WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2017 – 01:12 AM EDT

PDB ID	:	3LIF
Title	:	Crystal Structure of the extracellular domain of the putative histidine kinase rpHK1S-Z16
Authors	:	Zhang, Z.; Hendrickson, W.A.
Deposited on	:	unknown
Resolution	:	2.70 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 2.70 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	Percentile Ranks	Value
Rfree		0.255
Clashscore		36
Ramachandran outliers		4.2%
Sidechain outliers		17.3%
RSRZ outliers		2.1%

Worse — *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
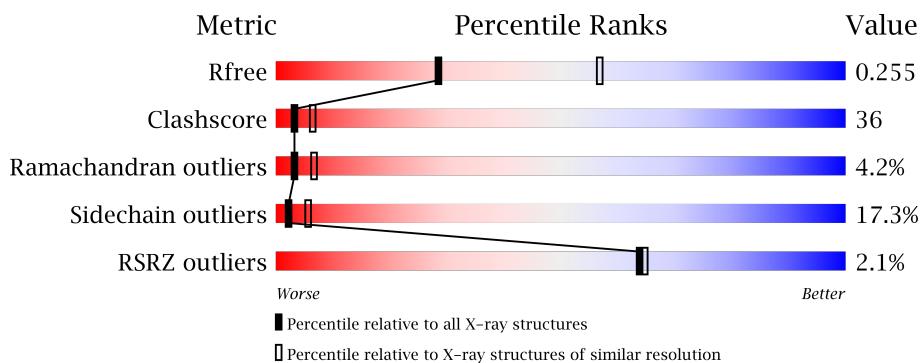
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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. 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	254	55% 26% 11% • •
1	B	254	4% 48% 33% 10% • 5%
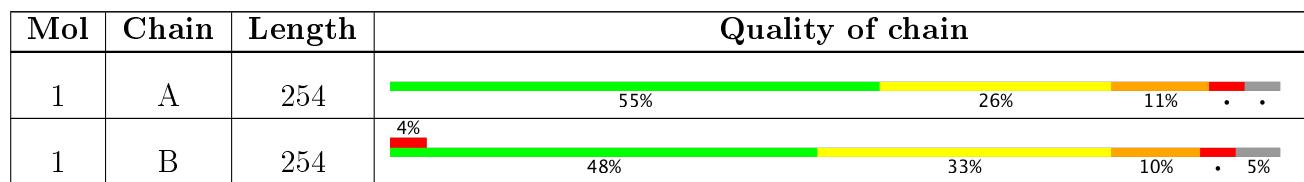
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	A	1	-	-	X	X
2	MPD	B	2	-	-	X	-
3	CIT	A	294	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3984 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 Putative diguanylate cyclase (GGDEF) with PAS/PAC domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	Se	0	1	0
			1929	1227	336	362	4			
1	B	241	Total	C	N	O	Se	0	1	0
			1920	1224	332	360	4			

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).
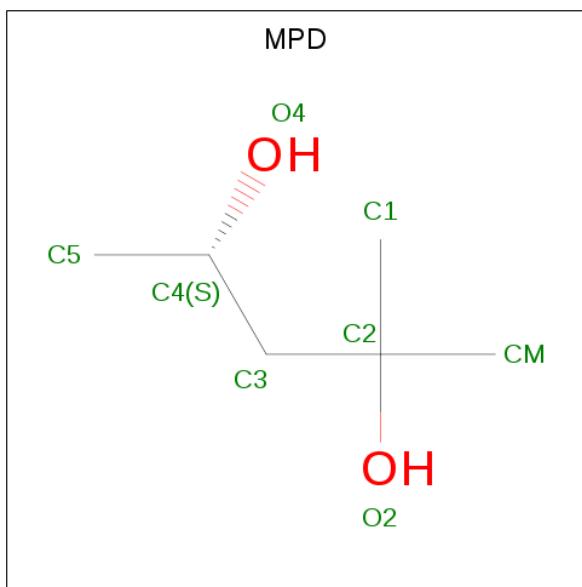
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
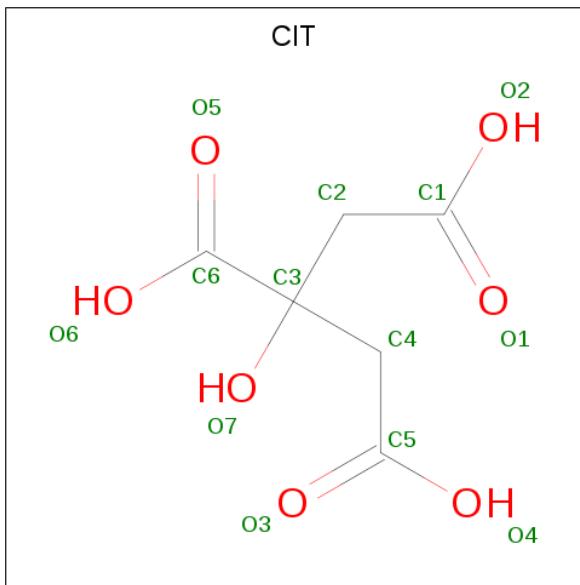
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 13	C 6	O 7	0	0
3	B	1	Total 13	C 6	O 7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total 57	O 57	0	0
4	B	36	Total 36	O 36	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: Putative diguanylate cyclase (GGDEF) with PAS/PAC domain

Chain A:

• Molecule 1: Putative diguanylate cyclase (GGDEF) with PAS/PAC domain

Chain B:
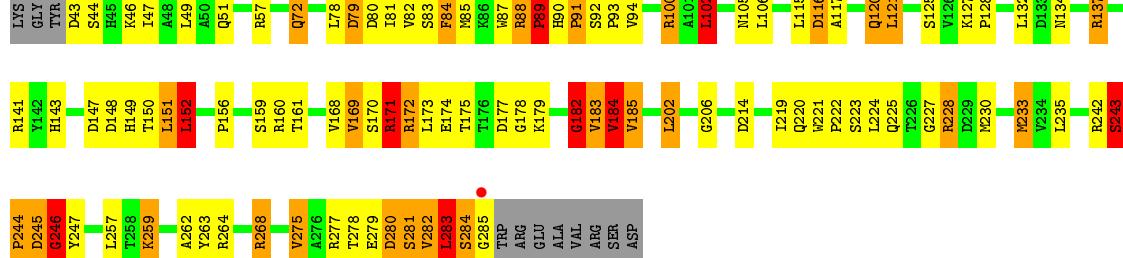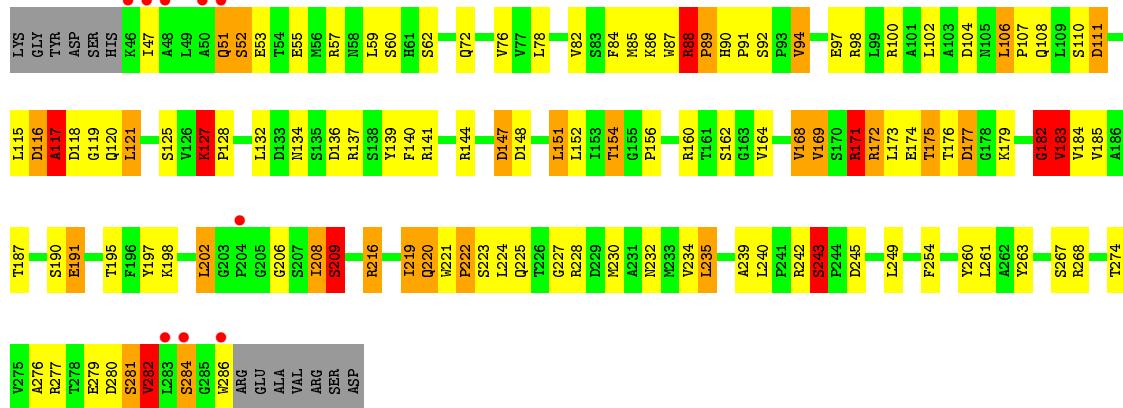
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α, β, γ	184.78Å 184.78Å 184.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.39 – 2.70 41.32 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.39-2.70) 100.0 (41.32-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	9.69 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.205 , 0.256 0.211 , 0.255	Depositor DCC
R_{free} test set	1500 reflections (5.23%)	DCC
Wilson B-factor (Å^2)	45.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.5	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3984	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MPD, CIT

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	0.99	1/1977 (0.1%)	1.18	16/2685 (0.6%)
1	B	0.94	0/1965	1.09	9/2670 (0.3%)
All	All	0.96	1/3942 (0.0%)	1.13	25/5355 (0.5%)

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	A	0	5
1	B	0	3
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	GLY	N-CA	5.16	1.53	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	184	VAL	CB-CA-C	-9.13	94.06	111.40
1	A	185	VAL	CB-CA-C	-8.38	95.48	111.40
1	A	117	ALA	N-CA-C	-7.29	91.31	111.00
1	A	275	VAL	CB-CA-C	-7.17	97.78	111.40
1	A	184	VAL	CB-CA-C	-7.12	97.86	111.40
1	A	89	PRO	N-CA-C	-7.11	93.62	112.10
1	A	79	ASP	CB-CG-OD1	-6.92	112.07	118.30
1	B	111	ASP	CB-CG-OD1	-6.75	112.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	GLY	N-CA-C	-6.74	96.26	113.10
1	B	183	VAL	N-CA-C	6.66	128.98	111.00
1	B	182	GLY	C-N-CA	6.35	137.56	121.70
1	A	171	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	A	245	ASP	N-CA-CB	-6.05	99.70	110.60
1	B	117	ALA	N-CA-C	-6.04	94.68	111.00
1	A	121	LEU	CA-CB-CG	5.99	129.06	115.30
1	A	116	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	246	GLY	N-CA-C	5.45	126.73	113.10
1	A	152	LEU	CB-CG-CD2	5.31	120.03	111.00
1	B	243	SER	N-CA-C	5.28	125.26	111.00
1	A	214	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	102	LEU	CB-CG-CD1	-5.24	102.10	111.00
1	A	233	MSE	CG-SE-CE	-5.12	87.64	98.90
1	A	228	ARG	CB-CG-CD	-5.10	98.34	111.60
1	B	209	SER	CB-CA-C	-5.08	100.44	110.10
1	B	171	ARG	CG-CD-NE	-5.00	101.29	111.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ASP	Peptide
1	A	182	GLY	Peptide
1	A	243	SER	Peptide
1	A	244	PRO	Peptide
1	A	88	ARG	Peptide
1	B	116	ASP	Peptide
1	B	182	GLY	Peptide
1	B	242	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1929	0	1893	133	0
1	B	1920	0	1883	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	8	0	14	18	0
2	B	8	0	14	7	0
3	A	13	0	5	7	0
3	B	13	0	5	4	0
4	A	57	0	0	10	0
4	B	36	0	0	5	0
All	All	3984	0	3814	279	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 36.

All (279) 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:B:116:ASP:HB2	1:B:117:ALA:CB	1.38	1.46
1:A:171:ARG:HH11	1:A:171:ARG:CG	1.31	1.36
1:A:230:MSE:HB3	1:A:233:MSE:CE	1.63	1.26
1:B:116:ASP:CB	1:B:117:ALA:HB3	1.64	1.25
1:A:160:ARG:H	2:A:1:MPD:C5	1.52	1.21
1:A:72:GLN:OE1	1:A:268:ARG:NH2	1.75	1.20
1:A:228:ARG:HG3	1:A:230:MSE:CE	1.74	1.18
3:A:294:CIT:H22	4:A:328:HOH:O	1.12	1.16
3:A:294:CIT:H42	4:A:328:HOH:O	1.11	1.14
1:B:127:LYS:HB3	1:B:128:PRO:CD	1.78	1.12
1:B:127:LYS:CB	1:B:128:PRO:HD3	1.80	1.12
1:A:284:SER:OG	1:A:285:GLY:HA2	1.49	1.11
1:A:171:ARG:NH1	1:A:171:ARG:HG2	1.18	1.11
1:B:219:ILE:HD12	1:B:219:ILE:N	1.62	1.08
1:B:139:TYR:OH	2:B:2:MPD:H52	1.55	1.06
1:B:208:ILE:HD12	1:B:209:SER:N	1.70	1.06
1:A:281:SER:O	1:A:282:VAL:HG23	1.53	1.06
1:B:137:ARG:HE	2:B:2:MPD:H51	1.16	1.05
1:A:230:MSE:CB	1:A:233:MSE:HE3	1.86	1.05
1:B:175:THR:HG22	1:B:179:LYS:H	1.18	1.05
1:A:161:THR:HG23	2:A:1:MPD:H12	1.38	1.04
1:B:127:LYS:HB3	1:B:128:PRO:HD3	1.05	1.04
1:A:245:ASP:HB2	1:A:246:GLY:HA3	1.40	1.03
1:B:116:ASP:CB	1:B:117:ALA:CB	2.28	1.03
1:A:228:ARG:HG3	1:A:230:MSE:HE3	1.04	1.02
1:A:88:ARG:O	1:A:91:PRO:HD3	1.61	1.00
1:B:111:ASP:HB2	1:B:125:SER:OG	1.61	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ARG:CG	1:A:230:MSE:HE3	1.90	1.00
1:A:160:ARG:H	2:A:1:MPD:H53	1.29	0.98
1:B:116:ASP:HB2	1:B:117:ALA:HB2	1.46	0.97
1:B:72:GLN:OE1	1:B:268:ARG:NH2	1.99	0.95
1:B:208:ILE:C	1:B:208:ILE:HD12	1.87	0.95
1:B:127:LYS:CB	1:B:128:PRO:CD	2.41	0.93
1:A:284:SER:CB	1:A:285:GLY:HA2	1.99	0.93
1:B:220:GLN:HG2	1:B:254:PHE:CZ	2.05	0.92
1:A:160:ARG:N	2:A:1:MPD:C5	2.32	0.92
1:A:242:ARG:O	1:A:243:SER:HB3	1.65	0.91
1:A:134:ASN:HD22	1:A:160:ARG:HH11	1.04	0.90
1:A:137:ARG:HH21	2:A:1:MPD:H51	1.36	0.90
1:B:243:SER:OG	3:B:294:CIT:O4	1.88	0.90
1:A:230:MSE:HB3	1:A:233:MSE:HE3	0.90	0.89
2:A:1:MPD:HM3	2:A:1:MPD:H52	1.57	0.87
1:B:219:ILE:HD12	1:B:219:ILE:H	1.33	0.86
1:A:283:LEU:HD22	1:A:283:LEU:H	1.40	0.85
1:A:283:LEU:HD22	1:A:283:LEU:N	1.91	0.85
1:B:134:ASN:HB2	1:B:137:ARG:HG2	1.57	0.85
1:A:150:THR:HG22	1:A:151:LEU:O	1.78	0.84
1:A:245:ASP:HA	1:A:263:TYR:CE1	2.12	0.84
1:B:147:ASP:HA	1:B:172:ARG:HD2	1.60	0.83
1:B:88:ARG:O	1:B:91:PRO:HD3	1.79	0.83
1:A:245:ASP:O	3:A:294:CIT:O6	1.96	0.82
1:B:116:ASP:HB2	1:B:117:ALA:HB3	0.82	0.81
1:B:175:THR:CG2	1:B:179:LYS:H	1.93	0.80
1:A:228:ARG:CG	1:A:230:MSE:CE	2.56	0.80
1:A:161:THR:CG2	2:A:1:MPD:H12	2.10	0.80
1:A:228:ARG:NH1	1:A:230:MSE:HE1	1.96	0.80
2:A:1:MPD:HM3	2:A:1:MPD:C5	2.02	0.79
1:B:134:ASN:HB3	1:B:160:ARG:NH1	1.98	0.78
1:A:127:LYS:HA	1:A:128:PRO:C	2.03	0.78
1:A:134:ASN:ND2	1:A:160:ARG:HH11	1.80	0.78
1:B:220:GLN:NE2	1:B:223:SER:H	1.81	0.78
1:A:230:MSE:CB	1:A:233:MSE:CE	2.53	0.77
1:A:283:LEU:N	1:A:283:LEU:CD2	2.47	0.77
3:A:294:CIT:C4	4:A:328:HOH:O	1.85	0.77
1:A:277:ARG:HD3	4:A:329:HOH:O	1.84	0.76
1:B:86:LYS:HG3	1:B:174:GLU:O	1.85	0.76
1:A:134:ASN:HD22	1:A:160:ARG:NH1	1.82	0.75
1:A:242:ARG:O	1:A:243:SER:CB	2.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:THR:O	1:A:178:GLY:N	2.18	0.73
1:B:147:ASP:HA	1:B:172:ARG:CD	2.17	0.73
1:A:228:ARG:CZ	1:A:230:MSE:HE1	2.18	0.73
1:A:279:GLU:O	1:A:280:ASP:HB2	1.87	0.73
1:A:245:ASP:HB2	1:A:246:GLY:CA	2.17	0.73
1:B:175:THR:HG22	1:B:179:LYS:N	2.00	0.72
1:B:151:LEU:HD21	1:B:169:VAL:HG13	1.70	0.72
1:A:279:GLU:O	1:A:280:ASP:CB	2.38	0.71
1:A:72:GLN:CD	1:A:268:ARG:HH21	1.95	0.71
1:B:136:ASP:HA	1:B:141:ARG:HH12	1.56	0.70
1:B:154:THR:HG23	1:B:168:VAL:HG12	1.73	0.70
1:B:137:ARG:NE	2:B:2:MPD:H51	1.98	0.70
1:A:43:ASP:O	1:A:47:ILE:HD12	1.92	0.70
1:A:87:TRP:O	1:A:88:ARG:CG	2.40	0.70
1:A:143:HIS:HE1	1:A:170:SER:OG	1.76	0.69
1:B:156:PRO:HD3	1:B:216:ARG:HG3	1.74	0.68
1:A:43:ASP:HB2	1:A:46:LYS:HG3	1.75	0.68
1:A:160:ARG:N	2:A:1:MPD:H53	2.01	0.68
1:B:228:ARG:HB3	1:B:230:MSE:HE1	1.76	0.67
1:B:106:LEU:O	4:B:12:HOH:O	2.13	0.67
1:B:175:THR:HG23	1:B:177:ASP:H	1.61	0.66
1:A:284:SER:CB	1:A:285:GLY:CA	2.74	0.66
1:B:88:ARG:H	1:B:89:PRO:CD	2.09	0.66
1:B:220:GLN:HG2	1:B:254:PHE:CE1	2.30	0.65
1:A:264:ARG:HD3	4:A:304:HOH:O	1.96	0.65
1:A:171:ARG:NH1	1:A:171:ARG:CG	2.07	0.65
1:A:282:VAL:HA	1:A:283:LEU:O	1.97	0.65
1:B:51:GLN:O	1:B:55:GLU:HG3	1.96	0.65
1:A:284:SER:OG	1:A:285:GLY:CA	2.37	0.65
1:B:88:ARG:H	1:B:89:PRO:HD3	1.62	0.65
3:A:294:CIT:C3	4:A:328:HOH:O	2.18	0.64
1:B:53:GLU:OE2	1:B:57:ARG:NH1	2.30	0.64
1:A:225:GLN:NE2	1:A:228:ARG:HE	1.96	0.64
1:A:106:LEU:O	4:A:11:HOH:O	2.16	0.62
1:B:132:LEU:HG	1:B:134:ASN:ND2	2.14	0.62
1:A:151:LEU:HD13	1:A:169:VAL:CG2	2.30	0.62
1:A:281:SER:O	1:A:282:VAL:CG2	2.38	0.61
1:B:92:SER:OG	1:B:94:VAL:HG22	2.00	0.61
3:A:294:CIT:O3	3:A:294:CIT:O5	2.18	0.61
1:B:141:ARG:HH11	1:B:141:ARG:HG3	1.65	0.61
1:B:134:ASN:HB3	1:B:160:ARG:HH11	1.63	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLN:HE22	1:A:228:ARG:HE	1.48	0.60
1:B:52:SER:O	1:B:53:GLU:C	2.40	0.60
1:A:102:LEU:C	1:A:102:LEU:HD12	2.23	0.59
1:A:160:ARG:CB	2:A:1:MPD:H53	2.32	0.59
1:A:280:ASP:O	1:A:281:SER:OG	2.20	0.59
1:A:47:ILE:O	1:A:51:GLN:HG3	2.02	0.59
1:B:177:ASP:OD1	1:B:177:ASP:N	2.35	0.59
1:B:228:ARG:CG	1:B:230:MSE:HE1	2.33	0.58
1:B:116:ASP:CA	1:B:117:ALA:CB	2.79	0.58
1:B:168:VAL:HG23	1:B:187:THR:HG22	1.86	0.58
1:A:159:SER:HA	2:A:1:MPD:H52	1.85	0.57
1:B:116:ASP:CB	1:B:117:ALA:HB2	2.17	0.57
1:B:162:SER:HB3	4:B:297:HOH:O	2.04	0.57
1:B:88:ARG:N	1:B:89:PRO:CD	2.67	0.57
1:B:286:TRP:CE3	1:B:286:TRP:C	2.78	0.57
1:B:190:SER:HB2	1:B:219:ILE:HG13	1.87	0.57
1:B:221:TRP:CD2	1:B:222:PRO:HA	2.39	0.57
1:B:202:LEU:HB3	1:B:206:GLY:HA3	1.87	0.57
1:A:160:ARG:N	2:A:1:MPD:H52	2.15	0.56
1:A:230:MSE:SE	1:A:233:MSE:CE	3.03	0.56
1:A:173:LEU:HD21	1:A:184:VAL:HG22	1.87	0.56
1:B:277:ARG:NH2	4:B:31:HOH:O	2.32	0.56
1:A:221:TRP:CE3	1:A:222:PRO:HA	2.41	0.56
1:B:191:GLU:HG3	4:B:304:HOH:O	2.05	0.56
1:B:88:ARG:O	1:B:90:HIS:N	2.39	0.56
1:A:102:LEU:O	1:A:102:LEU:HD12	2.06	0.56
1:A:87:TRP:O	1:A:88:ARG:HG2	2.05	0.56
1:B:147:ASP:CG	1:B:147:ASP:O	2.44	0.56
1:B:228:ARG:HG2	1:B:230:MSE:HE1	1.88	0.56
1:A:151:LEU:HD13	1:A:169:VAL:HG22	1.88	0.55
1:B:107:PRO:HD2	1:B:108:GLN:OE1	2.06	0.55
1:A:149:HIS:HB3	1:A:171:ARG:NH2	2.21	0.55
1:A:242:ARG:HD2	3:A:294:CIT:O2	2.07	0.55
1:B:171:ARG:NH1	1:B:171:ARG:CG	2.69	0.54
1:B:119:GLY:N	1:B:140:PHE:CE1	2.75	0.54
1:A:150:THR:CG2	1:A:151:LEU:O	2.54	0.54
1:B:281:SER:H	1:B:282:VAL:HG12	1.72	0.54
1:A:230:MSE:HB3	1:A:233:MSE:HE1	1.77	0.53
1:A:134:ASN:O	1:A:137:ARG:HB2	2.09	0.53
1:A:160:ARG:H	2:A:1:MPD:H51	1.62	0.53
1:B:147:ASP:CB	1:B:172:ARG:CZ	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HB3	1:A:206:GLY:HA3	1.90	0.53
1:B:121:LEU:C	1:B:121:LEU:HD13	2.29	0.53
1:A:259:LYS:HB3	1:A:277:ARG:O	2.09	0.53
1:B:267:SER:O	1:B:268:ARG:HB2	2.09	0.52
1:A:220:GLN:HG3	1:A:223:SER:OG	2.09	0.52
1:A:81:ILE:O	1:A:82:VAL:C	2.45	0.52
1:B:228:ARG:CB	1:B:230:MSE:HE1	2.38	0.52
1:A:221:TRP:CD2	1:A:222:PRO:HA	2.45	0.52
1:B:92:SER:OG	1:B:94:VAL:CG2	2.57	0.52
1:A:173:LEU:HD12	1:A:183:VAL:H	1.74	0.52
1:A:92:SER:O	1:A:94:VAL:N	2.43	0.52
1:B:209:SER:HB2	1:B:274:THR:OG1	2.10	0.52
1:B:94:VAL:O	1:B:97:GLU:N	2.41	0.52
1:B:111:ASP:CB	1:B:125:SER:OG	2.49	0.51
1:B:115:LEU:HA	1:B:120:GLN:O	2.11	0.51
1:B:191:GLU:CG	4:B:304:HOH:O	2.58	0.51
1:A:141:ARG:NH2	4:A:4:HOH:O	2.43	0.51
1:B:136:ASP:HA	1:B:141:ARG:NH1	2.22	0.51
1:A:160:ARG:HB2	2:A:1:MPD:H53	1.93	0.51
1:A:115:LEU:O	1:A:182:GLY:HA3	2.11	0.51
1:A:43:ASP:HB2	1:A:46:LYS:CG	2.41	0.51
1:B:171:ARG:HH11	1:B:171:ARG:CG	2.24	0.51
1:A:228:ARG:CD	1:A:230:MSE:HE1	2.42	0.50
1:A:230:MSE:SE	1:A:233:MSE:HE1	2.61	0.50
1:B:156:PRO:HD3	1:B:216:ARG:CG	2.42	0.50
1:A:87:TRP:O	1:A:88:ARG:HG3	2.11	0.50
1:A:88:ARG:O	1:A:91:PRO:CD	2.48	0.50
1:A:228:ARG:HH11	1:A:230:MSE:HE1	1.77	0.49
1:B:119:GLY:N	1:B:140:PHE:CZ	2.79	0.49
1:B:249:LEU:HD13	1:B:260:TYR:CE2	2.47	0.49
1:B:137:ARG:HE	2:B:2:MPD:C5	2.06	0.49
1:B:281:SER:H	1:B:282:VAL:CB	2.25	0.49
1:B:148:ASP:OD2	1:B:148:ASP:C	2.50	0.49
1:B:175:THR:HG23	1:B:177:ASP:N	2.28	0.49
1:B:147:ASP:HB3	1:B:172:ARG:CZ	2.43	0.49
1:B:220:GLN:HE22	1:B:223:SER:H	1.54	0.49
1:A:159:SER:HA	2:A:1:MPD:C5	2.43	0.49
1:A:152:LEU:O	1:A:169:VAL:HA	2.13	0.49
1:B:53:GLU:O	1:B:57:ARG:HG3	2.13	0.48
1:B:216:ARG:NH1	1:B:227:GLY:O	2.43	0.48
1:B:219:ILE:HA	1:B:225:GLN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ASP:O	3:B:294:CIT:C5	2.62	0.48
1:B:197:TYR:CE2	1:B:208:ILE:HD11	2.48	0.48
1:B:82:VAL:HG21	1:B:171:ARG:HG2	1.96	0.48
1:A:92:SER:C	1:A:94:VAL:H	2.17	0.48
1:A:127:LYS:CA	1:A:128:PRO:C	2.81	0.47
1:A:219:ILE:HG13	1:A:220:GLN:N	2.30	0.47
1:A:79:ASP:O	1:A:80:ASP:C	2.51	0.47
1:A:228:ARG:CG	1:A:230:MSE:HE1	2.42	0.47
1:B:195:THR:O	1:B:198:LYS:HG2	2.14	0.47
1:A:172:ARG:NH1	1:A:174:GLU:OE1	2.46	0.47
2:A:1:MPD:CM	2:A:1:MPD:H52	2.39	0.47
1:A:243:SER:CB	1:A:244:PRO:CD	2.92	0.47
1:B:121:LEU:CD1	1:B:121:LEU:C	2.83	0.47
1:B:221:TRP:CE3	1:B:222:PRO:HA	2.50	0.47
1:B:84:PHE:C	1:B:84:PHE:CD2	2.89	0.46
1:A:279:GLU:HB3	4:A:324:HOH:O	2.15	0.46
1:A:83:SER:O	1:A:84:PHE:C	2.52	0.46
3:B:294:CIT:H41	3:B:294:CIT:O1	2.15	0.46
1:B:127:LYS:HB2	1:B:128:PRO:CD	2.40	0.46
1:B:198:LYS:HE3	1:B:221:TRP:CH2	2.50	0.46
1:A:230:MSE:HE2	4:A:10:HOH:O	2.14	0.46
1:A:148:ASP:C	1:A:148:ASP:OD2	2.54	0.46
1:B:115:LEU:O	1:B:182:GLY:HA3	2.15	0.46
1:B:141:ARG:HH11	1:B:141:ARG:CG	2.25	0.46
1:A:282:VAL:O	1:A:282:VAL:HG12	2.15	0.46
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.80	0.46
1:A:161:THR:HG23	2:A:1:MPD:C1	2.29	0.45
1:B:151:LEU:CD2	1:B:169:VAL:HG13	2.43	0.45
1:B:175:THR:HG21	1:B:179:LYS:HB2	1.98	0.45
1:A:88:ARG:C	1:A:90:HIS:N	2.65	0.45
2:B:2:MPD:H11	2:B:2:MPD:H4	1.39	0.45
1:B:139:TYR:CZ	2:B:2:MPD:H52	2.45	0.45
1:B:139:TYR:HB3	1:B:154:THR:HG21	1.99	0.45
1:A:137:ARG:NH2	2:A:1:MPD:H51	2.18	0.44
1:B:100:ARG:HA	1:B:125:SER:HB2	1.99	0.44
1:B:127:LYS:HA	1:B:127:LYS:HD3	1.54	0.44
1:A:100:ARG:HA	1:A:125:SER:HB2	1.99	0.44
1:A:147:ASP:CG	1:A:147:ASP:O	2.54	0.44
3:B:294:CIT:O6	3:B:294:CIT:O1	2.35	0.44
1:A:88:ARG:HA	1:A:89:PRO:HD3	1.60	0.44
1:B:106:LEU:HD22	1:B:106:LEU:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:HIS:N	1:A:149:HIS:CD2	2.85	0.44
1:A:228:ARG:NE	1:A:230:MSE:HE1	2.33	0.44
1:B:235:LEU:HD22	1:B:240:LEU:HG	2.00	0.44
1:B:198:LYS:HE2	1:B:198:LYS:HB2	1.44	0.44
1:A:92:SER:C	1:A:94:VAL:N	2.71	0.44
1:B:220:GLN:HE21	1:B:223:SER:H	1.63	0.43
1:A:246:GLY:O	1:A:262:ALA:HA	2.19	0.43
1:A:219:ILE:HD12	1:A:220:GLN:H	1.83	0.43
1:A:223:SER:O	1:A:224:LEU:HB2	2.18	0.43
1:B:106:LEU:HA	1:B:106:LEU:HD13	1.49	0.43
1:B:139:TYR:HH	2:B:2:MPD:H52	1.71	0.43
1:A:282:VAL:HA	1:A:283:LEU:C	2.36	0.43
1:A:88:ARG:C	1:A:90:HIS:H	2.11	0.43
1:A:230:MSE:CB	1:A:233:MSE:HE1	2.42	0.42
1:B:281:SER:H	1:B:282:VAL:CG1	2.31	0.42
1:B:85:MSE:O	1:B:89:PRO:HD3	2.20	0.42
1:A:100:ARG:HE	1:A:100:ARG:HB2	1.21	0.42
1:B:260:TYR:O	1:B:276:ALA:HA	2.20	0.42
1:A:259:LYS:HB3	1:A:277:ARG:C	2.40	0.42
1:B:147:ASP:CA	1:B:172:ARG:NE	2.82	0.42
1:B:223:SER:O	1:B:224:LEU:HB2	2.20	0.42
1:A:177:ASP:CG	1:A:179:LYS:HG2	2.40	0.42
1:B:116:ASP:CG	1:B:117:ALA:HB3	2.32	0.41
1:B:141:ARG:NH1	1:B:141:ARG:CG	2.79	0.41
1:B:197:TYR:CZ	1:B:208:ILE:HD11	2.55	0.41
1:B:261:LEU:HD11	1:B:274:THR:HB	2.02	0.41
1:A:219:ILE:CG1	1:A:220:GLN:N	2.83	0.41
1:B:228:ARG:HG2	1:B:230:MSE:CE	2.50	0.41
1:A:279:GLU:O	1:A:280:ASP:CG	2.58	0.41
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.95	0.41
1:B:110:SER:O	1:B:111:ASP:HB3	2.20	0.41
1:B:173:LEU:HB2	1:B:182:GLY:C	2.41	0.41
1:B:87:TRP:O	1:B:88:ARG:HG2	2.20	0.41
1:A:88:ARG:O	1:A:90:HIS:N	2.54	0.41
1:A:156:PRO:HG3	1:A:227:GLY:HA2	2.03	0.41
1:A:283:LEU:HA	1:A:284:SER:HA	1.61	0.41
1:A:57:ARG:NH1	1:A:247:TYR:HB3	2.36	0.41
1:B:173:LEU:H	1:B:183:VAL:H	1.68	0.41
1:B:202:LEU:CB	1:B:206:GLY:HA3	2.51	0.41
1:B:234:VAL:O	1:B:235:LEU:C	2.59	0.41
1:B:280:ASP:HA	1:B:282:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:THR:CG2	1:B:179:LYS:HB2	2.51	0.41
1:B:239:ALA:HB1	1:B:263:TYR:CZ	2.56	0.41
1:A:263:TYR:CD1	1:A:263:TYR:C	2.94	0.40
1:A:257:LEU:HD13	1:A:278:THR:HG21	2.04	0.40
1:B:208:ILE:CD1	1:B:208:ILE:C	2.66	0.40
1:A:120:GLN:HE21	1:A:120:GLN:HB3	1.65	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	A	242/254 (95%)	213 (88%)	18 (7%)	11 (4%)	3	6
1	B	240/254 (94%)	213 (89%)	18 (8%)	9 (4%)	4	8
All	All	482/508 (95%)	426 (88%)	36 (8%)	20 (4%)	3	7

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	ASP
1	A	282	VAL
1	B	88	ARG
1	B	127	LYS
1	B	243	SER
1	B	281	SER
1	A	281	SER
1	B	89	PRO
1	B	117	ALA
1	B	183	VAL
1	A	84	PHE
1	A	246	GLY

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Mol	Chain	Res	Type
1	A	93	PRO
1	A	183	VAL
1	A	283	LEU
1	A	85	MSE
1	A	243	SER
1	B	284	SER
1	B	282	VAL
1	A	91	PRO

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	A	213/217 (98%)	186 (87%)	27 (13%)	5	12
1	B	211/217 (97%)	165 (78%)	46 (22%)	1	3
All	All	424/434 (98%)	351 (83%)	73 (17%)	2	6

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	72	GLN
1	A	78	LEU
1	A	89	PRO
1	A	100	ARG
1	A	102	LEU
1	A	105	ASN
1	A	120	GLN
1	A	121	LEU
1	A	132	LEU
1	A	137	ARG
1	A	151	LEU
1	A	152	LEU
1	A	168	VAL
1	A	169	VAL

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Mol	Chain	Res	Type
1	A	171	ARG
1	A	172	ARG
1	A	184	VAL
1	A	185	VAL
1	A	202	LEU
1	A	235	LEU
1	A	243	SER
1	A	259	LYS
1	A	268	ARG
1	A	275	VAL
1	A	283	LEU
1	A	284	SER
1	B	47	ILE
1	B	51	GLN
1	B	52	SER
1	B	59	LEU
1	B	60	SER
1	B	62	SER
1	B	76	VAL
1	B	78	LEU
1	B	88	ARG
1	B	94	VAL
1	B	98	ARG
1	B	102	LEU
1	B	104	ASP
1	B	106	LEU
1	B	118	ASP
1	B	121	LEU
1	B	127	LYS
1	B	144	ARG
1	B	147	ASP
1	B	151	LEU
1	B	152	LEU
1	B	154	THR
1	B	164	VAL
1	B	168	VAL
1	B	169	VAL
1	B	171	ARG
1	B	172	ARG
1	B	175	THR
1	B	176	THR
1	B	177	ASP

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Mol	Chain	Res	Type
1	B	183	VAL
1	B	185	VAL
1	B	191	GLU
1	B	202	LEU
1	B	208	ILE
1	B	209	SER
1	B	216	ARG
1	B	219	ILE
1	B	220	GLN
1	B	222	PRO
1	B	232	ASN
1	B	235	LEU
1	B	243	SER
1	B	279	GLU
1	B	282	VAL
1	B	284	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	120	GLN
1	A	134	ASN
1	A	143	HIS
1	A	146	ASN
1	A	149	HIS
1	A	158	GLN
1	A	220	GLN
1	A	225	GLN
1	B	105	ASN
1	B	120	GLN
1	B	134	ASN
1	B	143	HIS
1	B	149	HIS
1	B	158	GLN
1	B	220	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	MPD	A	1	-	7,7,7	1.71	1 (14%)	9,10,10	4.18	6 (66%)
3	CIT	A	294	-	3,12,12	1.41	1 (33%)	3,17,17	4.19	2 (66%)
2	MPD	B	2	-	7,7,7	0.72	0	9,10,10	0.60	0
3	CIT	B	294	-	3,12,12	0.72	0	3,17,17	3.52	3 (100%)

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	MPD	A	1	-	-	0/5/5/5	0/0/0/0
3	CIT	A	294	-	-	0/6/16/16	0/0/0/0
2	MPD	B	2	-	-	0/5/5/5	0/0/0/0
3	CIT	B	294	-	-	0/6/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	294	CIT	O7-C3	2.18	1.46	1.43
2	A	1	MPD	O2-C2	4.16	1.55	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	294	CIT	C4-C3-C2	-6.19	94.32	109.75
2	A	1	MPD	C1-C2-C3	-4.83	86.03	110.08
3	B	294	CIT	C3-C4-C5	-3.47	109.52	114.95
2	A	1	MPD	CM-C2-C3	-3.26	93.86	110.08
2	A	1	MPD	O4-C4-C5	-2.36	98.64	109.46
3	B	294	CIT	C3-C2-C1	-2.15	111.59	114.95
2	A	1	MPD	C5-C4-C3	3.19	127.99	112.11
3	A	294	CIT	C3-C2-C1	3.71	120.75	114.95
3	B	294	CIT	C4-C3-C2	4.53	121.03	109.75
2	A	1	MPD	O2-C2-C3	6.88	137.20	109.88
2	A	1	MPD	CM-C2-C1	7.67	127.54	110.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	MPD	18	0
3	A	294	CIT	7	0
2	B	2	MPD	7	0
3	B	294	CIT	4	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 (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	A	239/254 (94%)	-0.59	1 (0%)	92 93	20, 33, 57, 90	11 (4%)
1	B	237/254 (93%)	-0.30	9 (3%)	41 39	26, 43, 74, 100	1 (0%)
All	All	476/508 (93%)	-0.45	10 (2%)	64 65	20, 37, 70, 100	12 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	ALA	3.7
1	B	48	ALA	3.5
1	B	47	ILE	3.4
1	B	283	LEU	3.0
1	B	286	TRP	2.7
1	B	46	LYS	2.7
1	B	284	SER	2.4
1	B	51	GLN	2.2
1	B	204	PRO	2.1
1	A	285	GLY	2.1

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 carbohydrates in this entry.

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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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	MPD	A	1	8/8	0.83	0.23	8.27	23,30,34,36	0
3	CIT	A	294	13/13	0.90	0.17	1.48	45,48,54,56	13
3	CIT	B	294	13/13	0.83	0.15	0.46	52,57,59,60	13
2	MPD	B	2	8/8	0.90	0.14	0.25	39,44,47,48	0

6.5 Other polymers (i)

There are no such residues in this entry.