Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 10:39 PM EDT

PDB ID	:	3K8G
Title	:	Structure of crystal form I of TP0453
Authors	:	Zhu, G.; Luthra, A.; Desrosiers, D.; Koszelak-Rosenblum, M.; Mulay, V.; Radolf, J.D.; Malkowski, M.G.
Deposited on	:	2009-10-14
Resolution	:	1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

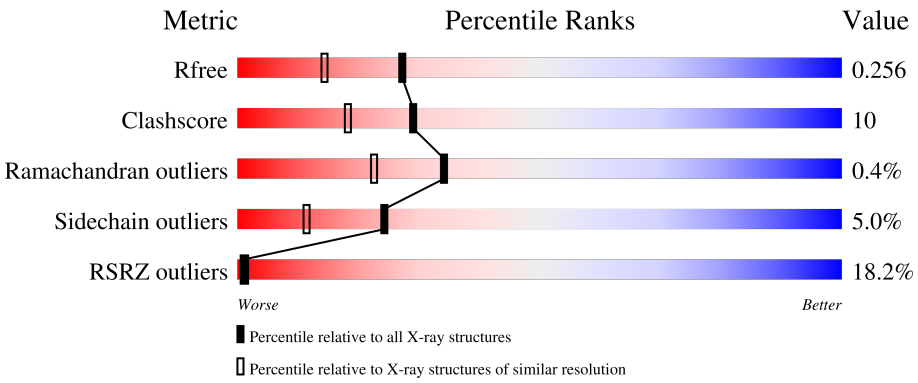
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	262	11% 81% 15% •
1	B	262	23% 72% 16% • 9%

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	300	X	-	-	-
2	MPD	A	301	X	-	X	-
2	MPD	A	303	X	-	-	-
2	MPD	B	302	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4116 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.

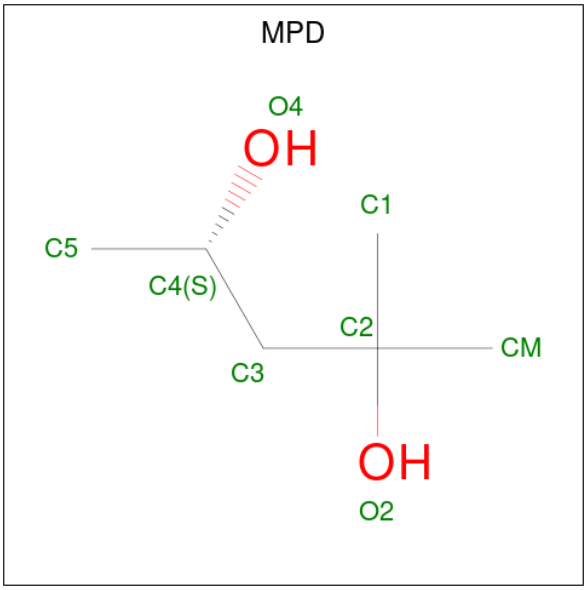
- Molecule 1 is a protein called 30kLP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	251	1988	1275	341	367	5	0	0	0
1	B	238	1883	1209	322	347	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP O67998
B	26	GLY	-	expression tag	UNP O67998

- 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
			Total	C	O		
2	A	1	8	6	2	0	0

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

- Molecule 3 is water.

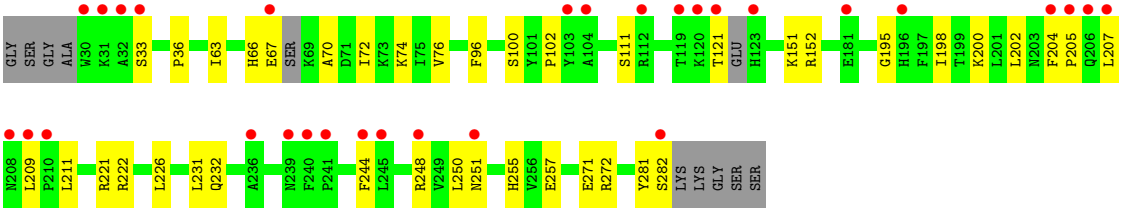
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	124	124	124	0	0
			Total	O		
3	B	89	89	89	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

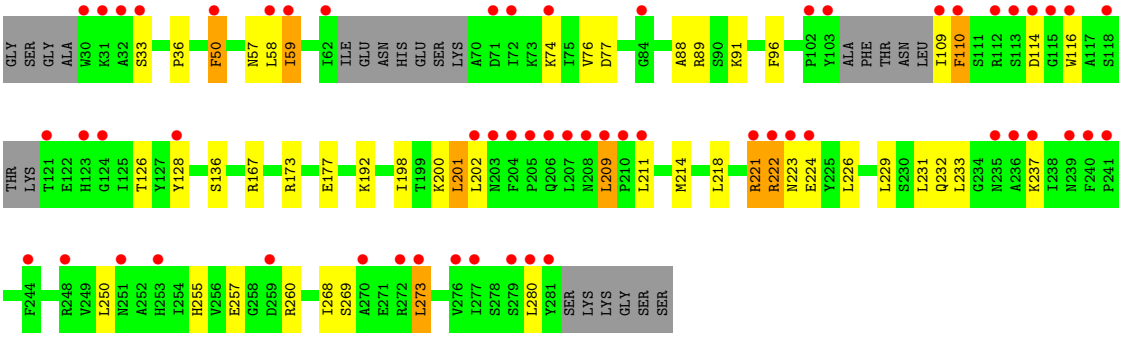
- Molecule 1: 30kLP

Chain A:



- Molecule 1: 30kLP

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	87.75Å 159.87Å 44.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.72 – 1.95 39.71 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.72-1.95) 99.5 (39.71-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.215 , 0.254 0.218 , 0.256	Depositor DCC
R_{free} test set	2336 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4116	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3432e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.70	0/2034	0.70	0/2753
1	B	0.66	0/1926	0.71	0/2606
All	All	0.68	0/3960	0.71	0/5359

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1988	0	1979	26	0
1	B	1883	0	1872	48	0
2	A	24	0	42	7	0
2	B	8	0	14	2	0
3	A	124	0	0	1	0
3	B	89	0	0	4	0
All	All	4116	0	3907	75	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 10.

All (75) 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:126:THR:HG22	1:B:128:TYR:CE2	1.68	1.27
1:B:126:THR:CG2	1:B:128:TYR:HE2	1.48	1.26
1:A:76:VAL:HG22	2:A:301:MPD:HM3	1.16	1.12
1:B:221:ARG:HH11	1:B:221:ARG:HG2	1.13	1.08
1:B:126:THR:CG2	1:B:128:TYR:CE2	2.33	1.07
1:B:126:THR:HG22	1:B:128:TYR:HE2	0.88	1.04
1:B:76:VAL:HG22	2:B:302:MPD:HM3	1.48	0.95
1:A:76:VAL:CG2	2:A:301:MPD:HM3	1.96	0.93
1:B:222:ARG:HH11	1:B:222:ARG:HG2	1.31	0.93
1:B:222:ARG:HG2	1:B:223:ASN:H	1.41	0.84
1:B:222:ARG:CG	1:B:223:ASN:H	1.95	0.80
1:B:222:ARG:HG2	1:B:223:ASN:N	1.97	0.79
1:A:76:VAL:HG22	2:A:301:MPD:CM	2.07	0.76
1:A:232:GLN:HG3	3:A:465:HOH:O	1.86	0.75
1:B:89:ARG:HG3	3:B:348:HOH:O	1.87	0.73
1:A:211:LEU:HD13	1:A:231:LEU:HD21	1.74	0.70
1:B:221:ARG:HG2	1:B:221:ARG:NH1	1.93	0.69
1:B:221:ARG:HH11	1:B:221:ARG:CG	2.00	0.68
1:B:198:ILE:HD13	1:B:231:LEU:HD22	1.76	0.68
1:B:222:ARG:HH11	1:B:222:ARG:CG	2.07	0.67
1:B:222:ARG:CG	1:B:223:ASN:N	2.57	0.66
1:A:195:GLY:O	1:A:198:ILE:HG22	1.99	0.62
1:A:151:LYS:NZ	1:B:33:SER:O	2.31	0.60
1:B:109:ILE:O	1:B:110:PHE:HB2	1.99	0.60
1:B:202:LEU:HG	1:B:250:LEU:HD21	1.82	0.60
1:A:221:ARG:HG3	1:A:226:LEU:HD12	1.83	0.59
1:A:281:TYR:O	1:A:282:SER:HB2	2.02	0.59
1:B:192:LYS:HE2	3:B:449:HOH:O	2.03	0.58
1:B:110:PHE:HB3	1:B:128:TYR:CE1	2.40	0.56
1:A:204:PHE:HB3	1:A:205:PRO:HD2	1.87	0.56
1:A:255:HIS:HE1	1:A:257:GLU:OE1	1.90	0.54
1:A:152:ARG:HG3	1:B:167:ARG:HH12	1.73	0.53
1:A:72:ILE:HG23	2:A:301:MPD:H13	1.91	0.52
1:B:211:LEU:HD13	1:B:231:LEU:HD21	1.92	0.52
1:B:221:ARG:HD3	1:B:226:LEU:HD12	1.92	0.51
2:A:301:MPD:O4	2:A:301:MPD:HM2	2.10	0.50
1:B:50:PHE:CZ	1:B:58:LEU:HD23	2.47	0.50
1:B:126:THR:HG23	1:B:128:TYR:CE2	2.42	0.49
1:A:70:ALA:HB1	1:A:74:LYS:NZ	2.27	0.49
1:A:222:ARG:HB3	1:A:222:ARG:NH1	2.27	0.49
1:B:167:ARG:NH1	3:B:399:HOH:O	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ARG:HG2	1:B:222:ARG:NH1	2.12	0.47
1:A:198:ILE:O	1:A:202:LEU:HG	2.15	0.47
1:A:63:ILE:HD11	1:A:76:VAL:HG21	1.96	0.47
1:B:58:LEU:HD11	1:B:273:LEU:HB3	1.97	0.46
1:B:88:ALA:O	1:B:91:LYS:HD2	2.16	0.46
1:A:36:PRO:HB3	1:A:96:PHE:CD2	2.50	0.46
1:B:57:ASN:HD22	1:B:223:ASN:HD21	1.64	0.46
1:B:221:ARG:NH1	1:B:221:ARG:CG	2.67	0.46
1:B:268:ILE:HG12	1:B:269:SER:N	2.30	0.46
1:B:222:ARG:CG	1:B:222:ARG:NH1	2.74	0.45
1:B:232:GLN:HB2	3:B:515:HOH:O	2.17	0.45
1:B:59:ILE:H	1:B:59:ILE:HG12	1.59	0.45
1:A:66:HIS:O	1:A:67:GLU:HB2	2.17	0.44
1:A:70:ALA:HB1	1:A:74:LYS:HZ2	1.82	0.44
1:B:114:ASP:HB2	1:B:116:TRP:HD1	1.82	0.44
1:B:173:ARG:O	1:B:177:GLU:HG2	2.18	0.44
1:A:72:ILE:HG23	2:A:301:MPD:C1	2.47	0.44
1:B:218:LEU:HD22	1:B:273:LEU:HD11	2.00	0.44
1:B:74:LYS:HA	1:B:77:ASP:OD2	2.18	0.43
1:B:109:ILE:O	1:B:110:PHE:CB	2.65	0.43
1:B:229:LEU:HD12	1:B:229:LEU:C	2.40	0.42
1:B:126:THR:O	1:B:136:SER:HA	2.19	0.42
1:A:202:LEU:HD13	1:A:250:LEU:HD11	2.02	0.42
1:B:50:PHE:CE1	1:B:59:ILE:HD13	2.55	0.41
1:A:200:LYS:O	1:A:272:ARG:NH1	2.50	0.41
2:B:302:MPD:O4	2:B:302:MPD:HM2	2.19	0.41
1:B:201:LEU:HD12	1:B:214:MET:HE1	2.03	0.41
1:B:222:ARG:C	1:B:224:GLU:H	2.24	0.41
1:A:204:PHE:HB3	1:A:205:PRO:CD	2.51	0.41
1:A:100:SER:C	1:A:102:PRO:HD3	2.41	0.41
2:A:300:MPD:O4	2:A:300:MPD:HM1	2.21	0.41
1:A:221:ARG:CG	1:A:226:LEU:HD12	2.49	0.40
1:B:36:PRO:HB3	1:B:96:PHE:CD2	2.56	0.40
1:B:255:HIS:CD2	1:B:257:GLU:HG3	2.56	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	245/262 (94%)	240 (98%)	5 (2%)	0	100 100
1	B	230/262 (88%)	218 (95%)	10 (4%)	2 (1%)	17 8
All	All	475/524 (91%)	458 (96%)	15 (3%)	2 (0%)	34 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	110	PHE
1	B	209	LEU

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	217/224 (97%)	208 (96%)	9 (4%)	30 18
1	B	205/224 (92%)	193 (94%)	12 (6%)	19 8
All	All	422/448 (94%)	401 (95%)	21 (5%)	24 11

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	111	SER
1	A	121	THR
1	A	207	LEU

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Mol	Chain	Res	Type
1	A	209	LEU
1	A	244	PHE
1	A	248	ARG
1	A	251	ASN
1	A	271	GLU
1	B	50	PHE
1	B	59	ILE
1	B	200	LYS
1	B	201	LEU
1	B	209	LEU
1	B	221	ARG
1	B	222	ARG
1	B	233	LEU
1	B	237	LYS
1	B	260	ARG
1	B	273	LEU
1	B	280	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	203	ASN
1	B	208	ASN
1	B	223	ASN
1	B	253	HIS

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 monosaccharides 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	300	-	7,7,7	0.35	0	9,10,10	0.79	1 (11%)
2	MPD	B	302	-	7,7,7	0.34	0	9,10,10	0.26	0
2	MPD	A	303	-	7,7,7	0.33	0	9,10,10	0.49	0
2	MPD	A	301	-	7,7,7	0.37	0	9,10,10	0.57	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	MPD	A	300	-	1/1/2/2	0/5/5/5	-
2	MPD	B	302	-	1/1/2/2	0/5/5/5	-
2	MPD	A	303	-	1/1/2/2	2/5/5/5	-
2	MPD	A	301	-	1/1/2/2	0/5/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	300	MPD	CM-C2-C1	-2.15	106.10	110.57

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	300	MPD	C4
2	A	301	MPD	C4
2	A	303	MPD	C4
2	B	302	MPD	C4

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	303	MPD	C2-C3-C4-C5
2	A	303	MPD	C2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	MPD	1	0
2	B	302	MPD	2	0
2	A	301	MPD	6	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	251/262 (95%)	0.79	30 (11%)	4	7	9, 24, 54, 65	0
1	B	238/262 (90%)	1.42	59 (24%)	0	0	10, 32, 67, 73	0
All	All	489/524 (93%)	1.10	89 (18%)	1	1	9, 26, 61, 73	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	LEU	8.9
1	B	209	LEU	7.1
1	A	208	ASN	7.0
1	A	32	ALA	6.8
1	B	221	ARG	6.6
1	B	240	PHE	6.6
1	A	30	TRP	6.4
1	B	208	ASN	5.9
1	B	62	ILE	5.8
1	B	204	PHE	5.7
1	B	206	GLN	5.7
1	B	72	ILE	5.5
1	B	210	PRO	5.3
1	B	71	ASP	5.3
1	A	121	THR	5.2
1	A	206	GLN	5.0
1	B	235	ASN	4.9
1	B	32	ALA	4.7
1	B	277	ILE	4.7
1	B	128	TYR	4.6
1	B	113	SER	4.3
1	B	239	ASN	4.2
1	B	244	PHE	4.2
1	B	205	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	276	VAL	4.0
1	B	281	TYR	3.8
1	B	30	TRP	3.8
1	B	59	ILE	3.8
1	B	74	LYS	3.7
1	A	207	LEU	3.7
1	B	31	LYS	3.7
1	B	124	GLY	3.7
1	A	205	PRO	3.6
1	B	202	LEU	3.4
1	B	224	GLU	3.4
1	A	31	LYS	3.3
1	A	244	PHE	3.3
1	B	222	ARG	3.3
1	B	109	ILE	3.3
1	A	123	HIS	3.3
1	B	121	THR	3.2
1	B	103	TYR	3.2
1	B	50	PHE	3.2
1	B	251	ASN	3.2
1	A	282	SER	3.2
1	B	115	GLY	3.2
1	A	204	PHE	3.2
1	A	240	PHE	3.2
1	B	280	LEU	3.0
1	A	104	ALA	3.0
1	A	33	SER	3.0
1	A	241	PRO	3.0
1	A	67	GLU	3.0
1	B	114	ASP	2.9
1	B	237	LYS	2.9
1	B	270	ALA	2.9
1	B	272	ARG	2.8
1	A	236	ALA	2.7
1	B	241	PRO	2.7
1	A	120	LYS	2.7
1	B	279	SER	2.7
1	A	103	TYR	2.6
1	A	210	PRO	2.6
1	A	245	LEU	2.6
1	B	203	ASN	2.6
1	B	123	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	102	PRO	2.5
1	A	239	ASN	2.4
1	B	223	ASN	2.4
1	B	248	ARG	2.4
1	B	33	SER	2.4
1	B	118	SER	2.4
1	B	110	PHE	2.3
1	B	253	HIS	2.3
1	B	211	LEU	2.3
1	B	116	TRP	2.3
1	A	251	ASN	2.3
1	A	181	GLU	2.2
1	A	119	THR	2.2
1	B	58	LEU	2.2
1	B	273	LEU	2.2
1	A	248	ARG	2.2
1	A	196	HIS	2.1
1	A	209	LEU	2.1
1	B	259	ASP	2.1
1	B	112	ARG	2.0
1	B	84	GLY	2.0
1	B	236	ALA	2.0
1	A	112	ARG	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MPD	A	300	8/8	0.78	0.25	43,46,52,54	0
2	MPD	A	303	8/8	0.78	0.24	44,53,57,58	0
2	MPD	B	302	8/8	0.89	0.30	38,45,48,49	0
2	MPD	A	301	8/8	0.90	0.19	28,37,38,39	0

6.5 Other polymers (i)

There are no such residues in this entry.