



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:40 am GMT

PDB ID : 2IO4
Title : Crystal structure of PCNA12 dimer from *Sulfolobus solfataricus*.
Authors : Hlinkova, V.; Ling, H.
Deposited on : 2006-10-09
Resolution : 2.60 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

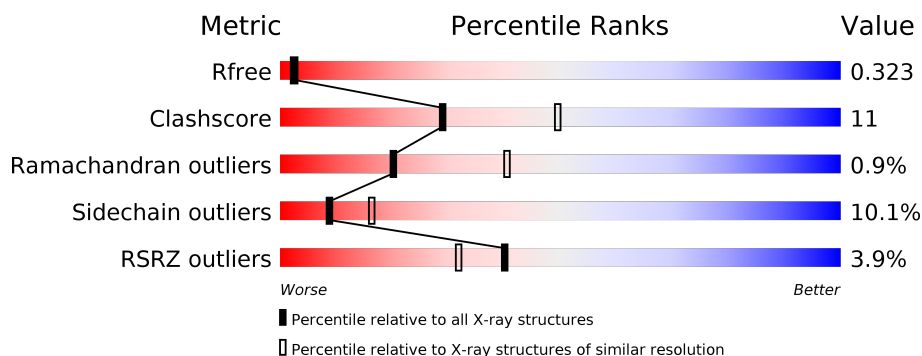
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	249	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>
1	C	249	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>29%</div> <div>•</div> </div> </div>
2	B	246	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>5% •</div> </div> </div>
2	D	246	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>29%</div> <div>• •</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPD	B	301	-	-	-	X
4	MPD	B	401	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7938 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 DNA polymerase sliding clamp B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1928	1227	310	382	9			
1	C	249	Total	C	N	O	S	0	1	0
			1932	1229	310	384	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	PHE	ENGINEERED	UNP P57766
C	2	VAL	PHE	ENGINEERED	UNP P57766

- Molecule 2 is a protein called DNA polymerase sliding clamp C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	246	Total	C	N	O	S	0	0	0
			1944	1249	304	386	5			
2	D	243	Total	C	N	O	S	0	0	0
			1922	1237	301	379	5			

There are 2 discrepancies between the modelled and reference sequences:

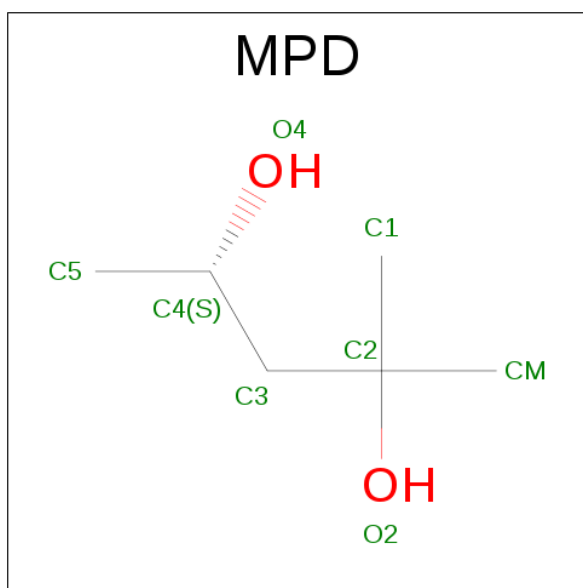
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	INITIATING METHIONINE	UNP Q97Z84
D	1	MET	-	INITIATING METHIONINE	UNP Q97Z84

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:

C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0

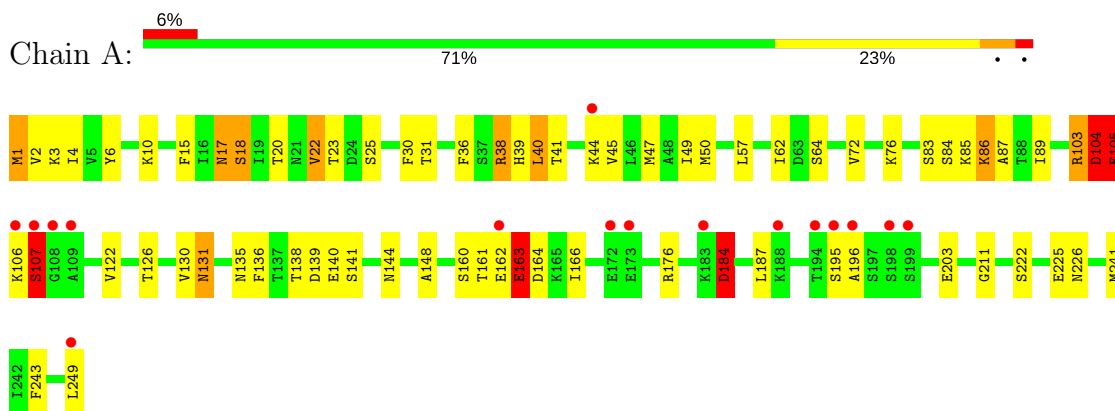
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	36	Total O 36 36	0	0
5	B	51	Total O 51 51	0	0
5	C	50	Total O 50 50	0	0
5	D	34	Total O 34 34	0	0

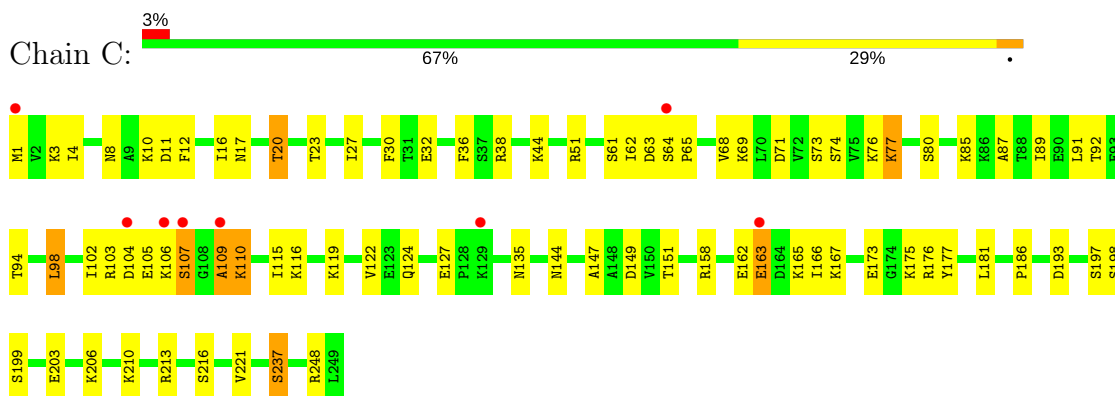
3 Residue-property plots [i](#)

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.

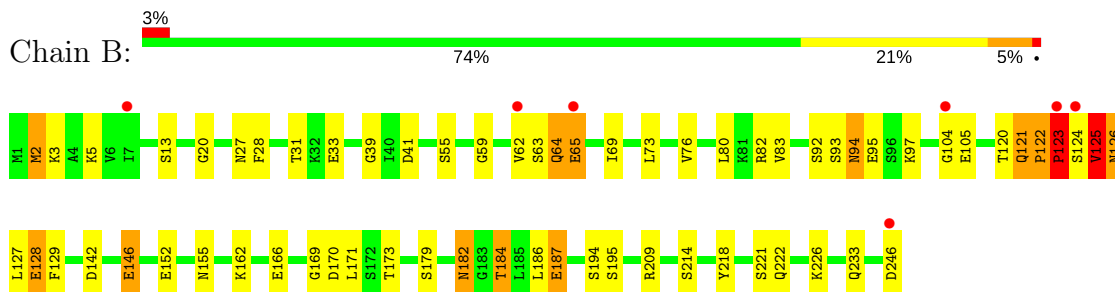
• Molecule 1: DNA polymerase sliding clamp B



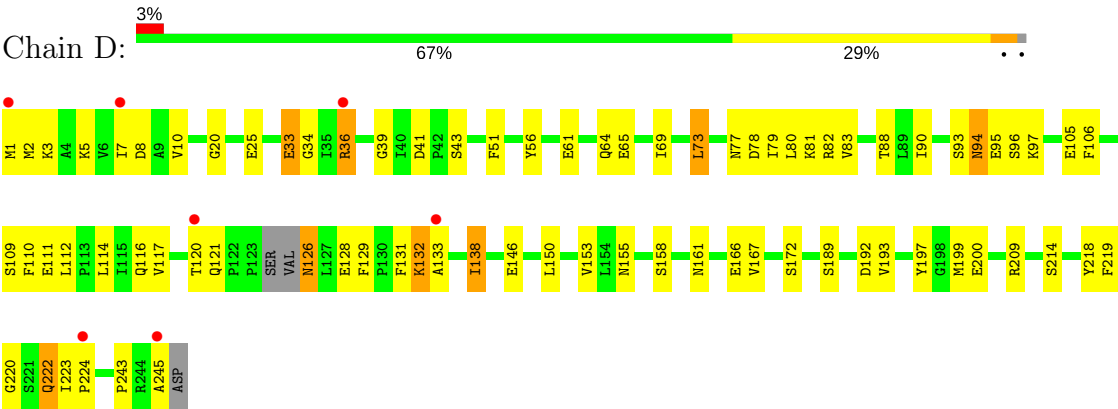
• Molecule 1: DNA polymerase sliding clamp B



• Molecule 2: DNA polymerase sliding clamp C



• Molecule 2: DNA polymerase sliding clamp C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.99Å 112.73Å 101.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.60) 99.9 (29.73-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.233 , 0.260 0.284 , 0.323	Depositor DCC
R_{free} test set	1152 reflections (3.05%)	DCC
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 26.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7938	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MPD

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	0.82	6/1955 (0.3%)	0.72	4/2632 (0.2%)
1	C	0.68	5/1964 (0.3%)	0.67	3/2644 (0.1%)
2	B	0.53	1/1979 (0.1%)	0.62	1/2673 (0.0%)
2	D	0.71	4/1956 (0.2%)	0.68	0/2641
All	All	0.69	16/7854 (0.2%)	0.67	8/10590 (0.1%)

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	3	0
2	B	0	4
2	D	1	1
All	All	4	5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	126	ASN	C-O	11.70	1.45	1.23
1	A	163	GLU	CG-CD	10.81	1.68	1.51
1	A	104	ASP	N-CA	9.80	1.66	1.46
1	A	163	GLU	CD-OE2	8.37	1.34	1.25
2	D	43	SER	CB-OG	7.19	1.51	1.42
2	D	128	GLU	CD-OE1	6.75	1.33	1.25
1	A	107	SER	CB-OG	6.47	1.50	1.42
2	D	65	GLU	CD-OE2	6.07	1.32	1.25
1	C	105	GLU	CD-OE1	5.98	1.32	1.25
1	A	131	ASN	CA-CB	5.98	1.68	1.53
1	C	163	GLU	CD-OE2	5.97	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	107	SER	CB-OG	5.91	1.50	1.42
1	C	64	SER	CB-OG	5.79	1.49	1.42
2	B	128	GLU	CA-CB	5.76	1.66	1.53
1	A	162	GLU	CD-OE2	5.60	1.31	1.25
1	C	94	THR	CB-OG1	5.17	1.53	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	GLU	N-CA-C	6.76	129.24	111.00
1	A	163	GLU	N-CA-C	6.34	128.11	111.00
1	A	163	GLU	OE1-CD-OE2	-6.22	115.84	123.30
1	A	184	ASP	N-CA-C	5.67	126.32	111.00
1	C	110	LYS	N-CA-C	5.33	125.38	111.00
1	A	105	GLU	N-CA-C	5.31	125.33	111.00
1	C	193	ASP	CB-CG-OD1	-5.20	113.62	118.30
2	B	128	GLU	N-CA-C	5.05	124.64	111.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	105	GLU	CA
1	A	163	GLU	CA
1	A	184	ASP	CA
2	D	145	ASP	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	122	PRO	Peptide
2	B	123	PRO	Peptide
2	B	125	VAL	Peptide
2	B	126	ASN	Peptide
2	D	126	ASN	Mainchain

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	1928	0	1987	40	0
1	C	1932	0	1989	46	0
2	B	1944	0	1941	39	0
2	D	1922	0	1922	50	0
3	B	1	0	0	0	0
4	A	8	0	14	2	0
4	B	32	0	56	8	0
5	A	36	0	0	1	0
5	B	51	0	0	2	0
5	C	50	0	0	2	0
5	D	34	0	0	2	0
All	All	7938	0	7909	171	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 11.

All (171) 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)
2:B:128:GLU:HG3	2:B:129:PHE:H	0.95	1.06
2:B:128:GLU:HG3	2:B:129:PHE:N	1.74	1.01
2:B:128:GLU:CG	2:B:129:PHE:H	1.75	1.00
1:A:10:LYS:HG3	1:A:84:SER:HA	1.56	0.87
2:D:158:SER:O	2:D:192:ASP:HB2	1.76	0.86
1:C:11:ASP:OD2	1:C:237:SER:HB3	1.79	0.82
2:D:167:VAL:HG21	2:D:199:MET:CE	2.11	0.81
2:B:122:PRO:HB2	2:B:123:PRO:HA	1.62	0.80
4:A:250:MPD:H12	4:A:250:MPD:H52	1.63	0.80
2:B:152:GLU:H	4:B:601:MPD:HM3	1.48	0.79
1:C:65:PRO:HB2	1:C:122:VAL:HG21	1.66	0.77
2:D:79:ILE:HD13	2:D:110:PHE:HB3	1.67	0.76
2:D:132:LYS:HG2	2:D:218:TYR:CE2	2.21	0.76
2:D:132:LYS:HG2	2:D:218:TYR:HE2	1.52	0.75
4:B:301:MPD:H53	5:B:751:HOH:O	1.87	0.74
2:B:221:SER:O	2:B:222:GLN:HG2	1.88	0.73
2:D:25:GLU:HB2	2:D:117:VAL:HG11	1.71	0.73
2:D:7:ILE:HG13	2:D:8:ASP:H	1.55	0.69
1:C:147:ALA:O	1:C:151:THR:HG23	1.92	0.69
1:C:71:ASP:HB3	1:C:74:SER:CB	2.22	0.69
2:B:169:GLY:HA2	4:B:601:MPD:HM1	1.74	0.69
2:B:80:LEU:O	2:B:83:VAL:HG12	1.96	0.65
1:A:17:ASN:O	1:A:20:THR:HB	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LYS:HD2	5:C:250:HOH:O	1.94	0.65
2:D:69:ILE:HG23	2:D:114:LEU:HD22	1.78	0.65
2:D:78:ASP:HA	2:D:81:LYS:HE2	1.79	0.64
2:B:2:MET:HG3	2:B:93:SER:OG	1.99	0.63
2:D:80:LEU:O	2:D:83:VAL:HG12	1.97	0.63
1:C:1:MET:HE1	1:C:3:LYS:HE3	1.82	0.62
1:C:71:ASP:HB3	1:C:74:SER:HB2	1.80	0.62
1:A:15:PHE:HD2	1:A:241:MET:HE2	1.64	0.62
2:D:34:GLY:HA2	5:D:280:HOH:O	1.99	0.62
1:A:23:THR:HG22	1:A:25:SER:H	1.64	0.61
2:B:28:PHE:HB2	2:B:69:ILE:HB	1.79	0.61
1:C:149:ASP:OD1	2:D:82:ARG:HD3	2.01	0.61
2:D:7:ILE:HG12	2:D:56:TYR:O	2.01	0.60
1:A:22:VAL:HG22	1:A:41:THR:HG23	1.83	0.60
2:B:121:GLN:HE21	2:B:121:GLN:H	1.50	0.60
1:C:8:ASN:HB2	1:C:237:SER:HB2	1.83	0.60
1:C:12:PHE:O	1:C:16:ILE:HG12	2.02	0.60
1:C:162[A]:GLU:HG3	1:C:167:LYS:HD2	1.83	0.59
1:C:210:LYS:HE3	1:C:213:ARG:HH12	1.66	0.59
1:C:173:GLU:CG	1:C:173:GLU:O	2.51	0.59
2:D:36:ARG:HD3	2:D:51:PHE:CD1	2.38	0.59
2:D:167:VAL:HG21	2:D:199:MET:HE3	1.84	0.58
1:A:83:SER:OG	1:A:85:LYS:HG3	2.02	0.58
2:D:167:VAL:HG21	2:D:199:MET:HE2	1.84	0.58
1:A:1:MET:HG3	1:A:2:VAL:N	2.19	0.58
4:B:601:MPD:HM2	5:B:712:HOH:O	2.03	0.57
1:A:15:PHE:HD2	1:A:241:MET:CE	2.18	0.57
1:A:87:ALA:CB	1:A:104:ASP:HA	2.35	0.57
1:A:6:TYR:HB2	1:A:89:ILE:HB	1.87	0.56
2:D:153:VAL:O	2:D:167:VAL:HG22	2.06	0.56
2:D:167:VAL:CG2	2:D:199:MET:HE2	2.36	0.55
1:A:40:LEU:CD2	1:A:44:LYS:HG3	2.36	0.55
2:B:128:GLU:CG	2:B:129:PHE:N	2.48	0.55
1:A:38:ARG:HG3	1:A:38:ARG:O	2.07	0.55
2:D:7:ILE:HG13	2:D:8:ASP:N	2.23	0.54
2:D:167:VAL:CG2	2:D:199:MET:CE	2.85	0.54
2:B:182:ASN:ND2	2:B:184:THR:OG1	2.42	0.53
1:A:161:THR:HG21	1:A:195:SER:HA	1.91	0.53
1:C:74:SER:OG	1:C:115:ILE:HG23	2.09	0.53
1:A:38:ARG:HB2	1:A:49:ILE:HG12	1.92	0.52
2:B:94:ASN:ND2	2:B:97:LYS:H	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:SER:O	2:B:125:VAL:C	2.47	0.52
2:D:2:MET:HG3	2:D:93:SER:OG	2.10	0.52
2:D:150:LEU:HD22	2:D:172:SER:HB3	1.92	0.52
2:B:105:GLU:OE2	2:B:105:GLU:N	2.40	0.51
1:C:104:ASP:HB3	1:C:109:ALA:HB3	1.93	0.51
1:A:148:ALA:HB3	2:B:82:ARG:NH1	2.26	0.51
1:C:30:PHE:HE1	1:C:68:VAL:CG2	2.23	0.51
1:A:136:PHE:CD2	1:A:166:ILE:HD12	2.45	0.51
2:B:186:LEU:C	2:B:187:GLU:HG2	2.31	0.51
1:C:3:LYS:HG3	1:C:92:THR:HG22	1.93	0.51
2:B:122:PRO:HB2	2:B:123:PRO:CA	2.38	0.50
1:A:103:ARG:O	1:A:103:ARG:HG3	2.10	0.50
1:C:175:LYS:HG2	2:D:112:LEU:HD23	1.92	0.50
2:B:94:ASN:C	2:B:94:ASN:HD22	2.15	0.50
1:C:17:ASN:O	1:C:20:THR:HB	2.10	0.50
1:C:27:ILE:HG12	1:C:69:LYS:HG2	1.92	0.50
1:C:87:ALA:HB1	1:C:103:ARG:O	2.11	0.50
1:C:30:PHE:HE1	1:C:68:VAL:HG23	1.76	0.50
1:C:71:ASP:HB3	1:C:74:SER:HB3	1.93	0.50
1:A:2:VAL:HG13	1:A:62:ILE:HG22	1.94	0.50
1:A:196:ALA:HA	1:A:225:GLU:OE1	2.12	0.49
1:A:47:MET:O	1:A:243:PHE:HA	2.13	0.48
2:B:20:GLY:HA2	2:B:73:LEU:HD13	1.95	0.48
2:D:77:ASN:O	2:D:81:LYS:HG3	2.13	0.48
1:C:166:ILE:HB	1:C:181:LEU:HB2	1.96	0.48
2:D:79:ILE:HD13	2:D:110:PHE:CB	2.39	0.48
1:A:31:THR:HG22	1:A:122:VAL:HG21	1.96	0.48
2:B:152:GLU:N	4:B:601:MPD:HM3	2.23	0.48
2:B:5:LYS:HB3	2:B:59:GLY:H	1.78	0.48
1:C:116:LYS:O	1:C:116:LYS:HG3	2.13	0.48
1:C:89:ILE:HD13	1:C:102:ILE:HG12	1.95	0.47
2:D:36:ARG:HD3	2:D:51:PHE:HD1	1.79	0.47
2:B:39:GLY:HA2	2:B:120:THR:HG21	1.96	0.47
1:A:15:PHE:CD2	1:A:50:MET:HG3	2.50	0.47
1:C:73:SER:HA	1:C:76:LYS:HG2	1.97	0.47
1:A:87:ALA:HA	1:A:104:ASP:HA	1.97	0.47
2:B:170:ASP:OD1	2:D:209:ARG:NH2	2.47	0.47
2:D:223:ILE:HB	2:D:224:PRO:CD	2.45	0.46
1:A:131:ASN:ND2	5:A:277:HOH:O	2.47	0.46
1:A:40:LEU:HD23	1:A:44:LYS:HG3	1.98	0.46
2:D:117:VAL:O	2:D:117:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:PHE:HE2	2:D:133:ALA:HB2	1.80	0.46
2:D:5:LYS:HG2	2:D:90:ILE:HG12	1.98	0.46
1:C:186:PRO:HD3	2:D:106:PHE:HB3	1.96	0.46
2:B:142:ASP:OD2	4:B:301:MPD:H32	2.16	0.46
2:B:222:GLN:OE1	1:C:213:ARG:NH1	2.49	0.46
2:D:120:THR:O	2:D:121:GLN:HG2	2.16	0.46
1:A:4:ILE:HD11	1:A:30:PHE:CE2	2.51	0.46
2:B:218:TYR:HB2	2:B:226:LYS:HB3	1.97	0.46
2:D:94:ASN:HD22	2:D:96:SER:H	1.64	0.46
2:D:39:GLY:HA2	2:D:120:THR:HB	1.97	0.45
1:A:87:ALA:HB2	1:A:104:ASP:HA	1.97	0.45
1:C:91:LEU:HG	1:C:98:LEU:HD21	1.98	0.45
2:D:20:GLY:CA	2:D:73:LEU:HD22	2.46	0.45
1:A:86:LYS:HB2	1:A:105:GLU:HG3	1.98	0.45
1:C:77:LYS:O	1:C:80:SER:HB2	2.17	0.45
1:A:226:ASN:HB3	1:A:249:LEU:O	2.17	0.45
1:A:72:VAL:O	1:A:76:LYS:HG3	2.16	0.45
1:C:173:GLU:HG3	1:C:173:GLU:O	2.17	0.44
2:B:246:ASP:HB2	1:C:213:ARG:CZ	2.46	0.44
1:C:106:LYS:NZ	5:C:298:HOH:O	2.45	0.44
1:C:106:LYS:HG3	1:C:107:SER:N	2.32	0.44
2:B:146:GLU:HG2	4:B:301:MPD:H11	1.99	0.44
2:D:138:ILE:O	2:D:138:ILE:HD13	2.17	0.44
1:A:138:THR:HG23	1:A:139:ASP:N	2.32	0.44
2:B:76:VAL:O	2:B:80:LEU:HG	2.18	0.44
1:C:176:ARG:NH1	2:D:111:GLU:OE2	2.51	0.43
1:C:135:ASN:HA	1:C:221:VAL:O	2.19	0.43
2:D:193:VAL:HG21	2:D:220:GLY:HA2	2.01	0.43
1:C:85:LYS:HD3	1:C:106:LYS:HE2	2.00	0.43
1:C:4:ILE:HD12	1:C:91:LEU:HD22	2.00	0.43
1:A:163:GLU:O	1:A:164:ASP:HB2	2.19	0.43
2:D:2:MET:HA	2:D:61:GLU:O	2.19	0.43
1:A:36:PHE:HA	1:A:50:MET:O	2.18	0.43
2:B:65:GLU:OE1	2:B:65:GLU:N	2.44	0.43
2:D:94:ASN:ND2	2:D:96:SER:H	2.17	0.43
2:B:63:SER:C	2:B:64:GLN:HG3	2.39	0.43
1:C:62:ILE:HG12	1:C:63:ASP:N	2.33	0.43
1:C:3:LYS:HB3	1:C:61:SER:OG	2.19	0.43
1:C:151:THR:HG21	1:C:206:LYS:HE2	2.00	0.42
2:B:27:ASN:HA	2:B:69:ILE:O	2.19	0.42
2:D:155:ASN:HB2	2:D:166:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LYS:O	1:A:107:SER:CB	2.67	0.42
2:B:155:ASN:HB2	2:B:166:GLU:HB3	2.02	0.42
2:D:33:GLU:HG3	5:D:258:HOH:O	2.19	0.42
4:B:401:MPD:H52	2:D:200:GLU:CG	2.50	0.42
2:D:161:ASN:ND2	2:D:189:SER:HA	2.35	0.42
2:D:132:LYS:HG2	2:D:218:TYR:CD2	2.55	0.42
2:D:222:GLN:NE2	2:D:245:ALA:O	2.53	0.41
1:A:18:SER:OG	1:A:211:GLY:O	2.39	0.41
1:A:22:VAL:CG2	1:A:41:THR:HG23	2.49	0.41
1:C:20:THR:HA	1:C:23:THR:O	2.20	0.41
1:C:149:ASP:HB3	1:C:177:TYR:CE1	2.55	0.41
1:A:86:LYS:HG2	1:A:86:LYS:H	1.68	0.41
4:A:250:MPD:H12	4:A:250:MPD:C5	2.43	0.41
2:D:129:PHE:HB3	2:D:218:TYR:HB3	2.01	0.41
1:A:249:LEU:HA	1:A:249:LEU:HD23	1.70	0.41
2:B:55:SER:HB3	2:B:233:GLN:OE1	2.21	0.41
1:A:23:THR:OG1	1:A:39:HIS:HB3	2.20	0.41
1:A:184:ASP:N	1:A:187:LEU:O	2.48	0.40
2:B:162:LYS:HG2	2:B:179:SER:HB3	2.02	0.40
2:D:81:LYS:HE3	2:D:81:LYS:HB2	1.91	0.40
2:D:197:TYR:CD2	2:D:243:PRO:HA	2.56	0.40
2:B:123:PRO:HA	2:B:124:SER:HA	1.86	0.40
2:B:31:THR:OG1	2:B:33:GLU:HG2	2.21	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	247/249 (99%)	230 (93%)	14 (6%)	3 (1%)	15	32
1	C	248/249 (100%)	224 (90%)	21 (8%)	3 (1%)	15	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	244/246 (99%)	233 (96%)	8 (3%)	3 (1%)	15	32
2	D	239/246 (97%)	226 (95%)	13 (5%)	0	100	100
All	All	978/990 (99%)	913 (93%)	56 (6%)	9 (1%)	20	40

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ASP
2	B	125	VAL
1	C	110	LYS
1	A	184	ASP
1	C	163	GLU
2	B	123	PRO
1	C	109	ALA
1	A	107	SER
2	B	104	GLY

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	220/220 (100%)	196 (89%)	24 (11%)	7	13
1	C	221/220 (100%)	200 (90%)	21 (10%)	10	19
2	B	220/220 (100%)	197 (90%)	23 (10%)	8	15
2	D	217/220 (99%)	196 (90%)	21 (10%)	9	18
All	All	878/880 (100%)	789 (90%)	89 (10%)	9	16

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LYS
1	A	17	ASN

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Mol	Chain	Res	Type
1	A	18	SER
1	A	22	VAL
1	A	38	ARG
1	A	40	LEU
1	A	45	VAL
1	A	57	LEU
1	A	64	SER
1	A	86	LYS
1	A	103	ARG
1	A	105	GLU
1	A	126	THR
1	A	130	VAL
1	A	135	ASN
1	A	140	GLU
1	A	141	SER
1	A	144	ASN
1	A	160	SER
1	A	163	GLU
1	A	176	ARG
1	A	203	GLU
1	A	222	SER
2	B	2	MET
2	B	3	LYS
2	B	13	SER
2	B	41	ASP
2	B	62	VAL
2	B	64	GLN
2	B	65	GLU
2	B	92	SER
2	B	94	ASN
2	B	95	GLU
2	B	121	GLN
2	B	126	ASN
2	B	127	LEU
2	B	146	GLU
2	B	171	LEU
2	B	173	THR
2	B	182	ASN
2	B	184	THR
2	B	187	GLU
2	B	194	SER
2	B	195	SER

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Mol	Chain	Res	Type
2	B	209	ARG
2	B	214	SER
1	C	10	LYS
1	C	20	THR
1	C	32	GLU
1	C	36	PHE
1	C	38	ARG
1	C	44	LYS
1	C	51	ARG
1	C	77	LYS
1	C	98	LEU
1	C	119	LYS
1	C	124	GLN
1	C	127	GLU
1	C	144	ASN
1	C	158	ARG
1	C	197	SER
1	C	198	SER
1	C	199	SER
1	C	203	GLU
1	C	216	SER
1	C	237	SER
1	C	248	ARG
2	D	1	MET
2	D	3	LYS
2	D	10	VAL
2	D	33	GLU
2	D	36	ARG
2	D	41	ASP
2	D	64	GLN
2	D	73	LEU
2	D	88	THR
2	D	94	ASN
2	D	95	GLU
2	D	97	LYS
2	D	105	GLU
2	D	109	SER
2	D	116	GLN
2	D	132	LYS
2	D	138	ILE
2	D	146	GLU
2	D	214	SER

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Mol	Chain	Res	Type
2	D	219	PHE
2	D	222	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	27	ASN
2	B	64	GLN
2	B	94	ASN
2	B	121	GLN
2	B	161	ASN
2	B	182	ASN
1	C	17	ASN
1	C	21	ASN
2	D	27	ASN
2	D	94	ASN
2	D	161	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	MPD	A	250	-	7,7,7	0.54	0	9,10,10	0.55	0
4	MPD	B	301	-	7,7,7	0.36	0	9,10,10	0.25	0
4	MPD	B	401	-	7,7,7	2.16	2 (28%)	9,10,10	0.78	0
4	MPD	B	501	-	7,7,7	0.44	0	9,10,10	0.21	0
4	MPD	B	601	-	7,7,7	0.29	0	9,10,10	0.55	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	MPD	A	250	-	-	0/5/5/5	0/0/0/0
4	MPD	B	301	-	-	0/5/5/5	0/0/0/0
4	MPD	B	401	-	-	0/5/5/5	0/0/0/0
4	MPD	B	501	-	-	0/5/5/5	0/0/0/0
4	MPD	B	601	-	-	0/5/5/5	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	MPD	O4-C4	3.55	1.59	1.43
4	B	401	MPD	C5-C4	4.08	1.70	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	250	MPD	2	0
4	B	301	MPD	3	0
4	B	401	MPD	1	0
4	B	601	MPD	4	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, 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	249/249 (100%)	0.32	16 (6%) 20 15	53, 61, 72, 79	0
1	C	249/249 (100%)	0.32	8 (3%) 48 40	42, 57, 67, 71	0
2	B	246/246 (100%)	0.17	7 (2%) 53 46	48, 60, 72, 76	0
2	D	243/246 (98%)	0.37	7 (2%) 52 45	55, 64, 73, 81	0
All	All	987/990 (99%)	0.30	38 (3%) 40 32	42, 61, 72, 81	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	107	SER	6.7
1	A	172	GLU	6.0
1	A	195	SER	5.0
1	C	106	LYS	4.2
1	A	109	ALA	4.0
1	A	106	LYS	4.0
2	D	120	THR	4.0
2	B	124	SER	3.7
2	B	123	PRO	3.4
2	D	133	ALA	3.3
1	A	173	GLU	3.2
1	C	109	ALA	3.1
1	A	194	THR	3.1
2	B	65	GLU	3.0
2	B	246	ASP	2.9
1	A	107	SER	2.8
2	B	7	ILE	2.8
1	C	1	MET	2.7
1	A	249	LEU	2.7
2	D	36	ARG	2.7
2	D	245	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	196	ALA	2.6
2	B	104	GLY	2.5
1	A	198	SER	2.4
1	A	44	LYS	2.4
1	A	108	GLY	2.4
2	B	62	VAL	2.3
1	C	104	ASP	2.3
2	D	7	ILE	2.3
1	A	162	GLU	2.2
1	A	183	LYS	2.2
2	D	1	MET	2.2
1	C	163	GLU	2.2
1	C	64	SER	2.1
2	D	224	PRO	2.1
1	A	199	SER	2.1
1	A	188	LYS	2.1
1	C	129	LYS	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.

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
4	MPD	B	301	8/8	0.84	0.33	5.41	83,83,84,85	0
4	MPD	B	401	8/8	0.85	0.33	3.18	76,77,77,78	0
4	MPD	A	250	8/8	0.60	0.34	1.37	77,78,78,78	0
4	MPD	B	501	8/8	0.89	0.24	0.51	74,75,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MPD	B	601	8/8	0.91	0.18	0.29	59,61,66,69	0
3	CA	B	701	1/1	0.74	0.13	-3.08	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.