Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:58 pm BST

PDB ID	:	6I7D
Title	:	Plasmodium falciparum Myosin A, post-rigor and rigor-like states
Authors	:	Robert-Paganin, J.; Auguin, D.; Moussaoui, D.; Jousset, G.; Baum, J.; Trybus, K.M.; Houdusse, A.
Deposited on	:	2018-11-16
Resolution	:	2.82 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 following versions of software and data (see references ⓘ) were used in the production of this report:

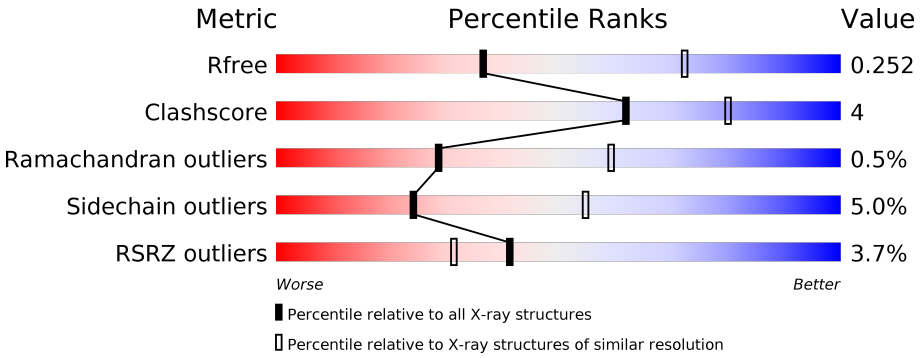
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 on 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	A	768	% 85% 14% ·
1	B	768	6% 87% 11% ·
1	C	768	4% 84% 13% · ·
1	D	768	3% 78% 19% · ·

2 Entry composition

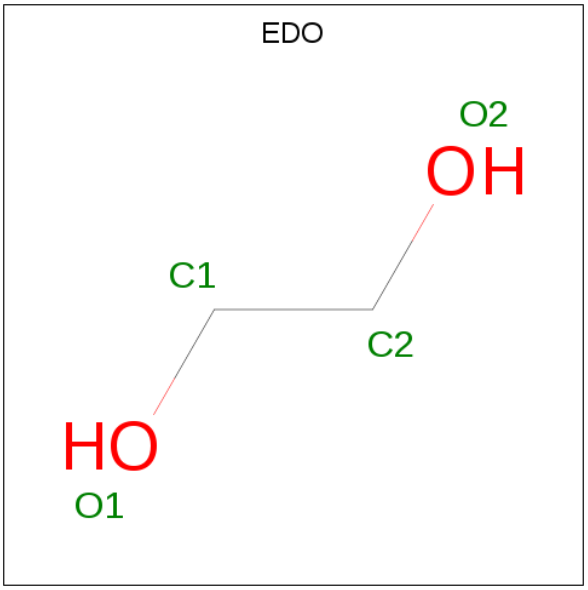
There are 4 unique types of molecules in this entry. The entry contains 24354 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Myosin-A.

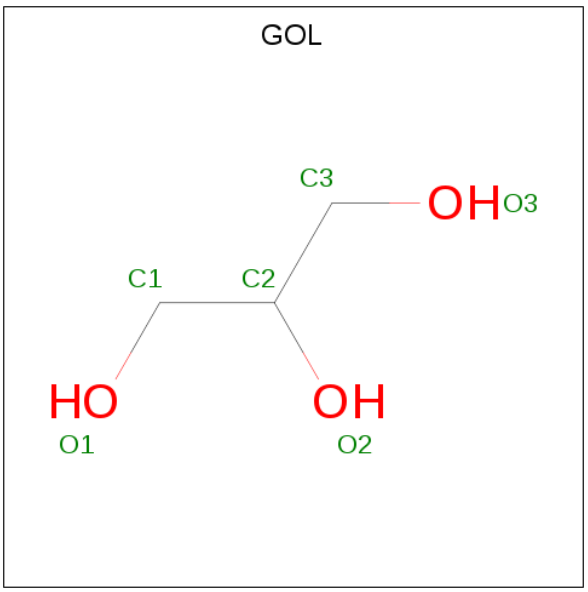
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	P	S	0	0	0
			6010	3819	1012	1147	1	31			
1	B	755	Total	C	N	O	P	S	0	1	0
			5952	3788	1002	1130	1	31			
1	C	755	Total	C	N	O	P	S	0	1	0
			5971	3798	1002	1139	1	31			
1	D	758	Total	C	N	O	P	S	0	1	0
			5984	3802	1007	1143	1	31			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O		0	0
			4	2	2			
2	D	1	Total	C	O		0	0
			4	2	2			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

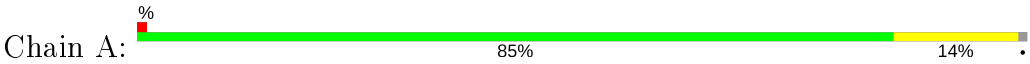
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	122	Total O 122 122	0	0
4	B	102	Total O 102 102	0	0
4	C	67	Total O 67 67	0	0
4	D	132	Total O 132 132	0	0

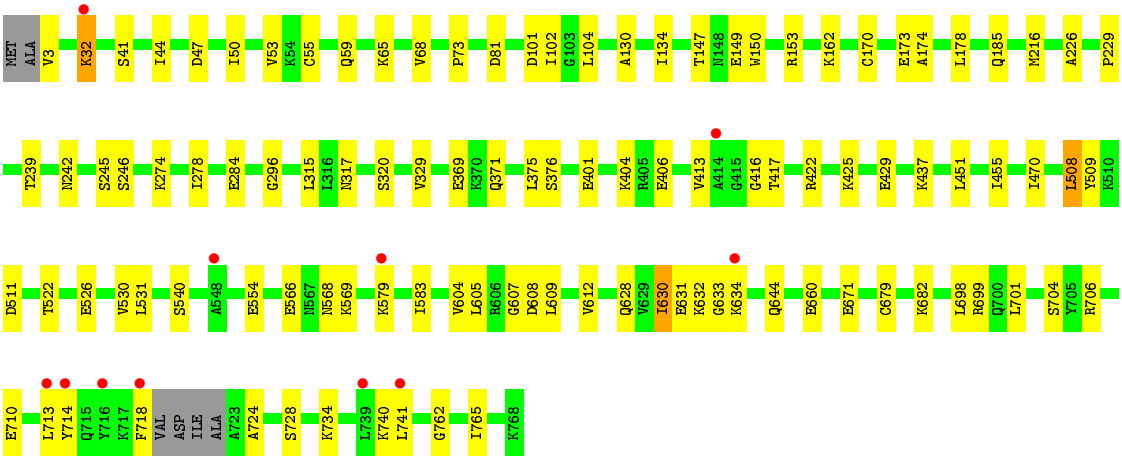
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Myosin-A

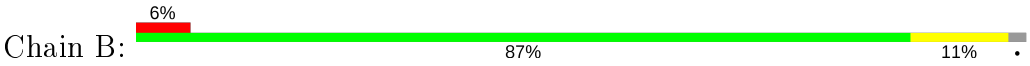
Chain A:

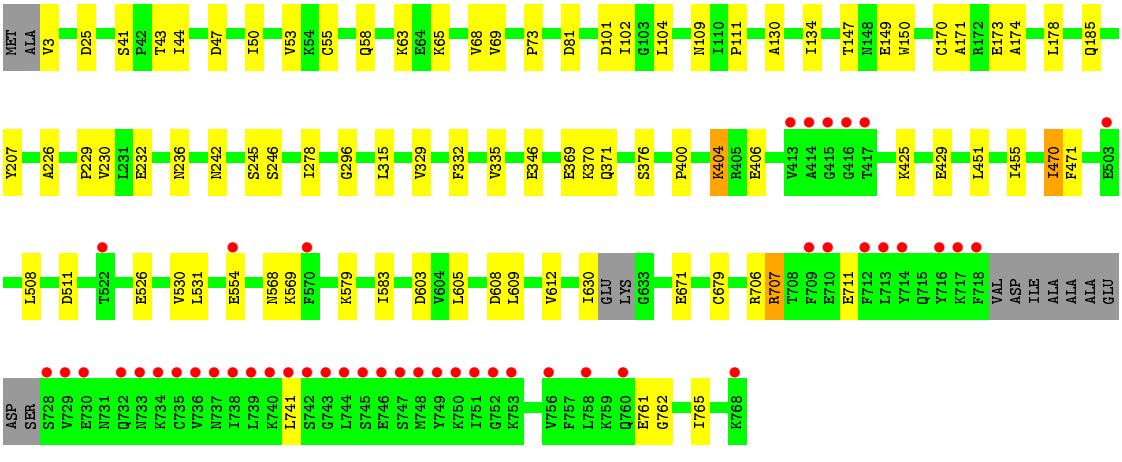




- Molecule 1: Myosin-A

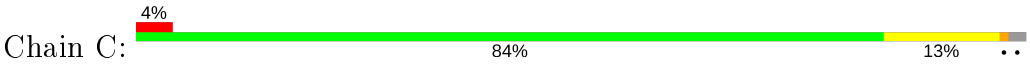
Chain B:

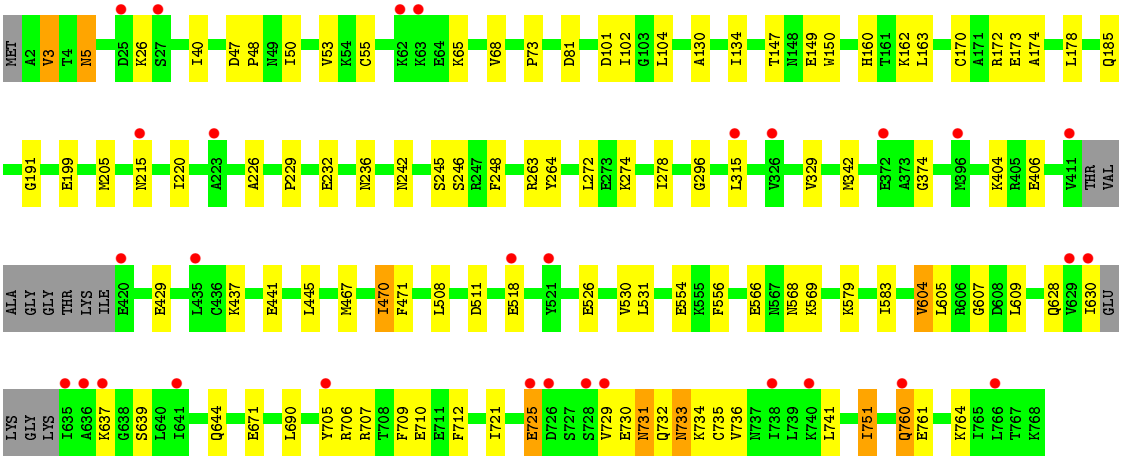




- Molecule 1: Myosin-A

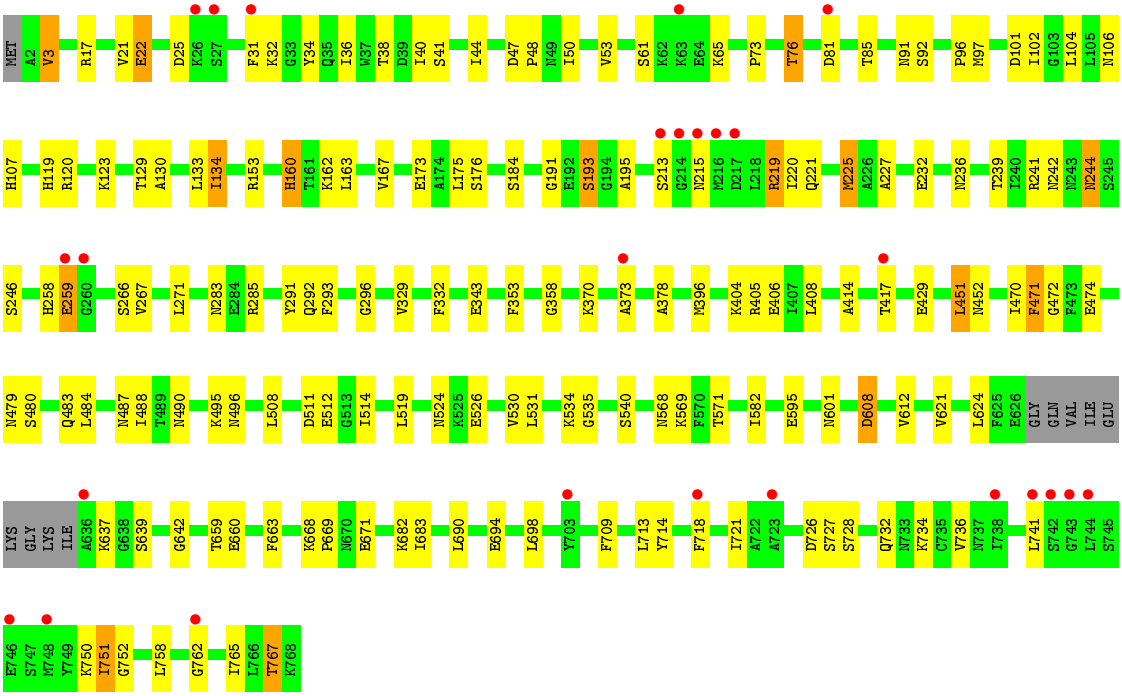
Chain C:





- Molecule 1: Myosin-A

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.52Å 258.73Å 103.09Å 90.00° 92.08° 90.00°	Depositor
Resolution (Å)	49.19 – 2.82 46.24 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.19-2.82) 98.8 (46.24-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.187 , 0.241 0.197 , 0.252	Depositor DCC
R_{free} test set	3938 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 69.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24354	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EDO, SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	0/6104	0.70	0/8236
1	B	0.48	0/6046	0.68	0/8161
1	C	0.49	0/6065	0.70	0/8187
1	D	0.54	0/6079	0.77	2/8198 (0.0%)
All	All	0.50	0/24294	0.71	2/32782 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	76	THR	N-CA-C	-6.12	94.48	111.00
1	D	225	MET	CB-CG-SD	5.14	127.82	112.40

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	6010	0	6050	43	0
1	B	5952	0	5973	40	0
1	C	5971	0	5996	55	0
1	D	5984	0	5999	77	0
2	B	4	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	4	0	6	0	0
3	D	6	0	8	0	0
4	A	122	0	0	0	0
4	B	102	0	0	0	0
4	C	67	0	0	1	0
4	D	132	0	0	1	0
All	All	24354	0	24038	209	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 4.

All (209) 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:C:470:ILE:CG1	1:C:470:ILE:CD1	1.75	1.64
1:A:153:ARG:HD3	1:D:76:THR:HB	1.49	0.93
1:D:474:GLU:H	1:D:487:ASN:HD21	1.20	0.90
1:A:32:LYS:HG2	1:D:714:TYR:O	1.75	0.87
1:D:97:MET:HE1	1:D:120:ARG:HA	1.57	0.86
1:D:479:ASN:HD22	1:D:483:GLN:HG2	1.41	0.84
1:D:97:MET:CE	1:D:120:ARG:HA	2.08	0.84
1:C:604:VAL:HG11	1:C:644:GLN:HE22	1.44	0.82
1:D:3:VAL:HG11	1:D:48:PRO:HB2	1.67	0.76
1:B:109:ASN:OD1	1:B:111:PRO:HD2	1.87	0.74
1:D:38:THR:HG22	1:D:40:ILE:H	1.52	0.74
1:D:91:ASN:HD21	1:D:107:HIS:H	1.36	0.73
1:D:239:THR:HG22	1:D:241:ARG:H	1.52	0.73
1:C:530:VAL:HG21	1:C:569:LYS:HB2	1.70	0.72
1:D:41:SER:HB3	1:D:44:ILE:HD12	1.71	0.72
1:A:530:VAL:HG21	1:A:569:LYS:HB2	1.70	0.72
1:B:530:VAL:HG21	1:B:569:LYS:HB2	1.72	0.72
1:C:205:MET:CE	1:C:467:MET:SD	2.77	0.72
1:D:530:VAL:HG21	1:D:569:LYS:HB2	1.72	0.72
1:D:474:GLU:H	1:D:487:ASN:ND2	1.87	0.71
1:B:242:ASN:HD21	2:B:801:EDO:H12	1.56	0.70
1:C:3:VAL:HG11	1:C:48:PRO:HB2	1.72	0.70
1:C:53:VAL:HG22	1:C:73:PRO:HD2	1.75	0.69
1:D:470:ILE:HG13	1:D:471:PHE:H	1.58	0.69
1:D:751:ILE:HG22	1:D:752:GLY:H	1.57	0.69
1:B:41:SER:HG	1:B:43:THR:HB	1.59	0.67
1:A:53:VAL:HG22	1:A:73:PRO:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:ASN:HD22	1:D:244:ASN:ND2	1.94	0.66
1:B:232:GLU:O	1:B:236:ASN:HB2	1.96	0.66
1:C:220[B]:ILE:HD11	1:C:264:TYR:HA	1.78	0.65
1:A:607:GLY:HA2	1:A:632:LYS:HA	1.78	0.65
1:D:53:VAL:HG22	1:D:73:PRO:HD2	1.78	0.65
1:B:58:GLN:NE2	1:B:69:VAL:HG22	2.12	0.65
1:D:474:GLU:N	1:D:487:ASN:HD21	1.91	0.65
1:C:761:GLU:HA	1:C:764:LYS:HE2	1.80	0.64
1:D:713:LEU:HD21	1:D:734:LYS:HB3	1.78	0.64
1:B:53:VAL:HG22	1:B:73:PRO:HD2	1.80	0.64
1:D:106:ASN:HD21	1:D:767:THR:HG21	1.63	0.64
1:C:518:GLU:HB2	4:C:810:HOH:O	1.97	0.63
1:D:242:ASN:HA	4:D:918:HOH:O	1.97	0.63
1:A:369:GLU:HG3	1:A:425:LYS:HB2	1.82	0.62
1:D:184:SER:HB3	1:D:659:THR:HG22	1.81	0.62
1:D:751:ILE:CG2	1:D:752:GLY:H	2.14	0.60
1:B:102:ILE:HD12	1:B:130:ALA:HB2	1.85	0.59
1:C:707:ARG:HG3	1:C:712:PHE:HB2	1.84	0.58
1:C:604:VAL:HG21	1:C:639:SER:O	2.04	0.57
1:D:526:GLU:O	1:D:530:VAL:HG23	2.04	0.57
1:D:671:GLU:HG2	1:D:682:LYS:HE2	1.84	0.57
1:A:630:ILE:HG12	1:C:5:ASN:HB3	1.85	0.57
1:A:102:ILE:HD12	1:A:130:ALA:HB2	1.86	0.57
1:B:41:SER:HB3	1:B:44:ILE:HD12	1.87	0.57
1:D:285:ARG:HB3	1:D:291:TYR:CZ	2.40	0.57
1:D:31:PHE:CZ	1:D:61:SER:HB3	2.39	0.57
1:D:195:ALA:HA	1:D:668:LYS:HB3	1.86	0.57
1:D:484:LEU:O	1:D:488:ILE:HG13	2.04	0.56
1:B:369:GLU:HG3	1:B:425:LYS:HB2	1.88	0.56
1:D:3:VAL:CG1	1:D:48:PRO:HB2	2.36	0.56
1:D:414:ALA:HB3	1:D:417:THR:HG23	1.87	0.55
1:C:160:HIS:HA	1:C:163:LEU:HD12	1.89	0.55
1:D:751:ILE:HG22	1:D:752:GLY:N	2.21	0.55
1:A:134:ILE:HD13	1:A:170:CYS:SG	2.47	0.55
1:C:134:ILE:HD13	1:C:170:CYS:SG	2.47	0.54
1:B:134:ILE:HD13	1:B:170:CYS:SG	2.47	0.54
1:C:205:MET:HE2	1:C:467:MET:SD	2.46	0.54
1:C:232:GLU:O	1:C:236:ASN:HB2	2.08	0.54
1:C:3:VAL:CG1	1:C:48:PRO:HB2	2.38	0.53
1:D:267:VAL:H	1:D:452:ASN:HD21	1.57	0.53
1:A:422:ARG:HB3	1:A:422:ARG:HH11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:VAL:HG22	1:B:679:CYS:SG	2.49	0.52
1:D:129:THR:HG22	1:D:134:ILE:HG22	1.92	0.52
1:D:102:ILE:HD12	1:D:130:ALA:HB2	1.91	0.52
1:D:232:GLU:O	1:D:236:ASN:HB2	2.10	0.52
1:A:605:LEU:HD11	1:A:609:LEU:HD13	1.91	0.52
1:D:267:VAL:H	1:D:452:ASN:ND2	2.09	0.51
1:C:721:ILE:O	1:C:725:GLU:HG3	2.11	0.51
1:C:736:VAL:HG22	1:C:751:ILE:HG12	1.92	0.51
1:B:608:ASP:O	1:B:612:VAL:HG23	2.11	0.51
1:D:293:PHE:CE1	1:D:353:PHE:HB3	2.46	0.51
1:C:102:ILE:HD12	1:C:130:ALA:HB2	1.92	0.51
1:D:227:ALA:HB2	1:D:451:LEU:HD13	1.93	0.50
1:A:416:GLY:HA3	1:C:40:ILE:HD11	1.92	0.50
1:A:3:VAL:HG22	1:A:679:CYS:SG	2.52	0.50
1:C:526:GLU:O	1:C:530:VAL:HG23	2.12	0.49
1:D:514:ILE:HG23	1:D:750:LYS:HD3	1.93	0.49
1:D:65:LYS:HD3	1:D:81:ASP:HB3	1.94	0.49
1:A:101:ASP:HB3	1:A:104:LEU:HG	1.94	0.49
1:B:371:GLN:HE21	1:B:376:SER:HA	1.77	0.49
1:C:65:LYS:HD3	1:C:81:ASP:HB3	1.95	0.49
1:B:346:GLU:CD	1:B:346:GLU:H	2.16	0.49
1:B:707:ARG:HG3	1:B:711:GLU:HB3	1.94	0.49
1:C:278:ILE:HA	1:C:315:LEU:HD22	1.94	0.48
1:A:630:ILE:HG13	1:C:5:ASN:HD22	1.79	0.48
1:A:242:ASN:HB3	1:A:245:SER:HB2	1.94	0.48
1:A:608:ASP:O	1:A:612:VAL:HG23	2.13	0.48
1:C:205:MET:HE1	1:C:467:MET:SD	2.54	0.48
1:D:96:PRO:HG2	1:D:119:HIS:CG	2.49	0.48
1:A:65:LYS:HD3	1:A:81:ASP:HB3	1.95	0.48
1:A:278:ILE:HA	1:A:315:LEU:HD22	1.96	0.48
1:C:160:HIS:HB3	1:C:172:ARG:CZ	2.44	0.47
1:B:242:ASN:HB3	1:B:245:SER:HB2	1.96	0.47
1:B:65:LYS:HD3	1:B:81:ASP:HB3	1.96	0.47
1:D:236:ASN:HD22	1:D:244:ASN:HD21	1.60	0.47
1:D:669:PRO:HA	1:D:683:ILE:HD11	1.96	0.47
1:D:17:ARG:HH21	1:D:85:THR:HG22	1.80	0.47
1:D:160:HIS:HA	1:D:163:LEU:HD12	1.96	0.47
1:C:705:TYR:HE2	1:C:760:GLN:HA	1.79	0.47
1:B:101:ASP:HB3	1:B:104:LEU:HG	1.98	0.46
1:B:526:GLU:O	1:B:530:VAL:HG23	2.15	0.46
1:C:160:HIS:HB2	1:C:163:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:GLY:HA2	1:C:329:VAL:HG13	1.97	0.46
1:A:406:GLU:HB3	1:A:609:LEU:HG	1.98	0.46
1:C:242:ASN:HB3	1:C:245:SER:HB2	1.96	0.46
1:D:119:HIS:O	1:D:123:LYS:HG3	2.16	0.46
1:C:470:ILE:HD12	1:C:471:PHE:H	1.81	0.46
1:C:531:LEU:HD21	1:C:583:ILE:HG21	1.97	0.46
1:D:495:LYS:HA	1:D:524[B]:ASN:HD21	1.81	0.46
1:D:709:PHE:CZ	1:D:732:GLN:HG3	2.50	0.46
1:B:55:CYS:HB3	1:B:68:VAL:HB	1.96	0.46
1:D:133:LEU:HD23	1:D:663:PHE:HB2	1.98	0.46
1:A:526:GLU:O	1:A:530:VAL:HG23	2.16	0.46
1:B:332:PHE:HA	1:B:335:VAL:HG12	1.97	0.46
1:D:608:ASP:O	1:D:612:VAL:HG23	2.16	0.46
1:A:724:ALA:O	1:A:728:SER:HB3	2.16	0.45
1:C:226:ALA:O	1:C:229:PRO:HD2	2.15	0.45
1:C:730:GLU:HB3	1:C:733:ASN:HB2	1.97	0.45
1:C:705:TYR:CE2	1:C:760:GLN:HA	2.51	0.45
1:B:706:ARG:O	1:B:707:ARG:HD3	2.17	0.45
1:D:762:GLY:HA2	1:D:765:ILE:HD12	1.97	0.45
1:D:296:GLY:HA2	1:D:329:VAL:HG13	1.99	0.45
1:B:406:GLU:HB3	1:B:609:LEU:HG	1.98	0.45
1:D:751:ILE:CG2	1:D:752:GLY:N	2.79	0.45
1:C:101:ASP:HB3	1:C:104:LEU:HG	1.99	0.45
1:B:226:ALA:O	1:B:229:PRO:HD2	2.17	0.45
1:B:296:GLY:HA2	1:B:329:VAL:HG13	1.98	0.45
1:B:531:LEU:HD21	1:B:583:ILE:HG21	1.98	0.44
1:B:762:GLY:HA2	1:B:765:ILE:HD12	2.00	0.44
1:D:292:GLN:HB2	1:D:332:PHE:HB2	1.98	0.44
1:A:554:GLU:HG3	1:A:579:LYS:HE3	1.99	0.44
1:B:278:ILE:HA	1:B:315:LEU:HD22	1.98	0.44
1:D:219:ARG:HG3	1:D:220:ILE:HD12	1.99	0.44
1:C:554:GLU:HG3	1:C:579:LYS:HE3	1.99	0.44
1:D:259:GLU:HG3	1:D:259:GLU:H	1.65	0.44
1:A:713:LEU:HD21	1:A:734:LYS:HB3	2.00	0.44
1:D:101:ASP:HB3	1:D:104:LEU:HG	1.99	0.44
1:C:47:ASP:HB3	1:C:50:ILE:HG12	2.00	0.44
1:C:220[B]:ILE:CD1	1:C:264:TYR:HA	2.46	0.44
1:A:226:ALA:O	1:A:229:PRO:HD2	2.18	0.44
1:B:47:ASP:HB3	1:B:50:ILE:HG12	1.98	0.44
1:C:174:ALA:O	1:C:185:GLN:HG3	2.18	0.44
1:D:571:THR:HB	1:D:582:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:VAL:HG21	1:A:644:GLN:HE22	1.83	0.43
1:C:406:GLU:HB3	1:C:609:LEU:HG	1.98	0.43
1:D:175:LEU:HA	1:D:175:LEU:HD23	1.87	0.43
1:B:230:VAL:HG22	1:B:335:VAL:HG23	1.99	0.43
1:C:147:THR:HG22	1:C:150:TRP:HD1	1.84	0.43
1:A:413:VAL:O	1:A:413:VAL:HG12	2.19	0.43
1:A:174:ALA:O	1:A:185:GLN:HG3	2.18	0.43
1:D:31:PHE:N	1:D:31:PHE:CD2	2.86	0.43
1:D:726:ASP:C	1:D:728:SER:H	2.23	0.43
1:D:732:GLN:O	1:D:736:VAL:HG13	2.19	0.43
1:A:274:LYS:HD2	1:A:437:LYS:HB3	2.01	0.42
1:C:729:VAL:HG13	1:C:734:LYS:HG3	2.01	0.42
1:A:508:LEU:HD23	1:A:509:TYR:HD1	1.84	0.42
1:B:554:GLU:HG3	1:B:579:LYS:HE3	2.00	0.42
1:A:47:ASP:HB3	1:A:50:ILE:HG12	2.00	0.42
1:A:762:GLY:HA2	1:A:765:ILE:HD12	2.01	0.42
1:A:531:LEU:HD21	1:A:583:ILE:HG21	2.01	0.42
1:C:55:CYS:HB3	1:C:68:VAL:HB	2.02	0.42
1:D:370:LYS:HB2	1:D:378:ALA:HB3	2.01	0.42
1:C:732:GLN:O	1:C:736:VAL:HG23	2.20	0.42
1:D:601:ASN:HD21	1:D:642:GLY:H	1.67	0.42
1:D:47:ASP:HB3	1:D:50:ILE:HG22	2.01	0.42
1:A:296:GLY:HA2	1:A:329:VAL:HG13	2.00	0.42
1:C:274:LYS:HD2	1:C:437:LYS:HB3	2.00	0.42
1:C:441:GLU:O	1:C:445:LEU:HG	2.19	0.42
1:D:472:GLY:HA2	1:D:490:ASN:OD1	2.20	0.42
1:B:605:LEU:HD11	1:B:609:LEU:HD13	2.02	0.42
1:D:22:GLU:O	1:D:34:TYR:CZ	2.73	0.42
1:A:41:SER:HB3	1:A:44:ILE:HD12	2.02	0.42
1:A:451:LEU:O	1:A:455:ILE:HG12	2.19	0.42
1:C:709:PHE:HD1	1:C:735:CYS:HG	1.67	0.42
1:A:698:LEU:HA	1:A:701:LEU:HD12	2.02	0.41
1:D:21:VAL:HG21	1:D:36:ILE:HG22	2.02	0.41
1:A:633:GLY:HA2	1:A:634:LYS:HA	1.83	0.41
1:C:248:PHE:HB3	1:C:272:LEU:HD12	2.02	0.41
1:D:358:GLY:HA3	1:D:396:MET:HG3	2.02	0.41
1:A:59:GLN:HB3	1:D:714:TYR:CZ	2.55	0.41
1:B:174:ALA:O	1:B:185:GLN:HG3	2.20	0.41
1:B:470:ILE:HD12	1:B:471:PHE:H	1.85	0.41
1:C:147:THR:HG22	1:C:150:TRP:CD1	2.55	0.41
1:D:512:GLU:HB2	1:D:514:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:PRO:O	1:B:404:LYS:HB2	2.21	0.41
1:D:191:GLY:HA2	1:D:690:LEU:HD21	2.03	0.41
1:C:220[B]:ILE:HG12	1:C:263:ARG:O	2.21	0.41
1:A:55:CYS:HB3	1:A:68:VAL:HB	2.02	0.41
1:C:191:GLY:HA2	1:C:690:LEU:HD21	2.03	0.41
1:A:147:THR:HG22	1:A:150:TRP:HD1	1.86	0.40
1:A:239:THR:HA	1:A:284:GLU:HG2	2.02	0.40
1:B:451:LEU:O	1:B:455:ILE:HG12	2.21	0.40
1:C:160:HIS:CA	1:C:163:LEU:HD12	2.51	0.40
1:D:106:ASN:ND2	1:D:767:THR:HG21	2.32	0.40
1:A:317:ASN:HB3	1:A:320:SER:OG	2.21	0.40
1:B:147:THR:HG22	1:B:150:TRP:HD1	1.84	0.40
1:C:731:ASN:HA	1:C:734:LYS:HE3	2.03	0.40
1:B:147:THR:HG22	1:B:150:TRP:CD1	2.55	0.40
1:B:171:ALA:HB1	1:B:207:TYR:CD1	2.56	0.40
1:D:193:SER:HB3	1:D:242:ASN:ND2	2.36	0.40
1:D:621:VAL:HA	1:D:624:LEU:HG	2.03	0.40
1:D:488:ILE:HG12	1:D:531:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	757/768 (99%)	723 (96%)	32 (4%)	2 (0%)	41	70
1	B	749/768 (98%)	723 (96%)	25 (3%)	1 (0%)	51	80
1	C	749/768 (98%)	714 (95%)	32 (4%)	3 (0%)	34	64
1	D	754/768 (98%)	711 (94%)	35 (5%)	8 (1%)	14	39
All	All	3009/3072 (98%)	2871 (95%)	124 (4%)	14 (0%)	29	59

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	631	GLU
1	C	607	GLY
1	C	751	ILE
1	D	213	SER
1	D	215	ASN
1	D	373	ALA
1	D	519	LEU
1	A	630	ILE
1	C	374	GLY
1	D	637	LYS
1	B	603	ASP
1	D	727	SER
1	D	535	GLY
1	D	751	ILE

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	670/679 (99%)	637 (95%)	33 (5%)	25 55
1	B	661/679 (97%)	643 (97%)	18 (3%)	44 77
1	C	666/679 (98%)	634 (95%)	32 (5%)	25 56
1	D	668/679 (98%)	619 (93%)	49 (7%)	14 37
All	All	2665/2716 (98%)	2533 (95%)	132 (5%)	24 55

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	149	GLU
1	A	162	LYS
1	A	173	GLU
1	A	178	LEU
1	A	216	MET
1	A	246	SER
1	A	371	GLN

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Mol	Chain	Res	Type
1	A	375	LEU
1	A	376	SER
1	A	401	GLU
1	A	404	LYS
1	A	417	THR
1	A	429	GLU
1	A	470	ILE
1	A	508	LEU
1	A	511	ASP
1	A	522	THR
1	A	540	SER
1	A	566	GLU
1	A	568	ASN
1	A	628	GLN
1	A	660	GLU
1	A	671	GLU
1	A	682	LYS
1	A	699	ARG
1	A	704	SER
1	A	706	ARG
1	A	710	GLU
1	A	714	TYR
1	A	718	PHE
1	A	740	LYS
1	A	741	LEU
1	B	25	ASP
1	B	63	LYS
1	B	149	GLU
1	B	173	GLU
1	B	178	LEU
1	B	246	SER
1	B	370	LYS
1	B	404	LYS
1	B	429	GLU
1	B	470	ILE
1	B	508	LEU
1	B	511	ASP
1	B	568	ASN
1	B	630	ILE
1	B	671	GLU
1	B	707	ARG
1	B	741	LEU

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Mol	Chain	Res	Type
1	B	761	GLU
1	C	3	VAL
1	C	5	ASN
1	C	26	LYS
1	C	149	GLU
1	C	162	LYS
1	C	173	GLU
1	C	178	LEU
1	C	199	GLU
1	C	215	ASN
1	C	246	SER
1	C	342	MET
1	C	404	LYS
1	C	429	GLU
1	C	470	ILE
1	C	508	LEU
1	C	511	ASP
1	C	556	PHE
1	C	566	GLU
1	C	568	ASN
1	C	604	VAL
1	C	605	LEU
1	C	628	GLN
1	C	630	ILE
1	C	637	LYS
1	C	671	GLU
1	C	706	ARG
1	C	710	GLU
1	C	725	GLU
1	C	731	ASN
1	C	733	ASN
1	C	741	LEU
1	C	760	GLN
1	D	3	VAL
1	D	22	GLU
1	D	25	ASP
1	D	32	LYS
1	D	92	SER
1	D	134	ILE
1	D	153	ARG
1	D	160	HIS
1	D	162	LYS

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Mol	Chain	Res	Type
1	D	167	VAL
1	D	173	GLU
1	D	176	SER
1	D	193	SER
1	D	219	ARG
1	D	221	GLN
1	D	225	MET
1	D	244	ASN
1	D	246	SER
1	D	258	HIS
1	D	259	GLU
1	D	266	SER
1	D	271	LEU
1	D	283	ASN
1	D	343	GLU
1	D	404	LYS
1	D	405	ARG
1	D	406	GLU
1	D	408	LEU
1	D	429	GLU
1	D	451	LEU
1	D	471	PHE
1	D	480	SER
1	D	496	ASN
1	D	508	LEU
1	D	511	ASP
1	D	534	LYS
1	D	540	SER
1	D	568	ASN
1	D	595	GLU
1	D	608	ASP
1	D	639	SER
1	D	660	GLU
1	D	694	GLU
1	D	698	LEU
1	D	718	PHE
1	D	721	ILE
1	D	741	LEU
1	D	758	LEU
1	D	767	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	70	GLN
1	A	107	HIS
1	A	644	GLN
1	A	731	ASN
1	A	732	GLN
1	B	58	GLN
1	B	70	GLN
1	B	242	ASN
1	B	258	HIS
1	B	371	GLN
1	B	700	GLN
1	C	5	ASN
1	C	58	GLN
1	C	70	GLN
1	C	644	GLN
1	C	731	ASN
1	D	49	ASN
1	D	70	GLN
1	D	91	ASN
1	D	106	ASN
1	D	145	ASN
1	D	185	GLN
1	D	203	GLN
1	D	221	GLN
1	D	242	ASN
1	D	244	ASN
1	D	452	ASN
1	D	479	ASN
1	D	487	ASN
1	D	601	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

4 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	$\#\|Z\| > 2$
1	SEP	A	19	1	8,9,10	1.04	0	8,12,14	2.22	1 (12%)
1	SEP	C	19	1	8,9,10	1.14	1 (12%)	8,12,14	3.10	4 (50%)
1	SEP	B	19	1	8,9,10	0.95	0	8,12,14	2.96	4 (50%)
1	SEP	D	19	1	8,9,10	1.27	1 (12%)	8,12,14	5.49	2 (25%)

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
1	SEP	A	19	1	-	1/5/8/10	-
1	SEP	C	19	1	-	1/5/8/10	-
1	SEP	B	19	1	-	1/5/8/10	-
1	SEP	D	19	1	-	4/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	19	SEP	CB-CA	2.50	1.59	1.52
1	C	19	SEP	P-OG	-2.06	1.53	1.60

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	19	SEP	OG-CB-CA	14.94	122.68	108.14
1	A	19	SEP	OG-CB-CA	5.51	113.50	108.14
1	C	19	SEP	OG-CB-CA	5.42	113.42	108.14
1	C	19	SEP	O2P-P-OG	-5.06	93.27	106.73
1	B	19	SEP	OG-CB-CA	5.05	113.06	108.14
1	B	19	SEP	OG-P-O1P	-4.78	93.06	106.47
1	C	19	SEP	OG-P-O1P	4.13	118.05	106.47
1	B	19	SEP	O2P-P-OG	3.71	116.60	106.73
1	D	19	SEP	O3P-P-OG	3.24	115.35	106.73
1	C	19	SEP	O3P-P-O2P	2.08	115.58	107.64
1	B	19	SEP	O3P-P-OG	2.03	112.14	106.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	19	SEP	N-CA-CB-OG
1	D	19	SEP	CB-OG-P-O1P
1	D	19	SEP	CB-OG-P-O2P
1	A	19	SEP	CA-CB-OG-P
1	C	19	SEP	CA-CB-OG-P
1	B	19	SEP	CA-CB-OG-P
1	D	19	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
2	EDO	B	801	-	3,3,3	1.02	0	2,2,2	0.51	0
2	EDO	D	801	-	3,3,3	0.35	0	2,2,2	0.72	0
3	GOL	D	802	-	5,5,5	0.16	0	5,5,5	0.44	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
2	EDO	B	801	-	-	0/1/1/1	-
2	EDO	D	801	-	-	0/1/1/1	-
3	GOL	D	802	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	802	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	EDO	1	0

5.7 Other polymers

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, 95^{th} 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	761/768 (99%)	-0.15	11 (1%)	75	69	36, 60, 95, 138	0
1	B	754/768 (98%)	0.18	46 (6%)	21	13	37, 70, 160, 182	0
1	C	754/768 (98%)	0.12	30 (3%)	38	28	34, 76, 122, 144	0
1	D	757/768 (98%)	-0.06	26 (3%)	45	35	36, 61, 106, 132	0
All	All	3026/3072 (98%)	0.02	113 (3%)	41	31	34, 66, 117, 182	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	741	LEU	10.2
1	B	712	PHE	8.6
1	B	751	ILE	8.4
1	B	728	SER	7.6
1	C	411	VAL	5.9
1	B	732	GLN	5.7
1	B	736	VAL	5.6
1	B	733	ASN	5.4
1	B	729	VAL	5.3
1	B	737	ASN	5.2
1	B	747	SER	5.2
1	B	739	LEU	5.1
1	C	705	TYR	5.1
1	D	215	ASN	4.7
1	D	214	GLY	4.7
1	D	742	SER	4.6
1	C	728	SER	4.5
1	B	740	LYS	4.5
1	B	730	GLU	4.5
1	C	635	ILE	4.5
1	A	741	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	716	TYR	4.4
1	B	742	SER	4.4
1	B	749	TYR	4.1
1	B	713	LEU	4.0
1	B	709	PHE	4.0
1	D	260	GLY	3.9
1	B	750	LYS	3.9
1	D	762	GLY	3.9
1	D	636	ALA	3.9
1	B	756	VAL	3.9
1	B	758	LEU	3.9
1	D	31	PHE	3.9
1	C	740	LYS	3.9
1	B	744	LEU	3.8
1	B	417	THR	3.8
1	D	27	SER	3.7
1	D	213	SER	3.7
1	A	634	LYS	3.7
1	C	637	LYS	3.7
1	B	710	GLU	3.7
1	B	746	GLU	3.7
1	C	215	ASN	3.7
1	B	413	VAL	3.6
1	D	259	GLU	3.6
1	D	723	ALA	3.5
1	B	752	GLY	3.4
1	C	726	ASP	3.4
1	D	217	ASP	3.4
1	B	760	GLN	3.3
1	C	725	GLU	3.3
1	B	748	MET	3.3
1	B	745	SER	3.2
1	B	714	TYR	3.2
1	A	713	LEU	3.0
1	D	216	MET	3.0
1	A	714	TYR	3.0
1	B	718	PHE	3.0
1	C	518	GLU	2.9
1	D	718	PHE	2.8
1	B	735	CYS	2.8
1	B	717	LYS	2.8
1	A	548	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	414	ALA	2.8
1	D	703	TYR	2.8
1	D	741	LEU	2.7
1	B	753	LYS	2.7
1	D	748	MET	2.7
1	A	579	LYS	2.6
1	C	372	GLU	2.6
1	D	743	GLY	2.6
1	D	744	LEU	2.5
1	C	760	GLN	2.5
1	C	396	MET	2.5
1	B	734	LYS	2.5
1	A	739	LEU	2.5
1	B	738	ILE	2.5
1	C	629	VAL	2.4
1	C	25	ASP	2.4
1	D	746	GLU	2.4
1	C	738	ILE	2.3
1	B	415	GLY	2.3
1	C	27	SER	2.3
1	C	315	LEU	2.3
1	B	416	GLY	2.2
1	C	63	LYS	2.2
1	D	738	ILE	2.2
1	C	630	ILE	2.2
1	C	62	LYS	2.2
1	D	63	LYS	2.2
1	A	718	PHE	2.2
1	D	373	ALA	2.2
1	D	417	THR	2.2
1	C	326	VAL	2.2
1	C	435	LEU	2.2
1	B	503	GLU	2.2
1	C	521	TYR	2.1
1	C	766	LEU	2.1
1	C	636	ALA	2.1
1	D	26	LYS	2.1
1	B	522	THR	2.1
1	D	81	ASP	2.1
1	C	223	ALA	2.1
1	C	729	VAL	2.1
1	A	716	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	641	ILE	2.1
1	C	420	GLU	2.1
1	A	32	LYS	2.1
1	A	414	ALA	2.0
1	B	570	PHE	2.0
1	B	768	LYS	2.0
1	B	743	GLY	2.0
1	B	554	GLU	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, 95^{th} 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
1	SEP	C	19	10/11	0.95	0.12	63,67,74,76	0
1	SEP	B	19	10/11	0.95	0.15	68,72,80,81	0
1	SEP	A	19	10/11	0.96	0.15	58,61,66,67	0
1	SEP	D	19	10/11	0.96	0.12	76,79,80,80	0

6.3 Carbohydrates (i)

There are no carbohydrates 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, 95^{th} 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	GOL	D	802	6/6	0.92	0.21	54,64,66,67	0
2	EDO	B	801	4/4	0.95	0.28	40,47,52,53	0
2	EDO	D	801	4/4	0.98	0.25	54,56,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.