Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 01:23 PM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

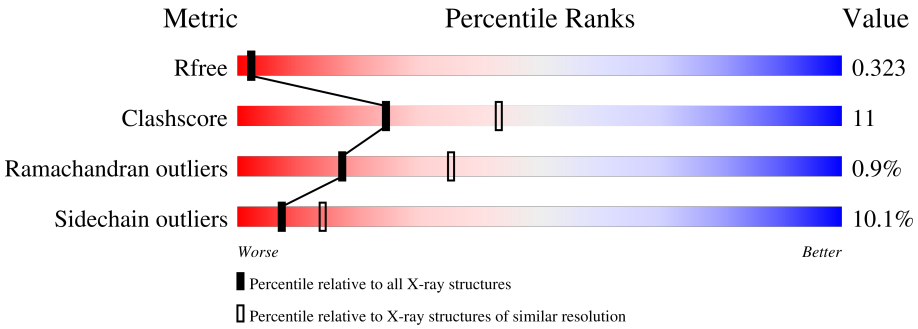
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	249	71% 23%
1	C	249	67% 29%
2	B	246	74% 21% 5%
2	D	246	67% 29%

2 Entry composition (i)

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 mutation	UNP P57766
C	2	VAL	PHE	engineered mutation	UNP P57766

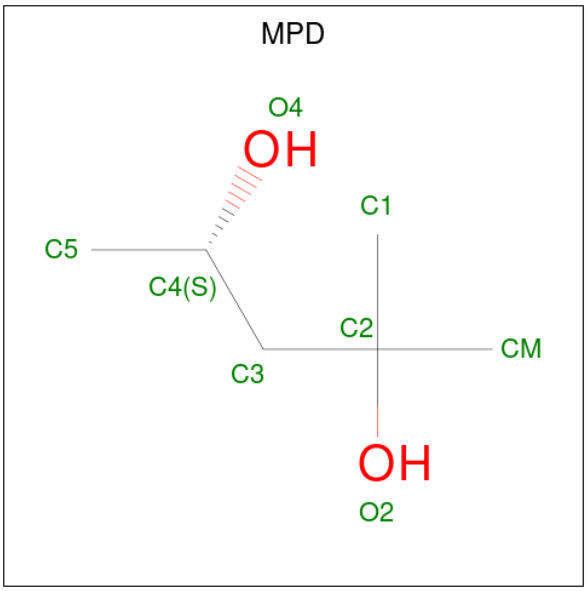
- Molecule 2 is a protein called DNA polymerase sliding clamp C.

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 (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	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

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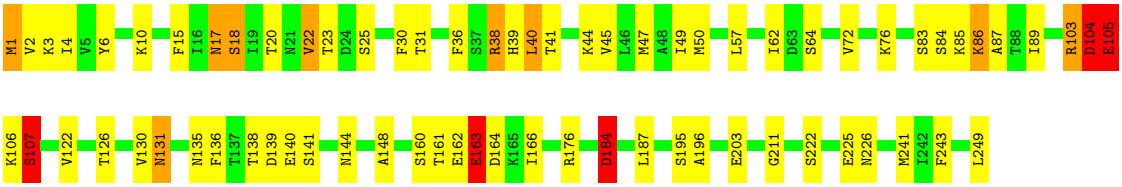
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	34	Total	O	0	0
			34	34		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

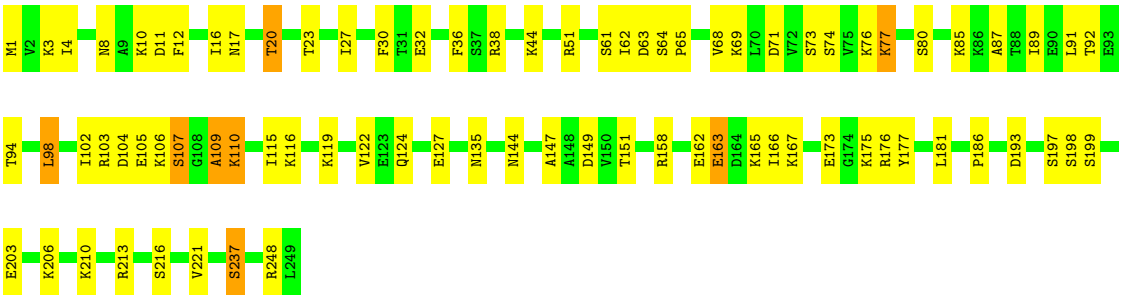
• Molecule 1: DNA polymerase sliding clamp B

Chain A:



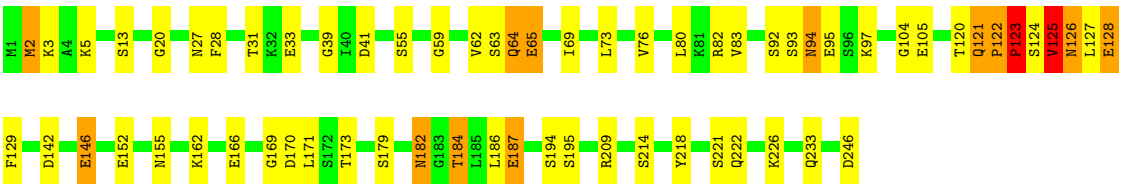
• Molecule 1: DNA polymerase sliding clamp B

Chain C:



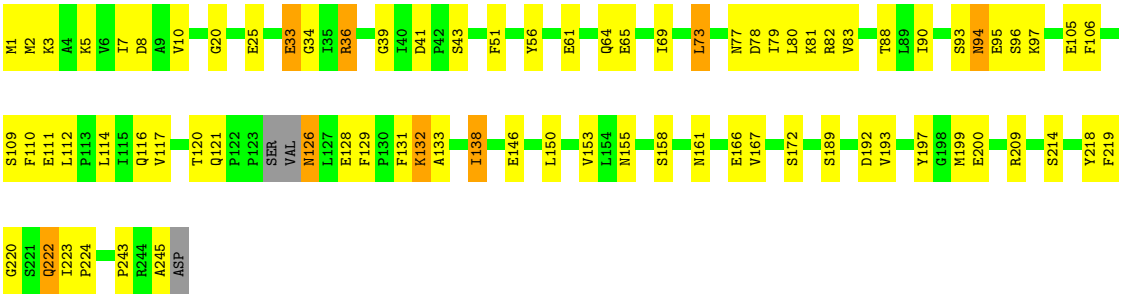
• Molecule 2: DNA polymerase sliding clamp C

Chain B:



• Molecule 2: DNA polymerase sliding clamp C

Chain D:


M1 M2 K3 A4 K5 V6 I7 D8 A9 V10 G20 E25 E33 G34 I35 R36 G39 I40 D41 P42 S43 F51 Y56 E61 Q64 E65 I69 L73 N77 D78 I79 L80 K81 R82 V83 T88 L89 I90 S93 N94 E95 S96 K97 E105 F106
S109 F110 E111 L112 P113 L114 I115 Q116 V117 T120 Q121 P122 P123 SER VAL N126 L127 E128 F129 P130 F131 K132 A133 I138 E146 L150 V153 L154 N155 S158 N161 E166 V167 S172 S189 D192 V193 Y197 G198 M199 E200 R209 S214 Y218 F219
G220 S221 Q222 I223 P224 P243 R244 A245 ASP

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.08 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.233 , 0.260 0.286 , 0.323	Depositor DCC
R_{free} test set	1151 reflections (3.05%)	wwPDB-VP
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]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[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, CA

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(^{o})	Ideal(^{o})
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 (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	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	A	8	0	14	2	0
3	B	32	0	56	8	0
4	B	1	0	0	0	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
3:A:250:MPD:H12	3:A:250:MPD:H52	1.63	0.80
2:B:152:GLU:H	3: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
3: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	3: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
3: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:O	1:A:38:ARG:HG3	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:N	2:B:105:GLU:OE2	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	3: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: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
1:C:73:SER:HA	1:C:76:LYS:HG2	1.97	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	3: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:72:VAL:O	1:A:76:LYS:HG3	2.16	0.45
1:A:226:ASN:HB3	1:A:249:LEU:O	2.17	0.45
2:B:246:ASP:HB2	1:C:213:ARG:CZ	2.46	0.44
1:C:173:GLU:O	1:C:173:GLU:HG3	2.17	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	3: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
3: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:H	1:A:86:LYS:HG2	1.68	0.41
1:A:249:LEU:HA	1:A:249:LEU:HD23	1.70	0.41
3:A:250:MPD:H12	3:A:250:MPD:C5	2.43	0.41
2:B:55:SER:HB3	2:B:233:GLN:OE1	2.21	0.41
2:D:129:PHE:HB3	2:D:218:TYR:HB3	2.01	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:31:THR:OG1	2:B:33:GLU:HG2	2.21	0.40
2:B:123:PRO:HA	2:B:124:SER:HA	1.86	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%)	13 27
1	C	248/249 (100%)	224 (90%)	21 (8%)	3 (1%)	13 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	244/246 (99%)	233 (96%)	8 (3%)	3 (1%)	13 27
2	D	239/246 (97%)	226 (95%)	13 (5%)	0	100 100
All	All	978/990 (99%)	913 (93%)	56 (6%)	9 (1%)	17 35

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 (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	220/220 (100%)	196 (89%)	24 (11%)	6 11
1	C	221/220 (100%)	200 (90%)	21 (10%)	8 16
2	B	220/220 (100%)	197 (90%)	23 (10%)	7 13
2	D	217/220 (99%)	196 (90%)	21 (10%)	8 15
All	All	878/880 (100%)	789 (90%)	89 (10%)	7 14

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

Sometimes 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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	MPD	A	250	-	7,7,7	0.57	0	9,10,10	0.60	0
3	MPD	B	301	-	7,7,7	0.39	0	9,10,10	0.27	0
3	MPD	B	501	-	7,7,7	0.47	0	9,10,10	0.23	0
3	MPD	B	601	-	7,7,7	0.30	0	9,10,10	0.59	0
3	MPD	B	401	-	7,7,7	2.28	2 (28%)	9,10,10	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	A	250	-	-	2/5/5/5	-
3	MPD	B	301	-	-	1/5/5/5	-
3	MPD	B	501	-	-	3/5/5/5	-
3	MPD	B	601	-	-	2/5/5/5	-
3	MPD	B	401	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	MPD	C5-C4	4.23	1.70	1.51
3	B	401	MPD	O4-C4	3.84	1.59	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	250	MPD	C2-C3-C4-O4
3	B	401	MPD	C2-C3-C4-C5
3	B	501	MPD	C2-C3-C4-O4
3	B	401	MPD	CM-C2-C3-C4
3	B	501	MPD	C1-C2-C3-C4
3	B	601	MPD	C1-C2-C3-C4
3	B	301	MPD	O2-C2-C3-C4
3	B	601	MPD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	A	250	MPD	C2-C3-C4-C5
3	B	501	MPD	C2-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	250	MPD	2	0
3	B	301	MPD	3	0
3	B	601	MPD	4	0
3	B	401	MPD	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.