	0.58
2:J:79:SER:CB	2:J:82:ALA:CB	2.81	0.57
1:A:52:TYR:OH	2:L:119:GLN:NE2	2.34	0.57
2:H:60:THR:HB	2:H:62:LYS:HG3	1.86	0.57
1:G:67:LEU:N	1:G:67:LEU:HD23	2.19	0.57
1:G:68:ALA:HB3	1:G:80:ILE:CD1	2.33	0.57
2:J:83:MET:HE2	2:J:83:MET:HA	1.85	0.56
1:G:68:ALA:CB	1:G:80:ILE:HD11	2.34	0.55
2:B:140:LYS:HG3	3:M:439:ASN:ND2	2.19	0.55
1:I:84:HIS:H	1:I:84:HIS:HD1	1.54	0.55
1:I:49:ALA:HB3	1:I:50:PRO:HD3	1.88	0.55
2:D:61:TYR:O	2:D:65:ILE:HG13	2.07	0.54
2:D:66:PHE:O	2:D:69:LEU:HB3	2.06	0.54
1:I:60:LEU:HD21	2:F:126:LEU:HD21	1.90	0.54
1:K:49:ALA:HB3	1:K:50:PRO:HD3	1.90	0.54
1:I:86:GLN:OE1	1:I:104:ILE:HD11	2.08	0.54
2:D:62:LYS:CB	2:D:83:MET:SD	2.97	0.54
1:A:19:ARG:HH21	4:A:201:GOL:H32	1.72	0.53
1:G:81:VAL:HG22	1:G:84:HIS:HD2	1.73	0.53
2:F:94:PHE:C	2:F:94:PHE:CD1	2.86	0.53
1:A:70:ASN:ND2	2:J:120:THR:OG1	2.42	0.53
1:I:99:LEU:HD12	1:I:99:LEU:H	1.73	0.53
1:I:81:VAL:HG12	1:I:84:HIS:CE1	2.43	0.53
1:I:26:GLN:N	1:I:58:GLU:OE2	2.41	0.53
1:A:77:LYS:O	2:F:107:TYR:OH	2.23	0.52
1:I:70:ASN:HD22	1:I:70:ASN:N	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:81:VAL:HG12	1:I:84:HIS:HE1	1.75	0.52
1:E:70:ASN:ND2	2:D:120:THR:HG23	2.25	0.51
1:G:68:ALA:C	1:G:80:ILE:HD11	2.36	0.51
2:D:72:VAL:HG22	2:D:72:VAL:O	2.12	0.50
1:G:25:LEU:C	1:G:25:LEU:HD23	2.36	0.50
1:K:70:ASN:N	1:K:70:ASN:ND2	2.60	0.50
1:G:60:LEU:HD21	2:H:126:LEU:HD21	1.92	0.50
1:G:70:ASN:N	1:G:70:ASN:ND2	2.60	0.50
1:G:81:VAL:HG22	1:G:84:HIS:CD2	2.47	0.50
2:F:116:ARG:HD3	3:O:432:GLU:CA	2.39	0.50
2:J:118:ILE:O	2:J:122:VAL:HG23	2.12	0.49
1:A:80:ILE:HA	1:A:84:HIS:HD2	1.77	0.49
1:G:25:LEU:C	1:G:25:LEU:CD2	2.85	0.49
1:I:56:VAL:HG21	2:F:122:VAL:HG21	1.93	0.49
2:J:79:SER:CB	2:J:82:ALA:HB2	2.42	0.49
1:I:99:LEU:HD12	1:I:99:LEU:N	2.28	0.49
2:F:60:THR:HG23	5:F:302:HOH:O	2.11	0.49
1:G:81:VAL:HG23	1:G:82:PRO:HD2	1.96	0.48
1:E:17:THR:HG22	1:E:17:THR:O	2.13	0.48
1:G:72:ALA:O	1:G:76:LYS:N	2.47	0.48
1:A:44:ARG:NH1	2:B:117:GLU:OE2	2.46	0.48
2:H:145:PHE:O	2:H:146:THR:CG2	2.62	0.48
2:D:102:SER:OG	1:G:41:TYR:O	2.31	0.48
1:K:56:VAL:HG21	2:B:122:VAL:HG21	1.95	0.48
1:C:80:ILE:HA	1:C:84:HIS:HD2	1.79	0.47
1:K:31:ARG:NH2	2:L:60:THR:O	2.47	0.47
2:J:123:ARG:HD3	2:J:135:VAL:HG21	1.96	0.47
1:G:86:GLN:NE2	1:G:102:VAL:O	2.40	0.47
2:H:73:HIS:HB3	2:H:76:ILE:HB	1.97	0.47
1:I:65:LEU:HD11	2:J:65:ILE:HG23	1.97	0.46
2:J:79:SER:CB	2:J:82:ALA:HB3	2.45	0.46
1:C:96:SER:O	1:C:100:GLY:N	2.43	0.46
2:D:73:HIS:HB3	2:D:76:ILE:CG1	2.46	0.46
2:D:67:LYS:CD	1:G:26:GLN:OE1	2.64	0.46
2:F:63:ILE:HG12	2:F:63:ILE:H	1.40	0.46
1:E:44:ARG:HD3	2:J:110:LYS:HB2	1.99	0.46
1:E:99:LEU:CD2	2:F:89:PHE:HD1	2.17	0.46
1:C:65:LEU:HD22	2:H:69:LEU:HD13	1.98	0.46
2:D:67:LYS:HD2	1:G:26:GLN:OE1	2.15	0.46
2:F:143:THR:HG21	3:O:436:GLU:OE1	2.16	0.45
1:C:26:GLN:HE21	1:C:26:GLN:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:PRO:HB3	1:E:104:ILE:HD12	1.98	0.45
2:D:83:MET:HA	2:D:83:MET:HE2	1.99	0.45
2:D:65:ILE:HG23	1:G:65:LEU:HD11	1.97	0.45
2:H:145:PHE:C	2:H:146:THR:CG2	2.89	0.45
2:F:116:ARG:NE	3:O:433:GLU:H	2.14	0.45
1:K:25:LEU:N	1:K:25:LEU:CD2	2.72	0.44
1:I:99:LEU:HD23	2:J:89:PHE:HB2	2.00	0.44
2:F:116:ARG:CD	3:O:432:GLU:HA	2.42	0.44
1:K:81:VAL:HG23	1:K:84:HIS:NE2	2.32	0.44
1:K:104:ILE:C	1:K:104:ILE:CD1	2.85	0.44
1:E:90:ARG:NH2	1:E:101:ASP:OD1	2.50	0.44
2:L:60:THR:OG1	2:L:62:LYS:CB	2.66	0.43
1:G:68:ALA:HB1	1:G:80:ILE:HD11	1.96	0.43
1:C:86:GLN:HA	1:C:102:VAL:HB	2.00	0.43
1:A:26:GLN:HE21	1:A:26:GLN:HA	1.84	0.43
1:E:99:LEU:HD21	2:F:89:PHE:HE1	1.57	0.43
2:L:92:ASP:OD1	2:L:96:LYS:HE2	2.18	0.42
1:E:17:THR:HA	1:E:19:ARG:NH2	2.34	0.42
2:F:116:ARG:HE	2:F:116:ARG:HB2	1.60	0.42
1:E:23:ALA:O	2:J:144:LYS:HD2	2.19	0.42
1:A:73:ARG:HG2	2:B:76:ILE:HD11	2.02	0.42
1:C:70:ASN:ND2	2:L:120:THR:OG1	2.53	0.42
1:G:64:VAL:HG12	1:G:65:LEU:N	2.34	0.42
2:H:93:ILE:HG23	2:H:93:ILE:HD12	1.79	0.42
2:H:94:PHE:CD1	2:H:94:PHE:C	2.97	0.42
1:A:72:ALA:HB2	1:A:84:HIS:CD2	2.55	0.42
1:E:82:PRO:CB	1:E:104:ILE:HD12	2.50	0.42
2:H:61:TYR:O	2:H:62:LYS:C	2.63	0.41
1:G:95:LEU:O	1:G:99:LEU:HD22	2.20	0.41
2:H:62:LYS:HD3	2:H:83:MET:HG3	2.03	0.41
1:A:73:ARG:NH1	2:B:76:ILE:HD12	2.35	0.41
2:D:91:ASN:HD22	2:D:91:ASN:N	2.18	0.41
2:F:102:SER:O	2:F:103:LYS:C	2.62	0.41
2:D:60:THR:O	1:G:31:ARG:NH2	2.53	0.41
1:E:66:GLU:O	2:F:73:HIS:HE1	2.04	0.41
1:E:73:ARG:HB3	2:H:104:LEU:HD22	2.03	0.41
1:I:86:GLN:O	1:I:90:ARG:HB2	2.20	0.41
2:H:145:PHE:O	2:H:146:THR:HG23	2.20	0.41
2:D:120:THR:O	2:D:124:LEU:HG	2.21	0.40
2:H:108:ASN:HD22	2:H:110:LYS:H	1.68	0.40
2:F:116:ARG:HD3	3:O:432:GLU:CB	2.52	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	86/93 (92%)	84 (98%)	2 (2%)	0	100	100
1	C	86/93 (92%)	84 (98%)	2 (2%)	0	100	100
1	E	86/93 (92%)	85 (99%)	1 (1%)	0	100	100
1	G	77/93 (83%)	70 (91%)	7 (9%)	0	100	100
1	I	78/93 (84%)	70 (90%)	8 (10%)	0	100	100
1	K	79/93 (85%)	70 (89%)	9 (11%)	0	100	100
2	B	84/98 (86%)	81 (96%)	3 (4%)	0	100	100
2	D	86/98 (88%)	83 (96%)	3 (4%)	0	100	100
2	F	84/98 (86%)	80 (95%)	4 (5%)	0	100	100
2	H	86/98 (88%)	84 (98%)	2 (2%)	0	100	100
2	J	87/98 (89%)	83 (95%)	4 (5%)	0	100	100
2	L	87/98 (89%)	81 (93%)	6 (7%)	0	100	100
3	M	8/105 (8%)	6 (75%)	2 (25%)	0	100	100
3	N	13/105 (12%)	11 (85%)	2 (15%)	0	100	100
3	O	11/105 (10%)	9 (82%)	1 (9%)	1 (9%)	0	0
All	All	1038/1461 (71%)	981 (94%)	56 (5%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	O	433	GLU

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	66/71 (93%)	62 (94%)	4 (6%)	17	35
1	C	66/71 (93%)	60 (91%)	6 (9%)	9	19
1	E	66/71 (93%)	62 (94%)	4 (6%)	17	35
1	G	52/71 (73%)	45 (86%)	7 (14%)	4	7
1	I	53/71 (75%)	47 (89%)	6 (11%)	5	11
1	K	44/71 (62%)	37 (84%)	7 (16%)	2	4
2	B	72/87 (83%)	62 (86%)	10 (14%)	3	6
2	D	73/87 (84%)	67 (92%)	6 (8%)	10	23
2	F	70/87 (80%)	59 (84%)	11 (16%)	2	4
2	H	71/87 (82%)	67 (94%)	4 (6%)	19	40
2	J	64/87 (74%)	57 (89%)	7 (11%)	6	12
2	L	71/87 (82%)	69 (97%)	2 (3%)	38	62
3	M	9/90 (10%)	8 (89%)	1 (11%)	6	12
3	N	14/90 (16%)	13 (93%)	1 (7%)	13	28
3	O	11/90 (12%)	10 (91%)	1 (9%)	9	19
All	All	802/1218 (66%)	725 (90%)	77 (10%)	8	17

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	18	SER
1	E	90	ARG
1	E	93	GLU
1	E	96	SER
1	A	44	ARG
1	A	93	GLU
1	A	96	SER
1	A	103	THR
1	C	17	THR
1	C	87	LEU

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Mol	Chain	Res	Type
1	C	90	ARG
1	C	93	GLU
1	C	96	SER
1	C	103	THR
2	D	63	ILE
2	D	66	PHE
2	D	75	ASP
2	D	78	ILE
2	D	116	ARG
2	D	146	THR
1	G	27	PHE
1	G	32	ILE
1	G	64	VAL
1	G	80	ILE
1	G	81	VAL
1	G	99	LEU
1	G	101	ASP
1	I	25	LEU
1	I	63	GLU
1	I	80	ILE
1	I	81	VAL
1	I	99	LEU
1	I	103	THR
1	K	25	LEU
1	K	40	LYS
1	K	70	ASN
1	K	81	VAL
1	K	99	LEU
1	K	103	THR
1	K	104	ILE
2	F	63	ILE
2	F	72	VAL
2	F	95	GLU
2	F	96	LYS
2	F	99	GLN
2	F	107	TYR
2	F	108	ASN
2	F	123	ARG
2	F	130	LEU
2	F	142	VAL
2	F	144	LYS
2	J	61	TYR

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Mol	Chain	Res	Type
2	J	85	ILE
2	J	87	ASN
2	J	88	SER
2	J	116	ARG
2	J	140	LYS
2	J	146	THR
2	H	95	GLU
2	H	108	ASN
2	H	115	SER
2	H	142	VAL
2	L	72	VAL
2	L	116	ARG
2	B	63	ILE
2	B	72	VAL
2	B	95	GLU
2	B	96	LYS
2	B	107	TYR
2	B	109	LYS
2	B	117	GLU
2	B	130	LEU
2	B	142	VAL
2	B	143	THR
3	M	434	ASP
3	N	433	GLU
3	O	444	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	26	GLN
1	E	70	ASN
1	E	75	ASN
1	E	84	HIS
1	A	26	GLN
1	A	70	ASN
1	A	75	ASN
1	A	84	HIS
1	C	26	GLN
1	C	70	ASN
1	C	75	ASN
1	C	84	HIS
1	C	91	ASN

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Mol	Chain	Res	Type
2	D	91	ASN
2	D	119	GLN
1	G	70	ASN
1	G	84	HIS
1	I	26	GLN
1	I	70	ASN
1	K	70	ASN
1	K	91	ASN
2	F	108	ASN
2	F	119	GLN
2	J	91	ASN
2	J	119	GLN
2	H	73	HIS
2	H	108	ASN
2	L	73	HIS
2	L	119	GLN
2	B	71	GLN
2	B	99	GLN
2	B	119	GLN
3	M	439	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](#)

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	C	201	-	5,5,5	0.72	0	5,5,5	1.27	1 (20%)
4	GOL	A	201	-	5,5,5	0.52	0	5,5,5	0.48	0
4	GOL	F	201	-	5,5,5	0.68	0	5,5,5	0.82	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	C	201	-	-	4/4/4/4	-
4	GOL	A	201	-	-	0/4/4/4	-
4	GOL	F	201	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	C	201	GOL	O3-C3-C2	2.14	120.02	110.38

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	201	GOL	O1-C1-C2-O2
4	C	201	GOL	O1-C1-C2-C3
4	C	201	GOL	C1-C2-C3-O3
4	C	201	GOL	O2-C2-C3-O3
4	F	201	GOL	O1-C1-C2-C3
4	F	201	GOL	C1-C2-C3-O3
4	F	201	GOL	O2-C2-C3-O3
4	F	201	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	201	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	88/93 (94%)	-0.30	0 100 100	27, 44, 75, 95	0
1	C	88/93 (94%)	-0.34	1 (1%) 78 73	26, 44, 77, 87	0
1	E	88/93 (94%)	-0.31	2 (2%) 61 52	26, 43, 74, 89	0
1	G	79/93 (84%)	0.86	13 (16%) 4 3	38, 79, 123, 134	0
1	I	80/93 (86%)	0.73	11 (13%) 6 5	37, 81, 123, 140	0
1	K	81/93 (87%)	0.97	17 (20%) 2 2	37, 78, 121, 133	0
2	B	86/98 (87%)	-0.22	2 (2%) 61 52	30, 48, 73, 92	0
2	D	88/98 (89%)	0.07	6 (6%) 23 17	29, 49, 106, 111	0
2	F	86/98 (87%)	-0.16	1 (1%) 76 71	30, 50, 75, 97	0
2	H	88/98 (89%)	-0.06	2 (2%) 61 52	31, 49, 82, 91	0
2	J	89/98 (90%)	0.32	11 (12%) 8 6	28, 50, 109, 122	0
2	L	89/98 (90%)	0.12	6 (6%) 24 17	28, 48, 106, 119	0
3	M	10/105 (9%)	0.87	1 (10%) 12 10	89, 95, 115, 117	0
3	N	15/105 (14%)	1.28	5 (33%) 1 1	85, 104, 145, 147	0
3	O	13/105 (12%)	1.11	2 (15%) 5 4	88, 95, 116, 128	0
All	All	1068/1461 (73%)	0.16	80 (7%) 20 14	26, 54, 109, 147	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	78	THR	4.2
1	G	74	ASP	4.0
2	L	65	ILE	4.0
1	K	71	ALA	3.9
3	N	445	VAL	3.8
1	K	74	ASP	3.7
1	E	18	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	80	ILE	3.7
1	G	71	ALA	3.7
2	D	108	ASN	3.6
2	L	109	LYS	3.5
1	K	101	ASP	3.5
1	I	71	ALA	3.4
1	K	80	ILE	3.4
3	N	443	VAL	3.3
2	H	129	GLU	3.3
1	G	72	ALA	3.2
2	B	129	GLU	3.2
2	J	75	ASP	3.2
1	G	75	ASN	3.2
2	F	129	GLU	3.2
1	I	37	LYS	3.1
1	K	77	LYS	3.0
2	J	78	ILE	3.0
1	G	103	THR	3.0
1	K	102	VAL	2.9
2	L	66	PHE	2.9
2	J	108	ASN	2.9
3	O	443	VAL	2.9
2	D	60	THR	2.9
2	J	76	ILE	2.9
2	D	72	VAL	2.9
2	H	146	THR	2.9
2	L	60	THR	2.8
1	I	72	ALA	2.8
2	J	66	PHE	2.8
1	K	104	ILE	2.8
1	K	75	ASN	2.8
1	G	77	LYS	2.7
1	I	80	ILE	2.7
1	G	62	ALA	2.6
1	E	23	ALA	2.6
2	J	69	LEU	2.6
1	I	69	GLY	2.6
3	N	446	GLU	2.5
1	I	68	ALA	2.5
3	M	435	ALA	2.5
3	O	435	ALA	2.5
2	J	70	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	J	63	ILE	2.5
1	K	73	ARG	2.5
1	G	73	ARG	2.4
2	B	144	LYS	2.4
1	G	69	GLY	2.4
1	I	25	LEU	2.4
1	C	17	THR	2.4
1	G	68	ALA	2.3
2	J	82	ALA	2.3
1	K	34	ARG	2.3
2	L	72	VAL	2.3
2	L	76	ILE	2.3
2	D	77	GLY	2.3
1	G	84	HIS	2.2
1	K	100	GLY	2.2
2	J	77	GLY	2.2
1	I	65	LEU	2.2
1	K	40	LYS	2.2
3	N	444	ASN	2.2
1	I	64	VAL	2.1
1	K	103	THR	2.1
1	K	72	ALA	2.1
1	I	77	LYS	2.1
1	K	37	LYS	2.1
2	D	66	PHE	2.1
1	K	68	ALA	2.1
1	I	75	ASN	2.1
1	G	25	LEU	2.1
2	J	72	VAL	2.0
3	N	435	ALA	2.0
2	D	109	LYS	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	F	201	6/6	0.72	0.17	61,70,76,76	0
4	GOL	C	201	6/6	0.83	0.15	63,65,71,72	0
4	GOL	A	201	6/6	0.86	0.13	58,60,62,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.