Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:46 PM EDT

PDB ID	:	1N0X
Title	:	Crystal Structure of a Broadly Neutralizing Anti-HIV-1 Antibody in Complex with a Peptide Mimotope
Authors	:	Saphire, E.O.; Montero, M.; Menendez, A.; Irving, M.B.; Zwick, M.B.; Parren, P.W.H.I.; Burton, D.R.; Scott, J.K.; Wilson, I.A.
Deposited on	:	2002-10-15
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

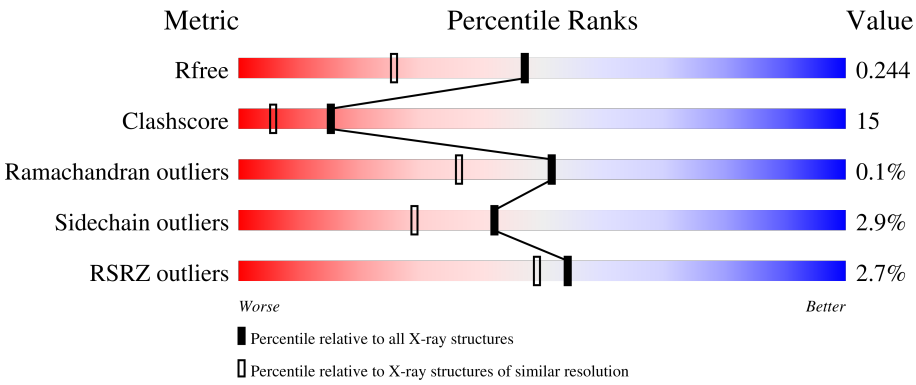
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	L	215	2%, 74%, 24%, •
1	M	215	2%, 73%, 25%, •
2	H	230	%, 77%, 18%, • •
2	K	230	3%, 77%, 18%, • •
3	P	21	14%, 52%, 43%, 5%

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Mol	Chain	Length	Quality of chain
3	R	21	10% 67% 24% 5% 5%

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
4	GOL	M	800	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7899 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 IMMUNOGLOBULIN LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	215	1668	1036	297	330	5	0	0	0
1	M	215	1668	1036	297	330	5	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	202	ARG	SER	conflict	UNP Q8TCD0
M	202	ARG	SER	conflict	UNP Q8TCD0

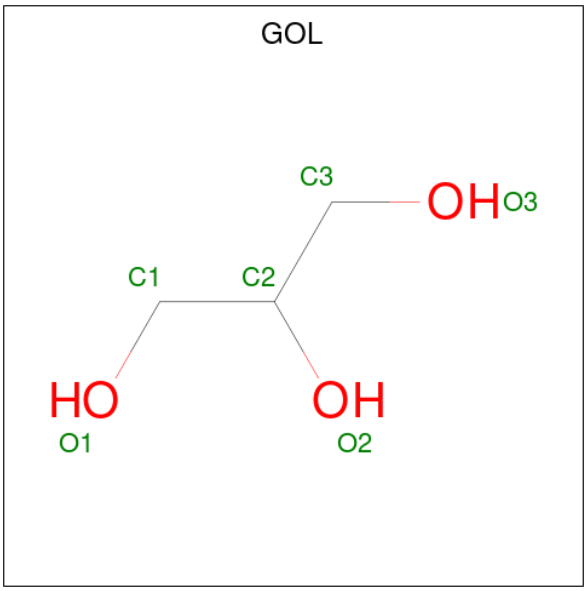
- Molecule 2 is a protein called IMMUNOGLOBULIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	222	1707	1084	288	328	7	0	0	0
2	K	224	1718	1089	290	331	8	0	0	0

- Molecule 3 is a protein called B2.1 peptide.

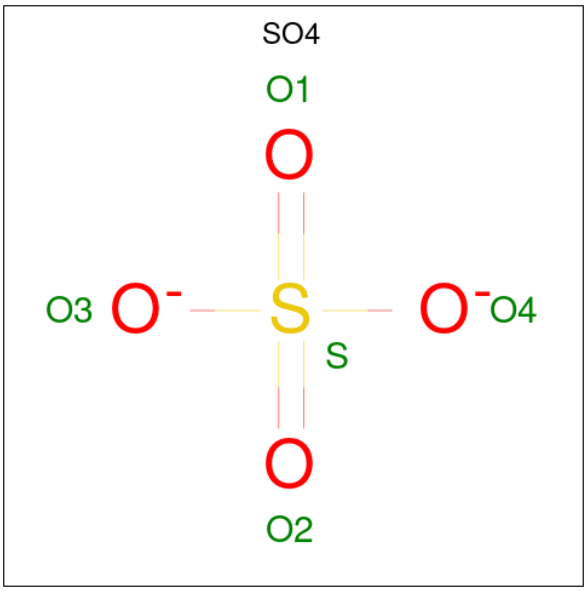
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	P	21	170	103	31	34	2	0	0	0
3	R	20	160	97	29	32	2	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



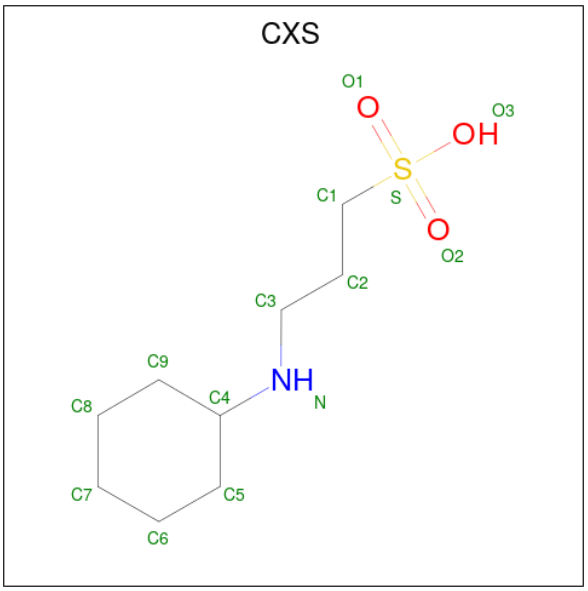
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	L	1	6	3	3	0	0
4	H	1	6	3	3	0	0
4	H	1	6	3	3	0	0
4	M	1	6	3	3	0	0
4	M	1	6	3	3	0	0
4	K	1	6	3	3	0	0
4	K	1	6	3	3	0	0
4	K	1	6	3	3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total O S 5 4 1	0	0
5	K	1	Total O S 5 4 1	0	0
5	R	1	Total O S 5 4 1	0	0
5	R	1	Total O S 5 4 1	0	0

- Molecule 6 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula: $C_9H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	H	1	14	9	1	3	1	0	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
7	P	1	1	1	0	0

- Molecule 8 is water.

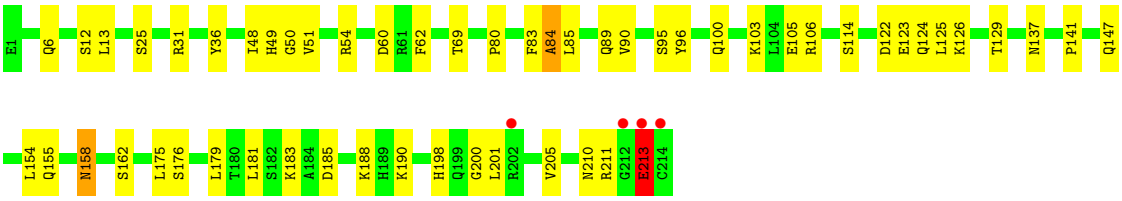
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	L	160	160	160	0	0
			Total	O		
8	H	187	187	187	0	0
			Total	O		
8	M	172	172	172	0	0
			Total	O		
8	K	179	179	179	0	0
			Total	O		
8	P	12	12	12	0	0
			Total	O		
8	R	15	15	15	0	0

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.

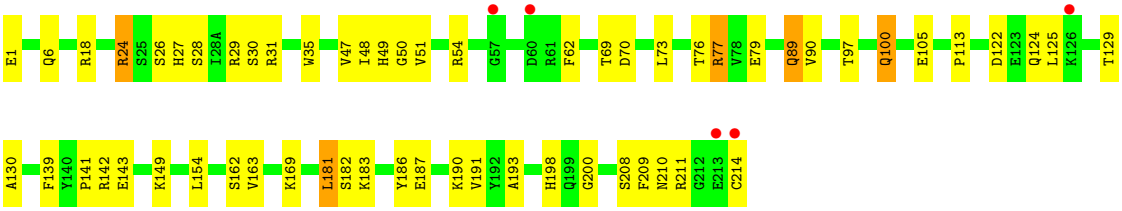
• Molecule 1: IMMUNOGLOBULIN LIGHT CHAIN

Chain L:



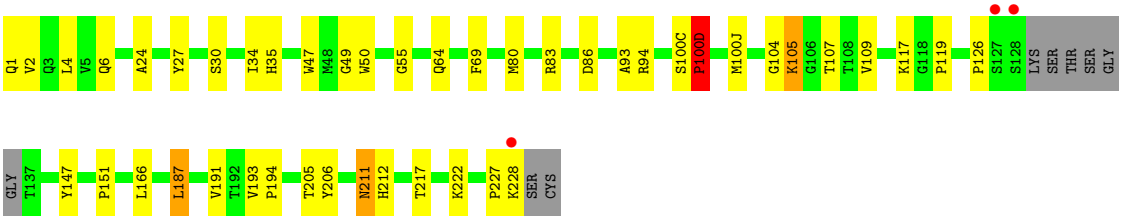
• Molecule 1: IMMUNOGLOBULIN LIGHT CHAIN

Chain M:



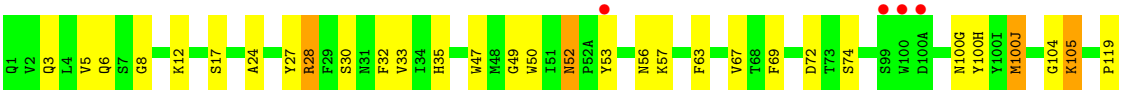
• Molecule 2: IMMUNOGLOBULIN HEAVY CHAIN

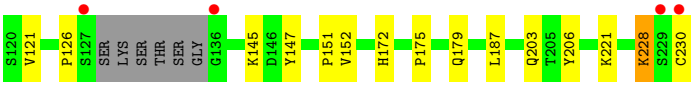
Chain H:



• Molecule 2: IMMUNOGLOBULIN HEAVY CHAIN

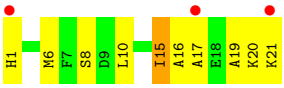
Chain K:





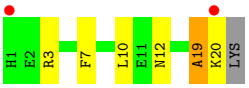
- Molecule 3: B2.1 peptide

Chain P:



- Molecule 3: B2.1 peptide

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.62Å 184.36Å 56.17Å 90.00° 103.05° 90.00°	Depositor
Resolution (Å)	45.00 – 1.80 33.45 – 1.75	Depositor EDS
% Data completeness (in resolution range)	92.0 (45.00-1.80) 92.0 (33.45-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.75Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.252 0.211 , 0.244	Depositor DCC
R_{free} test set	1832 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7899	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 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CXS, SO4, ORN, K, 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	L	0.44	2/1704 (0.1%)	0.64	2/2306 (0.1%)
1	M	0.32	0/1704	0.64	0/2306
2	H	0.38	1/1754 (0.1%)	0.68	2/2392 (0.1%)
2	K	0.33	0/1765	0.65	0/2405
3	P	0.35	0/166	0.44	0/217
3	R	0.50	0/156	0.57	0/206
All	All	0.38	3/7249 (0.0%)	0.65	4/9832 (0.0%)

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
1	L	0	1
2	H	0	1
3	R	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	84	ALA	C-N	11.92	1.61	1.34
2	H	100(D)	PRO	CA-C	6.39	1.65	1.52
1	L	83	PHE	C-N	-5.50	1.21	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	84	ALA	CA-C-N	-6.10	103.77	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	84	ALA	O-C-N	-6.05	113.02	122.70
2	H	100(D)	PRO	O-C-N	5.87	132.09	122.70
2	H	100(D)	PRO	N-CD-CG	-5.26	95.31	103.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	100(D)	PRO	Mainchain
1	L	84	ALA	Mainchain
3	R	19	ORN	Mainchain

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	L	1668	0	1622	46	0
1	M	1668	0	1621	67	0
2	H	1707	0	1652	39	0
2	K	1718	0	1659	50	0
3	P	170	0	152	13	0
3	R	160	0	138	9	0
4	H	12	0	16	1	0
4	K	18	0	24	4	0
4	L	6	0	8	1	0
4	M	12	0	16	0	0
5	H	5	0	0	0	0
5	K	5	0	0	0	0
5	R	10	0	0	1	0
6	H	14	0	19	0	0
7	P	1	0	0	0	0
8	H	187	0	0	9	0
8	K	179	0	0	1	0
8	L	160	0	0	8	0
8	M	172	0	0	14	0
8	P	12	0	0	6	0
8	R	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7899	0	6927	212	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (212) 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:M:191:VAL:HA	8:M:968:HOH:O	1.35	1.27
2:K:28:ARG:HD3	2:K:28:ARG:H	1.24	1.01
1:L:211:ARG:HH11	1:L:211:ARG:HB3	1.23	0.99
1:M:210:ASN:HA	8:M:968:HOH:O	1.63	0.98
2:K:105:LYS:HE3	2:K:105:LYS:H	1.32	0.95
1:L:31:ARG:HD2	1:M:29:ARG:HH21	1.30	0.93
1:M:100:GLN:NE2	1:M:100:GLN:H	1.64	0.93
1:M:24:ARG:HH11	1:M:24:ARG:HB2	1.31	0.91
1:M:100:GLN:H	1:M:100:GLN:HE21	0.91	0.88
1:M:100:GLN:HE21	1:M:100:GLN:N	1.70	0.88
2:K:35:HIS:HD2	2:K:47:TRP:HE1	1.17	0.87
1:M:181:LEU:HD11	1:M:186:TYR:HB2	1.58	0.86
2:H:100(C):SER:HB3	8:P:730:HOH:O	1.74	0.85
2:K:28:ARG:HD3	2:K:28:ARG:N	1.93	0.83
1:L:147:GLN:NE2	1:L:154:LEU:HG	1.94	0.82
1:L:211:ARG:HB3	1:L:211:ARG:NH1	1.96	0.81
1:M:76:THR:HA	8:M:967:HOH:O	1.81	0.80
3:P:8:SER:HB2	3:P:15:ILE:HD12	1.66	0.78
2:K:228:LYS:HE3	2:K:228:LYS:H	1.50	0.76
1:M:29:ARG:HG3	1:M:29:ARG:HH11	1.48	0.76
2:K:8:GLY:H	4:K:805:GOL:H2	1.51	0.74
2:K:28:ARG:H	2:K:28:ARG:CD	1.98	0.74
1:L:158:ASN:HD22	1:L:158:ASN:H	1.35	0.74
1:M:6:GLN:H	1:M:100:GLN:HE22	1.36	0.73
2:K:105:LYS:H	2:K:105:LYS:CE	2.02	0.73
1:M:1:GLU:HB3	3:R:10:LEU:HD11	1.70	0.72
2:K:228:LYS:HE3	2:K:228:LYS:N	2.04	0.71
1:M:181:LEU:CD1	1:M:186:TYR:HB2	2.20	0.71
1:M:198:HIS:CD2	1:M:200:GLY:H	2.09	0.70
2:K:56:ASN:HB3	3:R:19:ORN:CB	2.21	0.70
2:H:193:VAL:HG13	2:H:194:PRO:HD2	1.74	0.69
2:K:35:HIS:CD2	2:K:47:TRP:HE1	2.06	0.68
3:P:6:MET:O	3:P:15:ILE:HD13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:25:SER:O	1:L:69:THR:HG23	1.93	0.68
1:M:24:ARG:HB2	1:M:24:ARG:NH1	2.08	0.68
1:M:18:ARG:HD3	8:M:967:HOH:O	1.93	0.67
2:K:145:LYS:HE2	2:K:179:GLN:HE22	1.58	0.67
2:K:50:TRP:CH2	3:R:19:ORN:CB	2.78	0.67
1:M:125:LEU:HA	8:M:920:HOH:O	1.95	0.66
1:L:176:SER:HB3	8:L:869:HOH:O	1.94	0.66
2:H:109:VAL:HG22	8:H:1303:HOH:O	1.94	0.66
2:H:93:ALA:HB3	2:H:100(J):MET:HE3	1.78	0.65
2:K:228:LYS:H	2:K:228:LYS:CE	2.11	0.64
3:P:20:LYS:HB2	8:P:693:HOH:O	1.98	0.64
2:H:100(D):PRO:HD2	8:P:730:HOH:O	1.96	0.64
1:L:201:LEU:HD13	1:L:205:VAL:HG23	1.78	0.64
1:L:198:HIS:CD2	1:L:200:GLY:H	2.15	0.63
1:L:122:ASP:O	1:L:126:LYS:HG3	1.99	0.63
1:M:210:ASN:ND2	8:M:968:HOH:O	2.11	0.62
2:K:52:ASN:C	2:K:52:ASN:HD22	2.02	0.62
1:L:183:LYS:HB2	8:L:911:HOH:O	1.99	0.61
2:H:1:GLN:CD	2:H:2:VAL:H	2.04	0.61
3:P:6:MET:HA	8:P:730:HOH:O	1.98	0.61
1:M:209:PHE:O	8:M:968:HOH:O	2.16	0.61
3:P:17:ALA:HA	3:P:21:LYS:OXT	2.00	0.60
1:L:211:ARG:HH11	1:L:211:ARG:CB	2.05	0.60
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.49	0.60
1:M:90:VAL:HG22	1:M:97:THR:HG22	1.84	0.60
2:K:63:PHE:O	2:K:67:VAL:HG12	2.02	0.60
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.19	0.60
2:H:193:VAL:HG11	2:H:206:TYR:CZ	2.37	0.60
3:P:15:ILE:HD13	3:P:15:ILE:H	1.67	0.60
1:M:26:SER:OG	1:M:27:HIS:HD2	1.85	0.59
1:M:1:GLU:HB3	3:R:10:LEU:CD1	2.32	0.59
1:M:90:VAL:CG2	1:M:97:THR:HG22	2.33	0.59
3:R:19:ORN:O	3:R:20:LYS:CB	2.45	0.59
8:H:1206:HOH:O	3:P:21:LYS:HA	2.02	0.59
2:K:126:PRO:HA	8:K:1018:HOH:O	2.02	0.59
2:K:100(G):ASN:HD21	4:K:801:GOL:H11	1.68	0.58
1:L:158:ASN:H	1:L:158:ASN:ND2	2.02	0.58
1:L:190:LYS:HE2	1:L:210:ASN:ND2	2.18	0.58
1:M:79:GLU:HG2	8:M:961:HOH:O	2.04	0.58
1:M:198:HIS:HD2	1:M:200:GLY:H	1.51	0.57
1:M:29:ARG:HH11	1:M:29:ARG:CG	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:54:ARG:HD3	1:L:62:PHE:O	2.05	0.57
1:L:162:SER:HB3	8:L:869:HOH:O	2.05	0.57
1:L:155:GLN:HB3	1:L:158:ASN:HD21	1.70	0.56
1:L:36:TYR:OH	2:H:100(J):MET:HG2	2.05	0.56
1:L:85:LEU:HD12	8:L:940:HOH:O	2.05	0.56
2:K:121:VAL:O	2:K:221:LYS:HE3	2.06	0.56
1:M:31:ARG:O	1:M:51:VAL:HG23	2.06	0.56
2:K:33:VAL:HG23	4:K:801:GOL:H31	1.89	0.55
1:L:31:ARG:HD2	1:M:29:ARG:NH2	2.11	0.55
2:K:147:TYR:CE2	2:K:152:VAL:HG13	2.42	0.55
2:H:107:THR:HG22	8:H:1303:HOH:O	2.06	0.55
1:L:6:GLN:HB2	1:L:100:GLN:NE2	2.23	0.54
1:L:154:LEU:C	1:L:154:LEU:HD23	2.28	0.54
1:M:113:PRO:HB3	1:M:139:PHE:HB3	1.89	0.54
1:L:89:GLN:HG2	1:L:90:VAL:N	2.22	0.54
1:L:125:LEU:HA	8:L:911:HOH:O	2.08	0.54
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.43	0.54
2:K:228:LYS:H	2:K:228:LYS:CD	2.21	0.54
1:L:141:PRO:O	1:L:198:HIS:HE1	1.92	0.53
1:M:47:VAL:HG12	1:M:48:ILE:HG12	1.91	0.53
3:R:7:PHE:HZ	3:R:12:ASN:HD22	1.56	0.53
2:K:32:PHE:HA	4:K:801:GOL:O3	2.09	0.52
1:M:54:ARG:HD3	1:M:62:PHE:O	2.08	0.52
2:H:117:LYS:HE2	8:H:1299:HOH:O	2.09	0.52
2:K:126:PRO:O	2:K:228:LYS:HE2	2.09	0.52
1:L:123:GLU:HB2	4:L:803:GOL:O3	2.10	0.52
2:K:35:HIS:HD2	2:K:47:TRP:NE1	1.98	0.52
1:M:24:ARG:HD3	1:M:70:ASP:OD1	2.10	0.52
2:K:100(H):TYR:O	2:K:100(J):MET:HE1	2.10	0.52
1:M:190:LYS:HE2	1:M:211:ARG:O	2.10	0.52
2:K:57:LYS:HD3	2:K:69:PHE:HB2	1.92	0.51
2:H:35:HIS:CD2	2:H:50:TRP:HB3	2.45	0.51
2:H:187:LEU:C	2:H:187:LEU:HD12	2.30	0.51
2:H:211:ASN:HD22	2:H:212:HIS:N	2.09	0.51
2:H:211:ASN:ND2	8:H:1386:HOH:O	2.44	0.51
2:K:105:LYS:H	2:K:105:LYS:CD	2.24	0.51
3:P:16:ALA:HB1	8:P:504:HOH:O	2.11	0.51
1:L:158:ASN:HD22	1:L:158:ASN:N	1.99	0.50
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.93	0.50
2:K:187:LEU:C	2:K:187:LEU:HD12	2.32	0.50
1:M:181:LEU:HD13	1:M:182:SER:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:12:SER:O	1:L:13:LEU:HD23	2.11	0.50
1:M:193:ALA:HB2	1:M:208:SER:HB3	1.93	0.50
2:K:100(J):MET:SD	2:K:100(J):MET:N	2.85	0.50
2:H:193:VAL:HG13	2:H:194:PRO:CD	2.40	0.50
1:M:162:SER:OG	2:K:175:PRO:HD2	2.12	0.50
2:K:105:LYS:CD	2:K:105:LYS:N	2.75	0.49
1:L:69:THR:HG22	1:L:69:THR:O	2.12	0.49
1:L:213:GLU:HG2	1:L:213:GLU:O	2.12	0.49
1:M:30:SER:O	1:M:31:ARG:HB2	2.13	0.49
1:M:49:HIS:HD2	8:M:861:HOH:O	1.96	0.49
2:K:119:PRO:HB3	2:K:147:TYR:HB3	1.94	0.49
1:M:77:ARG:HG3	8:M:961:HOH:O	2.12	0.49
2:K:47:TRP:CZ2	2:K:49:GLY:HA2	2.48	0.49
1:L:158:ASN:ND2	1:L:158:ASN:N	2.60	0.48
2:H:6:GLN:HE21	2:H:104:GLY:HA3	1.75	0.48
2:K:121:VAL:HG12	2:K:221:LYS:HD2	1.95	0.48
2:H:55:GLY:HA3	4:H:809:GOL:H12	1.95	0.48
1:M:142:ARG:NH2	1:M:163:VAL:HG21	2.28	0.48
3:P:19:ORN:O	3:P:20:LYS:HG3	2.13	0.47
1:L:114:SER:HB2	1:L:137:ASN:HB3	1.96	0.47
1:L:95:SER:OG	3:P:10:LEU:HB2	2.15	0.47
2:K:50:TRP:HH2	3:R:19:ORN:CB	2.25	0.47
1:M:124:GLN:HG2	1:M:129:THR:O	2.15	0.47
2:H:187:LEU:HA	8:H:1221:HOH:O	2.15	0.47
1:M:77:ARG:HH11	1:M:77:ARG:HB2	1.80	0.47
1:L:124:GLN:HG2	1:L:129:THR:O	2.14	0.46
1:L:80:PRO:HG2	8:L:876:HOH:O	2.15	0.46
2:H:228:LYS:O	2:H:228:LYS:HG3	2.14	0.46
2:K:105:LYS:HE3	2:K:105:LYS:N	2.15	0.46
1:M:130:ALA:HB3	1:M:181:LEU:HD12	1.98	0.46
2:K:203:GLN:HG2	2:K:206:TYR:CZ	2.50	0.46
2:H:217:THR:N	8:H:1386:HOH:O	2.47	0.46
1:L:175:LEU:HD23	1:L:176:SER:N	2.30	0.46
1:M:141:PRO:O	1:M:198:HIS:HE1	1.99	0.46
1:M:1:GLU:HG2	1:M:1:GLU:O	2.14	0.46
1:M:28:SER:HB2	1:M:29:ARG:NH1	2.31	0.46
1:M:129:THR:HG22	8:M:902:HOH:O	2.16	0.46
1:M:214:CYS:N	2:K:230:CYS:SG	2.90	0.45
1:M:143:GLU:CD	1:M:143:GLU:H	2.19	0.45
2:K:72:ASP:OD1	2:K:74:SER:HB3	2.15	0.45
3:R:3:ARG:HG2	5:R:901:SO4:O2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:GLN:NE2	2:H:2:VAL:H	2.14	0.45
2:H:34:ILE:HD13	2:H:94:ARG:HA	1.99	0.45
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.52	0.45
2:H:30:SER:HB2	8:H:1383:HOH:O	2.15	0.45
1:M:149:LYS:HD3	1:M:154:LEU:HA	1.98	0.45
2:H:193:VAL:CG1	2:H:206:TYR:OH	2.64	0.45
1:L:103:LYS:HE2	8:L:923:HOH:O	2.17	0.45
1:M:29:ARG:CG	1:M:29:ARG:NH1	2.76	0.44
1:M:142:ARG:CZ	1:M:163:VAL:HG21	2.46	0.44
1:M:28:SER:CB	1:M:29:ARG:NH1	2.80	0.44
1:M:100:GLN:NE2	1:M:100:GLN:N	2.45	0.44
1:M:181:LEU:HD12	1:M:181:LEU:O	2.16	0.44
2:K:12:LYS:HE2	2:K:17:SER:O	2.17	0.44
2:H:83:ARG:HG2	2:H:86:ASP:OD2	2.17	0.44
2:H:105:LYS:HG3	8:H:1263:HOH:O	2.17	0.44
2:H:126:PRO:HG2	2:H:227:PRO:HG3	1.99	0.44
1:L:69:THR:O	1:L:69:THR:CG2	2.65	0.44
1:L:185:ASP:HA	1:L:188:LYS:HD3	1.98	0.44
1:M:169:LYS:HE3	8:M:954:HOH:O	2.18	0.44
2:K:24:ALA:HB1	2:K:27:TYR:CE1	2.53	0.44
2:H:193:VAL:CG1	2:H:194:PRO:N	2.81	0.43
2:K:35:HIS:CD2	2:K:50:TRP:HB3	2.54	0.43
1:L:90:VAL:O	1:L:96:TYR:HA	2.19	0.43
1:L:201:LEU:HD13	1:L:205:VAL:CG2	2.44	0.43
2:H:205:THR:HG23	2:H:222:LYS:HE3	2.00	0.43
2:K:3:GLN:HE21	2:K:5:VAL:CG2	2.31	0.43
2:H:105:LYS:NZ	2:H:105:LYS:HB3	2.34	0.43
1:L:105:GLU:HG2	1:L:106:ARG:N	2.33	0.43
3:P:6:MET:HG3	3:P:15:ILE:HD11	2.00	0.43
2:H:105:LYS:NZ	2:H:105:LYS:CB	2.82	0.43
1:M:28:SER:OG	1:M:29:ARG:NH1	2.52	0.43
2:K:30:SER:O	2:K:53:TYR:HB2	2.19	0.43
2:K:105:LYS:N	2:K:105:LYS:HD3	2.34	0.43
2:H:193:VAL:HG11	2:H:206:TYR:OH	2.18	0.42
3:P:20:LYS:NZ	3:P:20:LYS:HB3	2.33	0.42
1:L:179:LEU:HG	1:L:181:LEU:CD1	2.49	0.42
2:H:69:PHE:HE2	2:H:80:MET:HG2	1.84	0.42
2:K:57:LYS:O	3:R:19:ORN:HA	2.20	0.42
1:M:35:TRP:CD2	1:M:73:LEU:HB2	2.55	0.42
3:P:1:HIS:HB2	8:P:675:HOH:O	2.20	0.42
1:L:50:GLY:O	1:L:51:VAL:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6:GLN:H	1:M:100:GLN:NE2	2.11	0.41
1:L:49:HIS:HD2	8:L:832:HOH:O	2.03	0.41
1:M:89:GLN:HE21	1:M:89:GLN:HB3	1.70	0.41
1:M:130:ALA:HB3	1:M:181:LEU:CD1	2.50	0.41
1:M:183:LYS:O	1:M:187:GLU:HG3	2.21	0.41
8:M:857:HOH:O	2:K:172:HIS:HD2	2.03	0.41
1:M:50:GLY:O	1:M:51:VAL:HB	2.21	0.41
1:M:69:THR:HG22	8:M:917:HOH:O	2.21	0.41
1:M:181:LEU:HD12	1:M:181:LEU:C	2.41	0.41
1:M:193:ALA:CB	1:M:208:SER:HB3	2.51	0.41
1:M:129:THR:OG1	1:M:130:ALA:N	2.54	0.41
2:K:6:GLN:HE21	2:K:104:GLY:HA3	1.85	0.40
1:L:48:ILE:HD13	1:L:54:ARG:HA	2.02	0.40
2:H:166:LEU:HD21	2:H:191:VAL:HG21	2.04	0.40
2:K:35:HIS:CD2	2:K:47:TRP:NE1	2.81	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	L	213/215 (99%)	205 (96%)	7 (3%)	1 (0%)	29	15
1	M	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
2	H	218/230 (95%)	212 (97%)	6 (3%)	0	100	100
2	K	220/230 (96%)	214 (97%)	6 (3%)	0	100	100
3	P	18/21 (86%)	16 (89%)	2 (11%)	0	100	100
3	R	17/21 (81%)	15 (88%)	2 (12%)	0	100	100
All	All	899/932 (96%)	867 (96%)	31 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	213	GLU

5.3.2 Protein sidechains (i)

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	L	187/187 (100%)	184 (98%)	3 (2%)	62	54
1	M	187/187 (100%)	180 (96%)	7 (4%)	34	19
2	H	190/196 (97%)	184 (97%)	6 (3%)	39	25
2	K	191/196 (97%)	185 (97%)	6 (3%)	40	25
3	P	17/18 (94%)	16 (94%)	1 (6%)	19	7
3	R	16/18 (89%)	16 (100%)	0	100	100
All	All	788/802 (98%)	765 (97%)	23 (3%)	42	29

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	60	ASP
1	L	158	ASN
1	L	213	GLU
2	H	4	LEU
2	H	64	GLN
2	H	105	LYS
2	H	151	PRO
2	H	187	LEU
2	H	211	ASN
1	M	24	ARG
1	M	77	ARG
1	M	89	GLN
1	M	100	GLN
1	M	105	GLU
1	M	122	ASP
1	M	181	LEU
2	K	28	ARG
2	K	52	ASN

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Mol	Chain	Res	Type
2	K	100(J)	MET
2	K	105	LYS
2	K	151	PRO
2	K	228	LYS
3	P	15	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	42	GLN
1	L	49	HIS
1	L	138	ASN
1	L	147	GLN
1	L	158	ASN
1	L	198	HIS
1	L	199	GLN
1	L	210	ASN
2	H	1	GLN
2	H	6	GLN
2	H	35	HIS
2	H	56	ASN
2	H	64	GLN
2	H	76	ASN
2	H	172	HIS
2	H	179	GLN
2	H	211	ASN
1	M	27	HIS
1	M	42	GLN
1	M	49	HIS
1	M	89	GLN
1	M	100	GLN
1	M	147	GLN
1	M	198	HIS
1	M	210	ASN
2	K	3	GLN
2	K	6	GLN
2	K	31	ASN
2	K	35	HIS
2	K	43	GLN
2	K	52	ASN
2	K	76	ASN
2	K	172	HIS

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Mol	Chain	Res	Type
2	K	179	GLN
3	R	12	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ORN	P	19	3	3,4,8	0.58	0	2,4,9	0.81	0
3	ORN	R	19	3	3,4,8	0.45	0	2,4,9	1.10	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
3	ORN	P	19	3	-	0/0/2/8	-
3	ORN	R	19	3	-	0/0/2/8	-

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.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	19	ORN	1	0
3	R	19	ORN	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	$\#\|Z\| > 2$
5	SO4	H	903	-	4,4,4	0.27	0	6,6,6	0.05	0
4	GOL	M	804	-	5,5,5	0.99	0	5,5,5	0.32	0
5	SO4	K	904	-	4,4,4	0.24	0	6,6,6	0.08	0
4	GOL	K	806	-	5,5,5	0.93	0	5,5,5	0.25	0
6	CXS	H	1201	-	14,14,14	1.60	3 (21%)	18,18,18	1.40	2 (11%)
4	GOL	K	801	-	5,5,5	0.88	0	5,5,5	0.22	0
5	SO4	R	901	-	4,4,4	0.25	0	6,6,6	0.08	0
4	GOL	M	800	-	5,5,5	0.99	0	5,5,5	0.28	0
4	GOL	H	808	-	5,5,5	0.95	0	5,5,5	0.28	0
4	GOL	H	809	-	5,5,5	0.93	0	5,5,5	0.28	0
4	GOL	K	805	-	5,5,5	0.97	0	5,5,5	0.27	0
4	GOL	L	803	-	5,5,5	0.89	0	5,5,5	0.24	0
5	SO4	R	902	-	4,4,4	0.28	0	6,6,6	0.05	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	M	804	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	K	806	-	-	2/4/4/4	-
6	CXS	H	1201	-	-	0/8/16/16	0/1/1/1
4	GOL	K	801	-	-	2/4/4/4	-
4	GOL	M	800	-	-	4/4/4/4	-
4	GOL	H	808	-	-	3/4/4/4	-
4	GOL	H	809	-	-	4/4/4/4	-
4	GOL	K	805	-	-	2/4/4/4	-
4	GOL	L	803	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	1201	CXS	C1-S	3.96	1.83	1.77
6	H	1201	CXS	C9-C4	2.78	1.58	1.52
6	H	1201	CXS	C5-C4	2.59	1.58	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	1201	CXS	C3-N-C4	4.49	122.95	114.14
6	H	1201	CXS	O3-S-C1	2.45	109.73	105.77

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	803	GOL	O1-C1-C2-C3
4	L	803	GOL	C1-C2-C3-O3
4	H	808	GOL	O1-C1-C2-C3
4	H	809	GOL	O1-C1-C2-C3
4	H	809	GOL	C1-C2-C3-O3
4	M	804	GOL	O1-C1-C2-C3
4	M	800	GOL	O1-C1-C2-C3
4	K	801	GOL	O1-C1-C2-C3
4	K	805	GOL	O1-C1-C2-C3
4	K	806	GOL	O1-C1-C2-C3
4	L	803	GOL	O1-C1-C2-O2
4	H	808	GOL	O1-C1-C2-O2
4	H	809	GOL	O1-C1-C2-O2
4	M	800	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	K	801	GOL	O1-C1-C2-O2
4	K	805	GOL	O1-C1-C2-O2
4	K	806	GOL	O1-C1-C2-O2
4	M	804	GOL	C1-C2-C3-O3
4	H	809	GOL	O2-C2-C3-O3
4	M	804	GOL	O1-C1-C2-O2
4	M	804	GOL	O2-C2-C3-O3
4	L	803	GOL	O2-C2-C3-O3
4	M	800	GOL	C1-C2-C3-O3
4	H	808	GOL	C1-C2-C3-O3
4	M	800	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	801	GOL	3	0
5	R	901	SO4	1	0
4	H	809	GOL	1	0
4	K	805	GOL	1	0
4	L	803	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	R	2
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	84:ALA	C	85:LEU	N	1.61
1	R	18:GLU	C	19:ORN	N	1.15
1	R	19:ORN	C	20:LYS	N	1.14

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	L	215/215 (100%)	0.04	4 (1%)	66	63	20, 31, 46, 110	0
1	M	215/215 (100%)	-0.09	5 (2%)	60	56	18, 28, 46, 101	1 (0%)
2	H	222/230 (96%)	-0.21	3 (1%)	75	72	19, 28, 43, 77	0
2	K	224/230 (97%)	-0.08	8 (3%)	42	37	18, 29, 51, 103	0
3	P	20/21 (95%)	0.84	3 (15%)	2	1	27, 42, 92, 98	0
3	R	19/21 (90%)	0.77	2 (10%)	6	4	28, 36, 70, 79	1 (5%)
All	All	915/932 (98%)	-0.05	25 (2%)	54	49	18, 30, 49, 110	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	214	CYS	11.4
1	M	214	CYS	9.3
2	K	230	CYS	7.6
3	P	1	HIS	6.1
2	K	100	TRP	5.9
1	L	213	GLU	5.5
1	L	202	ARG	5.3
2	H	127	SER	4.6
3	P	21	LYS	4.5
3	R	1	HIS	4.4
2	K	136	GLY	4.2
2	K	229	SER	4.1
1	M	213	GLU	3.9
1	L	212	GLY	3.4
3	R	20	LYS	3.3
2	K	53	TYR	3.3
1	M	60	ASP	3.2
2	K	127	SER	3.1
2	K	100(A)	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	228	LYS	2.6
2	K	99	SER	2.5
1	M	57	GLY	2.3
2	H	128	SER	2.2
1	M	126	LYS	2.1
3	P	17	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	ORN	P	19	5/9	0.80	0.25	78,81,84,85	0
3	ORN	R	19	5/9	0.92	0.25	71,73,75,76	0

6.3 Carbohydrates (i)

There are no monosaccharides 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	L	803	6/6	0.62	0.30	66,70,71,74	0
4	GOL	M	800	6/6	0.63	0.41	78,79,79,79	0
4	GOL	H	809	6/6	0.68	0.33	62,63,65,67	0
4	GOL	K	806	6/6	0.69	0.28	81,81,82,82	0
4	GOL	K	805	6/6	0.72	0.22	66,67,68,68	0
4	GOL	K	801	6/6	0.78	0.19	50,50,51,58	0
4	GOL	M	804	6/6	0.84	0.13	46,56,58,59	0
4	GOL	H	808	6/6	0.86	0.28	74,75,76,76	0
7	K	P	1001	1/1	0.89	0.07	35,35,35,35	0
5	SO4	K	904	5/5	0.94	0.10	71,71,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CXS	H	1201	14/14	0.95	0.09	27,31,36,39	0
5	SO4	R	902	5/5	0.95	0.23	73,73,74,75	0
5	SO4	R	901	5/5	0.97	0.13	50,51,53,54	0
5	SO4	H	903	5/5	0.97	0.13	47,47,48,50	0

6.5 Other polymers (i)

There are no such residues in this entry.