Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 01:12 PM EDT

PDB ID	:	3AIM
Title	:	R267E mutant of a HSL-like carboxylesterase from Sulfolobus tokodaii
Authors	:	Angkawidjaja, C.; Kanaya, S.
Deposited on	:	2010-05-16
Resolution	:	2.30 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 (1)) were used in the production of this report:

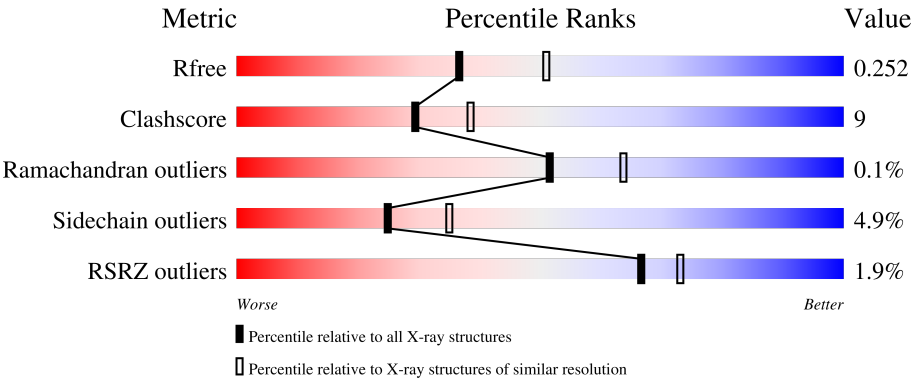
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	323	69% 18% • 12%
1	B	323	% 69% 17% • 12%
1	C	323	2% 73% 14% • 12%
1	D	323	3% 68% 18% • 12%

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	B	305	-	-	X	-
4	MRD	B	306	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9203 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 303aa long hypothetical esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2235	1448	365	419	3			
1	B	283	Total	C	N	O	S	0	0	0
			2235	1448	365	419	3			
1	C	283	Total	C	N	O	S	0	0	0
			2235	1448	365	419	3			
1	D	283	Total	C	N	O	S	0	0	0
			2235	1448	365	419	3			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q976W8
A	-18	GLY	-	expression tag	UNP Q976W8
A	-17	SER	-	expression tag	UNP Q976W8
A	-16	SER	-	expression tag	UNP Q976W8
A	-15	HIS	-	expression tag	UNP Q976W8
A	-14	HIS	-	expression tag	UNP Q976W8
A	-13	HIS	-	expression tag	UNP Q976W8
A	-12	HIS	-	expression tag	UNP Q976W8
A	-11	HIS	-	expression tag	UNP Q976W8
A	-10	HIS	-	expression tag	UNP Q976W8
A	-9	SER	-	expression tag	UNP Q976W8
A	-8	SER	-	expression tag	UNP Q976W8
A	-7	GLY	-	expression tag	UNP Q976W8
A	-6	LEU	-	expression tag	UNP Q976W8
A	-5	VAL	-	expression tag	UNP Q976W8
A	-4	PRO	-	expression tag	UNP Q976W8
A	-3	ARG	-	expression tag	UNP Q976W8
A	-2	GLY	-	expression tag	UNP Q976W8
A	-1	SER	-	expression tag	UNP Q976W8
A	0	HIS	-	expression tag	UNP Q976W8
A	267	GLU	ARG	engineered mutation	UNP Q976W8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q976W8
B	-18	GLY	-	expression tag	UNP Q976W8
B	-17	SER	-	expression tag	UNP Q976W8
B	-16	SER	-	expression tag	UNP Q976W8
B	-15	HIS	-	expression tag	UNP Q976W8
B	-14	HIS	-	expression tag	UNP Q976W8
B	-13	HIS	-	expression tag	UNP Q976W8
B	-12	HIS	-	expression tag	UNP Q976W8
B	-11	HIS	-	expression tag	UNP Q976W8
B	-10	HIS	-	expression tag	UNP Q976W8
B	-9	SER	-	expression tag	UNP Q976W8
B	-8	SER	-	expression tag	UNP Q976W8
B	-7	GLY	-	expression tag	UNP Q976W8
B	-6	LEU	-	expression tag	UNP Q976W8
B	-5	VAL	-	expression tag	UNP Q976W8
B	-4	PRO	-	expression tag	UNP Q976W8
B	-3	ARG	-	expression tag	UNP Q976W8
B	-2	GLY	-	expression tag	UNP Q976W8
B	-1	SER	-	expression tag	UNP Q976W8
B	0	HIS	-	expression tag	UNP Q976W8
B	267	GLU	ARG	engineered mutation	UNP Q976W8
C	-19	MET	-	expression tag	UNP Q976W8
C	-18	GLY	-	expression tag	UNP Q976W8
C	-17	SER	-	expression tag	UNP Q976W8
C	-16	SER	-	expression tag	UNP Q976W8
C	-15	HIS	-	expression tag	UNP Q976W8
C	-14	HIS	-	expression tag	UNP Q976W8
C	-13	HIS	-	expression tag	UNP Q976W8
C	-12	HIS	-	expression tag	UNP Q976W8
C	-11	HIS	-	expression tag	UNP Q976W8
C	-10	HIS	-	expression tag	UNP Q976W8
C	-9	SER	-	expression tag	UNP Q976W8
C	-8	SER	-	expression tag	UNP Q976W8
C	-7	GLY	-	expression tag	UNP Q976W8
C	-6	LEU	-	expression tag	UNP Q976W8
C	-5	VAL	-	expression tag	UNP Q976W8
C	-4	PRO	-	expression tag	UNP Q976W8
C	-3	ARG	-	expression tag	UNP Q976W8
C	-2	GLY	-	expression tag	UNP Q976W8
C	-1	SER	-	expression tag	UNP Q976W8
C	0	HIS	-	expression tag	UNP Q976W8
C	267	GLU	ARG	engineered mutation	UNP Q976W8

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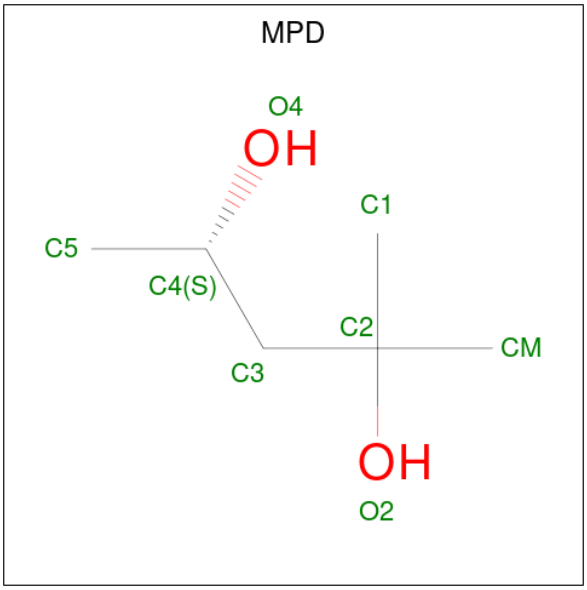
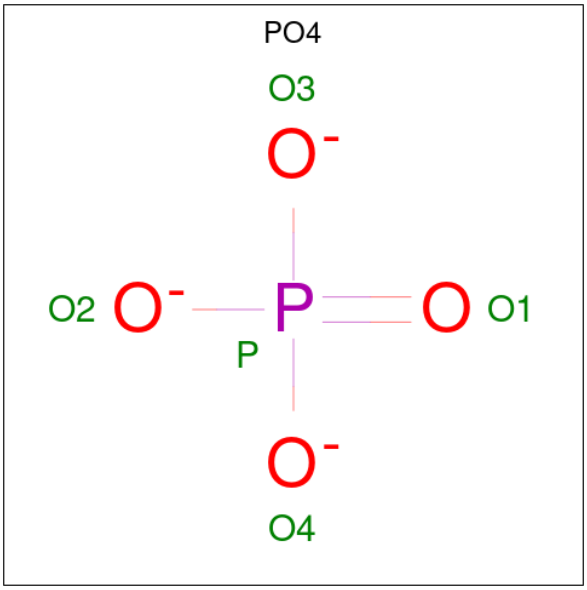
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP Q976W8
D	-18	GLY	-	expression tag	UNP Q976W8
D	-17	SER	-	expression tag	UNP Q976W8
D	-16	SER	-	expression tag	UNP Q976W8
D	-15	HIS	-	expression tag	UNP Q976W8
D	-14	HIS	-	expression tag	UNP Q976W8
D	-13	HIS	-	expression tag	UNP Q976W8
D	-12	HIS	-	expression tag	UNP Q976W8
D	-11	HIS	-	expression tag	UNP Q976W8
D	-10	HIS	-	expression tag	UNP Q976W8
D	-9	SER	-	expression tag	UNP Q976W8
D	-8	SER	-	expression tag	UNP Q976W8
D	-7	GLY	-	expression tag	UNP Q976W8
D	-6	LEU	-	expression tag	UNP Q976W8
D	-5	VAL	-	expression tag	UNP Q976W8
D	-4	PRO	-	expression tag	UNP Q976W8
D	-3	ARG	-	expression tag	UNP Q976W8
D	-2	GLY	-	expression tag	UNP Q976W8
D	-1	SER	-	expression tag	UNP Q976W8
D	0	HIS	-	expression tag	UNP Q976W8
D	267	GLU	ARG	engineered mutation	UNP Q976W8

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



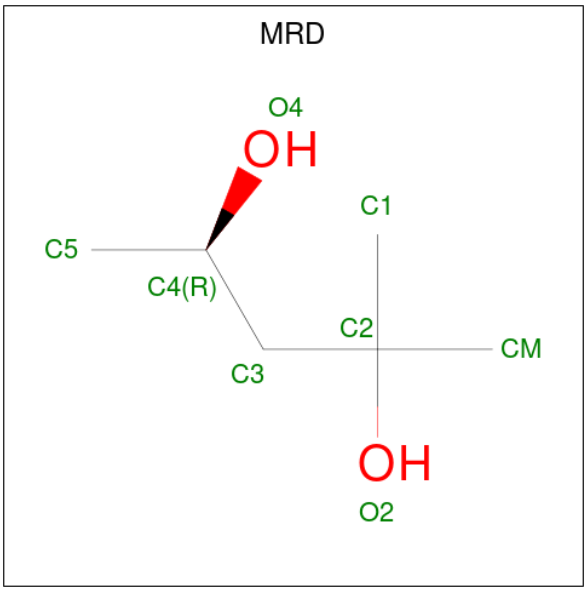
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 6 2	0	0
2	B	1	Total C O 8 6 2	0	0
2	B	1	Total C O 8 6 2	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



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

- Molecule 5 is water.

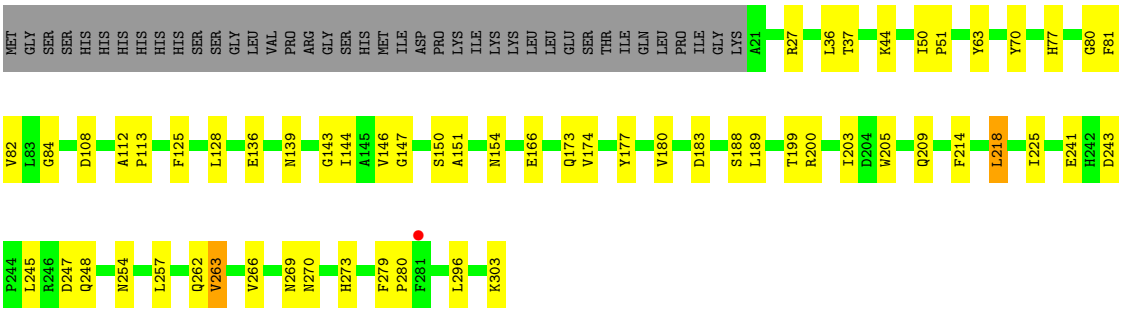
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	51	Total O 51 51	0	0
5	B	44	Total O 44 44	0	0
5	C	38	Total O 38 38	0	0
5	D	25	Total O 25 25	0	0

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.

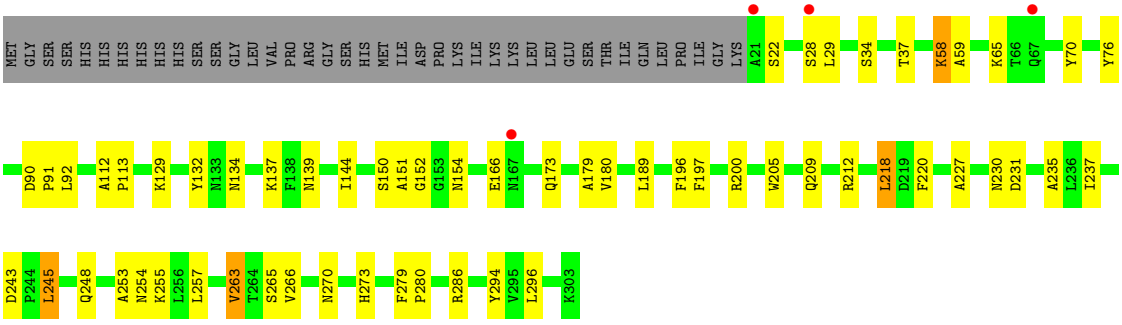
• Molecule 1: 303aa long hypothetical esterase

Chain A:



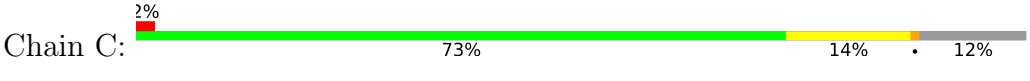
• Molecule 1: 303aa long hypothetical esterase

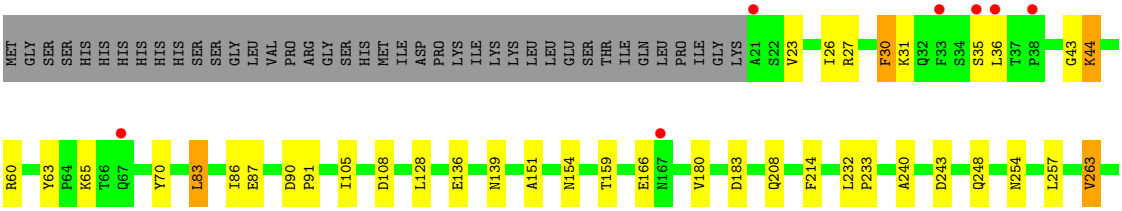
Chain B:



• Molecule 1: 303aa long hypothetical esterase

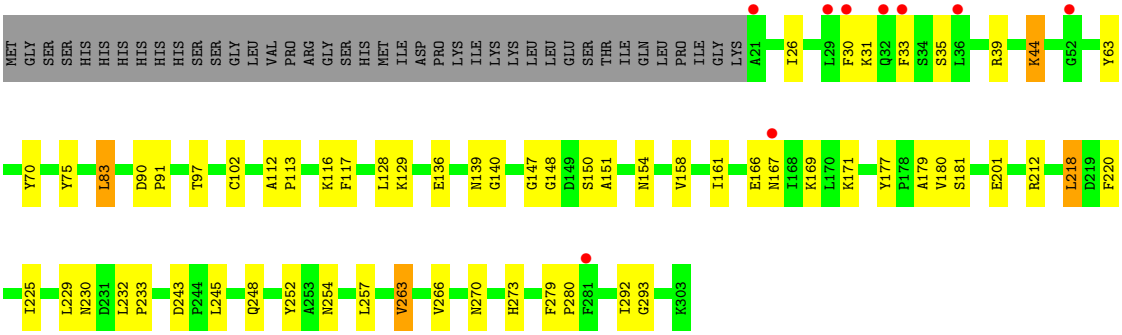
Chain C:





• Molecule 1: 303aa long hypothetical esterase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.21Å 114.83Å 102.22Å 90.00° 109.74° 90.00°	Depositor
Resolution (Å)	32.46 – 2.30 30.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (32.46-2.30) 96.7 (30.42-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.210 , 0.249 0.214 , 0.252	Depositor DCC
R_{free} test set	3588 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9203	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, PO4, MRD

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	0.61	2/2290 (0.1%)	0.56	1/3106 (0.0%)
1	B	0.56	1/2290 (0.0%)	0.51	0/3106
1	C	0.58	0/2290	0.55	1/3106 (0.0%)
1	D	0.53	1/2290 (0.0%)	0.51	0/3106
All	All	0.57	4/9160 (0.0%)	0.53	2/12424 (0.0%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	177	TYR	CD1-CE1	-6.50	1.29	1.39
1	A	177	TYR	CD2-CE2	-5.94	1.30	1.39
1	B	265	SER	CB-OG	-5.42	1.35	1.42
1	A	82	VAL	CB-CG2	-5.38	1.41	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	183	ASP	CB-CG-OD1	7.11	124.70	118.30
1	C	183	ASP	CB-CG-OD1	6.08	123.77	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	TYR	Peptide
1	B	70	TYR	Peptide
1	C	70	TYR	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	2235	0	2198	45	0
1	B	2235	0	2198	51	0
1	C	2235	0	2200	34	0
1	D	2235	0	2198	43	0
2	A	8	0	14	5	0
2	B	16	0	28	10	0
3	A	10	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	B	16	0	28	6	0
4	C	24	0	42	6	0
4	D	16	0	28	2	0
5	A	51	0	0	2	0
5	B	44	0	0	0	0
5	C	38	0	0	0	0
5	D	25	0	0	1	0
All	All	9203	0	8934	170	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 9.

All (170) 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)
4:D:306:MRD:H5C2	4:D:306:MRD:O2	1.52	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:307:MRD:O4	4:C:307:MRD:CM	2.03	1.06
4:C:307:MRD:O4	4:C:307:MRD:HMC2	1.56	1.04
4:B:306:MRD:O2	4:B:306:MRD:H5C2	1.59	0.98
1:A:270:ASN:HD21	1:D:254:ASN:HD21	1.18	0.90
1:A:37:THR:HG23	1:A:280:PRO:HG3	1.52	0.89
1:D:180:VAL:H	1:D:248:GLN:HE21	1.18	0.88
2:B:304:MPD:H52	2:B:304:MPD:H12	1.58	0.85
4:D:306:MRD:O2	4:D:306:MRD:C5	2.24	0.83
2:A:304:MPD:H51	5:A:578:HOH:O	1.80	0.82
1:C:30:PHE:HD2	1:C:30:PHE:O	1.63	0.81
1:B:180:VAL:H	1:B:248:GLN:HE21	1.28	0.81
1:B:270:ASN:HD21	1:C:254:ASN:HD21	1.26	0.81
1:B:37:THR:OG1	2:B:305:MPD:H13	1.82	0.80
4:B:306:MRD:H5C3	4:B:306:MRD:H1C2	1.62	0.80
1:B:151:ALA:O	1:B:154:ASN:HB3	1.82	0.79
1:D:180:VAL:H	1:D:248:GLN:NE2	1.79	0.79
1:B:132:TYR:HA	1:B:144:ILE:CD1	2.16	0.76
1:A:254:ASN:HD21	1:D:270:ASN:HD21	1.35	0.74
1:C:180:VAL:H	1:C:248:GLN:HE21	1.34	0.74
1:B:34:SER:HA	2:B:305:MPD:H11	1.70	0.74
1:B:254:ASN:HD21	1:C:270:ASN:HD21	1.38	0.71
1:B:180:VAL:H	1:B:248:GLN:NE2	1.89	0.70
1:D:243:ASP:OD2	1:D:273:HIS:HD2	1.75	0.69
1:A:270:ASN:HD21	1:D:254:ASN:ND2	1.92	0.68
4:B:306:MRD:O2	4:B:306:MRD:C5	2.35	0.68
1:C:151:ALA:O	1:C:154:ASN:HB3	1.94	0.68
1:A:243:ASP:OD2	1:A:273:HIS:HD2	1.78	0.67
1:B:270:ASN:HD21	1:C:254:ASN:ND2	1.92	0.66
2:B:304:MPD:H12	2:B:304:MPD:C5	2.26	0.66
1:B:257:LEU:HG	1:B:263:VAL:HG13	1.77	0.66
1:A:180:VAL:H	1:A:248:GLN:HE21	1.41	0.66
1:C:26:ILE:HG22	1:C:83:LEU:HD22	1.78	0.66
1:D:128:LEU:O	1:D:128:LEU:HG	1.93	0.65
1:D:26:ILE:HG22	1:D:83:LEU:CD2	2.27	0.65
1:C:128:LEU:HD22	1:C:159:THR:HG22	1.79	0.64
1:B:34:SER:OG	2:B:305:MPD:H11	1.97	0.64
1:C:30:PHE:O	1:C:30:PHE:CD2	2.50	0.64
1:A:279:PHE:CD1	1:A:280:PRO:HD3	2.33	0.64
1:D:232:LEU:HB3	1:D:233:PRO:HD2	1.81	0.63
1:A:199:THR:O	1:A:203:ILE:HD12	1.99	0.63
1:B:90:ASP:HB3	1:B:91:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:HG13	1:D:266:VAL:HG13	1.81	0.62
2:A:304:MPD:H52	2:A:304:MPD:H11	1.80	0.62
1:A:180:VAL:H	1:A:248:GLN:NE2	1.97	0.62
1:A:257:LEU:HG	1:A:263:VAL:HG13	1.80	0.62
4:C:307:MRD:HMC2	4:C:307:MRD:HA	1.59	0.62
4:B:306:MRD:H1C2	4:B:306:MRD:C5	2.28	0.61
1:B:132:TYR:HA	1:B:144:ILE:HD13	1.82	0.60
1:B:237:ILE:HD12	1:B:253:ALA:HB2	1.83	0.60
1:C:232:LEU:HB3	1:C:233:PRO:HD2	1.82	0.60
1:C:257:LEU:HG	1:C:263:VAL:CG1	2.32	0.60
1:B:266:VAL:HG13	1:C:266:VAL:HG13	1.83	0.60
1:C:208:GLN:HG3	4:C:305:MRD:H1C1	1.84	0.59
4:C:307:MRD:O4	4:C:307:MRD:HMC1	1.97	0.58
1:A:254:ASN:ND2	1:D:270:ASN:HD21	2.00	0.58
1:D:26:ILE:HG22	1:D:83:LEU:HD22	1.85	0.58
1:D:90:ASP:HB3	1:D:91:PRO:HD3	1.85	0.58
1:D:112:ALA:HB1	1:D:113:PRO:HA	1.85	0.58
1:B:243:ASP:OD2	1:B:273:HIS:HD2	1.86	0.57
1:B:132:TYR:HD1	1:B:144:ILE:HD12	1.68	0.57
1:D:243:ASP:OD2	1:D:273:HIS:CD2	2.56	0.57
1:B:205:TRP:O	1:B:209:GLN:HG2	2.05	0.57
1:A:279:PHE:CG	1:A:280:PRO:HD3	2.40	0.56
1:D:201:GLU:N	1:D:201:GLU:OE1	2.35	0.56
1:B:254:ASN:HD21	1:C:270:ASN:ND2	2.04	0.56
1:C:243:ASP:OD2	1:C:273:HIS:HD2	1.87	0.55
1:C:26:ILE:HG22	1:C:83:LEU:CD2	2.37	0.55
1:B:92:LEU:HB2	2:B:305:MPD:H51	1.88	0.55
1:B:279:PHE:N	1:B:280:PRO:CD	2.71	0.54
1:A:218:LEU:HD22	1:B:218:LEU:HD22	1.90	0.54
1:A:243:ASP:OD2	1:A:273:HIS:CD2	2.61	0.54
1:B:132:TYR:CD1	1:B:144:ILE:HD12	2.41	0.54
1:B:279:PHE:CG	1:B:280:PRO:HD3	2.43	0.53
1:A:112:ALA:HB1	1:A:113:PRO:HA	1.89	0.53
1:A:270:ASN:ND2	1:D:254:ASN:HD21	1.99	0.53
1:C:128:LEU:HD22	1:C:159:THR:CG2	2.38	0.53
1:D:158:VAL:HA	1:D:161:ILE:HD12	1.91	0.53
1:A:279:PHE:N	1:A:280:PRO:HD2	2.24	0.52
1:C:279:PHE:N	1:C:280:PRO:CD	2.72	0.52
1:A:241:GLU:HB2	1:A:269:ASN:HA	1.92	0.52
1:B:189:LEU:HD11	1:B:200:ARG:NE	2.24	0.52
1:B:266:VAL:CG1	1:C:266:VAL:HG13	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:TYR:CE1	1:D:148:GLY:HA2	2.44	0.52
1:D:150:SER:OG	1:D:273:HIS:HE1	1.93	0.51
1:A:125:PHE:HZ	1:A:166:GLU:HG3	1.75	0.51
1:D:31:LYS:NZ	5:D:314:HOH:O	2.40	0.51
1:B:270:ASN:ND2	1:C:254:ASN:HD21	2.03	0.51
1:D:70:TYR:O	1:D:140:GLY:HA2	2.11	0.50
4:B:306:MRD:C5	4:B:306:MRD:C1	2.88	0.49
1:A:279:PHE:CG	1:A:280:PRO:CD	2.96	0.49
1:C:43:GLY:O	1:C:44:LYS:HB3	2.12	0.49
1:D:26:ILE:CG2	1:D:83:LEU:HD21	2.43	0.49
1:B:58:LYS:HG3	1:B:59:ALA:N	2.28	0.49
1:A:27:ARG:HG2	5:A:617:HOH:O	2.12	0.49
1:B:34:SER:OG	2:B:305:MPD:C1	2.59	0.49
1:C:90:ASP:HB3	1:C:91:PRO:HD3	1.95	0.48
1:D:26:ILE:CG2	1:D:83:LEU:CD2	2.91	0.48
1:C:180:VAL:H	1:C:248:GLN:NE2	2.07	0.48
1:D:279:PHE:CG	1:D:280:PRO:HD3	2.47	0.48
1:A:128:LEU:HD13	1:A:146:VAL:HG12	1.95	0.48
1:A:266:VAL:HG13	1:D:266:VAL:CG1	2.43	0.48
1:B:112:ALA:HB1	1:B:113:PRO:HA	1.95	0.48
1:A:143:GLY:C	1:A:144:ILE:HD13	2.34	0.47
1:B:189:LEU:HD11	1:B:200:ARG:CD	2.44	0.47
1:C:30:PHE:CD2	1:C:30:PHE:C	2.86	0.47
1:C:44:LYS:HE3	1:C:63:TYR:CE2	2.50	0.47
1:A:80:GLY:HA2	2:A:304:MPD:HM1	1.97	0.47
1:D:116:LYS:O	1:D:117:PHE:C	2.54	0.46
1:D:279:PHE:N	1:D:280:PRO:CD	2.78	0.46
1:C:30:PHE:HD2	1:C:30:PHE:C	2.16	0.46
1:C:151:ALA:HB2	4:C:304:MRD:HMC1	1.97	0.46
1:A:245:LEU:HD11	2:A:304:MPD:H13	1.97	0.45
1:B:173:GLN:HG3	1:B:235:ALA:HB2	1.98	0.45
1:B:34:SER:CA	2:B:305:MPD:H11	2.43	0.45
1:A:150:SER:OG	1:A:273:HIS:HE1	2.00	0.45
1:A:81:PHE:HE2	2:A:304:MPD:H53	1.82	0.45
1:D:179:ALA:HA	1:D:245:LEU:HD13	1.99	0.44
1:D:167:ASN:O	1:D:169:LYS:HE3	2.17	0.44
1:D:181:SER:HB2	1:D:225:ILE:CG2	2.48	0.44
1:C:86:ILE:HD12	1:C:108:ASP:HB2	1.98	0.44
1:D:136:GLU:H	1:D:136:GLU:CD	2.21	0.44
1:D:218:LEU:HD12	1:D:218:LEU:HA	1.78	0.44
1:A:147:GLY:HA2	1:A:174:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:VAL:O	1:C:27:ARG:HG3	2.18	0.44
1:A:146:VAL:O	1:A:173:GLN:HA	2.17	0.44
1:D:212:ARG:HE	1:D:212:ARG:HB2	1.58	0.44
1:A:279:PHE:CE1	1:A:280:PRO:HD3	2.52	0.44
1:D:75:TYR:HA	1:D:147:GLY:O	2.18	0.43
1:D:292:ILE:O	1:D:293:GLY:C	2.57	0.43
1:D:26:ILE:HG21	1:D:83:LEU:HD21	2.00	0.43
1:A:50:ILE:HG23	1:A:51:PRO:HD2	2.00	0.43
1:B:37:THR:HG1	2:B:305:MPD:H13	1.80	0.43
1:A:189:LEU:HD11	1:A:200:ARG:CD	2.49	0.43
1:D:97:THR:HG23	1:D:102:CYS:O	2.19	0.43
1:A:150:SER:OG	1:A:273:HIS:CE1	2.72	0.43
1:A:151:ALA:O	1:A:154:ASN:HB3	2.18	0.43
1:A:218:LEU:CD2	1:B:218:LEU:HD22	2.48	0.43
4:B:306:MRD:H5C2	4:B:306:MRD:H2	1.76	0.43
1:A:188:SER:HB3	1:A:247:ASP:CG	2.39	0.42
1:B:196:PHE:O	1:B:197:PHE:HB3	2.19	0.42
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.86	0.42
1:B:76:TYR:O	1:B:152:GLY:HA3	2.19	0.42
1:B:237:ILE:HD12	1:B:253:ALA:CB	2.49	0.42
1:B:286:ARG:HD2	1:C:294:TYR:OH	2.19	0.42
1:C:240:ALA:HB3	1:C:243:ASP:HB2	2.01	0.42
1:A:205:TRP:O	1:A:209:GLN:HG2	2.20	0.42
1:B:230:ASN:O	1:B:231:ASP:HB2	2.20	0.41
1:A:189:LEU:HD11	1:A:200:ARG:NE	2.35	0.41
1:A:128:LEU:HD13	1:A:146:VAL:CG1	2.50	0.41
1:B:270:ASN:ND2	1:C:254:ASN:ND2	2.65	0.41
1:C:60:ARG:O	1:C:105:ILE:HA	2.20	0.41
1:B:294:TYR:OH	1:C:286:ARG:HD2	2.21	0.41
1:A:77:HIS:CE1	1:A:84:GLY:O	2.74	0.41
1:B:134:ASN:HB3	1:B:137:LYS:HG3	2.02	0.41
1:B:179:ALA:HA	1:B:245:LEU:HD13	2.03	0.41
2:B:304:MPD:C5	2:B:304:MPD:C1	2.97	0.41
1:D:44:LYS:HE2	1:D:63:TYR:HB2	2.03	0.41
1:A:214:PHE:CD1	1:B:218:LEU:HG	2.56	0.40
1:A:296:LEU:HD23	1:A:296:LEU:HA	1.87	0.40
1:B:227:ALA:O	1:B:255:LYS:NZ	2.54	0.40
1:A:44:LYS:HB3	1:A:63:TYR:HB2	2.04	0.40
1:B:150:SER:OG	1:B:273:HIS:HE1	2.04	0.40
1:B:212:ARG:NH2	3:B:308:PO4:O4	2.40	0.40
1:B:294:TYR:CD2	1:B:294:TYR:C	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:PHE:CD1	1:D:220:PHE:C	2.95	0.40
1:D:151:ALA:O	1:D:154:ASN:HB3	2.20	0.40
1:D:229:LEU:HD11	1:D:252:TYR:CE1	2.57	0.40
1:B:220:PHE:CD1	1:B:220:PHE:C	2.95	0.40
1:D:257:LEU:HG	1:D:263:VAL:HG13	2.03	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	281/323 (87%)	264 (94%)	16 (6%)	1 (0%)	34 42
1	B	281/323 (87%)	268 (95%)	13 (5%)	0	100 100
1	C	281/323 (87%)	265 (94%)	16 (6%)	0	100 100
1	D	281/323 (87%)	259 (92%)	22 (8%)	0	100 100
All	All	1124/1292 (87%)	1056 (94%)	67 (6%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	ILE

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	239/275 (87%)	231 (97%)	8 (3%)	38	53
1	B	239/275 (87%)	228 (95%)	11 (5%)	27	38
1	C	239/275 (87%)	224 (94%)	15 (6%)	18	24
1	D	239/275 (87%)	226 (95%)	13 (5%)	22	30
All	All	956/1100 (87%)	909 (95%)	47 (5%)	25	35

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	108	ASP
1	A	136	GLU
1	A	139	ASN
1	A	218	LEU
1	A	262	GLN
1	A	263	VAL
1	A	303	LYS
1	B	22	SER
1	B	28	SER
1	B	29	LEU
1	B	58	LYS
1	B	65	LYS
1	B	129	LYS
1	B	139	ASN
1	B	166	GLU
1	B	218	LEU
1	B	245	LEU
1	B	263	VAL
1	C	30	PHE
1	C	31	LYS
1	C	35	SER
1	C	36	LEU
1	C	44	LYS
1	C	65	LYS
1	C	83	LEU
1	C	87	GLU
1	C	136	GLU
1	C	139	ASN
1	C	166	GLU
1	C	214	PHE
1	C	263	VAL
1	C	281	PHE

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Mol	Chain	Res	Type
1	C	303	LYS
1	D	30	PHE
1	D	33	PHE
1	D	35	SER
1	D	39	ARG
1	D	44	LYS
1	D	83	LEU
1	D	129	LYS
1	D	139	ASN
1	D	166	GLU
1	D	171	LYS
1	D	218	LEU
1	D	230	ASN
1	D	263	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	154	ASN
1	A	209	GLN
1	A	248	GLN
1	A	254	ASN
1	A	262	GLN
1	A	273	HIS
1	B	139	ASN
1	B	192	ASN
1	B	248	GLN
1	B	254	ASN
1	B	269	ASN
1	B	273	HIS
1	C	67	GLN
1	C	139	ASN
1	C	154	ASN
1	C	192	ASN
1	C	209	GLN
1	C	248	GLN
1	C	254	ASN
1	C	273	HIS
1	D	139	ASN
1	D	154	ASN
1	D	248	GLN

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Mol	Chain	Res	Type
1	D	254	ASN
1	D	262	GLN
1	D	269	ASN
1	D	273	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)

15 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	$\#\|Z\| > 2$
3	PO4	B	308	-	4,4,4	0.93	0	6,6,6	0.40	0
3	PO4	D	305	-	4,4,4	0.81	0	6,6,6	0.51	0
4	MRD	B	306	-	7,7,7	0.28	0	9,10,10	0.34	0
2	MPD	B	305	-	7,7,7	0.29	0	9,10,10	0.26	0
3	PO4	C	306	-	4,4,4	0.89	0	6,6,6	0.38	0
2	MPD	B	304	-	7,7,7	0.33	0	9,10,10	0.34	0
3	PO4	A	306	-	4,4,4	0.86	0	6,6,6	0.47	0
4	MRD	C	304	-	7,7,7	0.21	0	9,10,10	0.37	0
3	PO4	A	305	-	4,4,4	0.80	0	6,6,6	0.55	0
4	MRD	D	304	-	7,7,7	0.26	0	9,10,10	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MRD	B	307	-	7,7,7	0.27	0	9,10,10	0.22	0
4	MRD	D	306	-	7,7,7	0.29	0	9,10,10	0.23	0
4	MRD	C	305	-	7,7,7	0.26	0	9,10,10	0.35	0
2	MPD	A	304	-	7,7,7	0.32	0	9,10,10	0.58	0
4	MRD	C	307	-	7,7,7	0.27	0	9,10,10	0.28	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	MRD	B	306	-	-	2/5/5/5	-
2	MPD	B	305	-	-	4/5/5/5	-
4	MRD	C	304	-	-	2/5/5/5	-
2	MPD	B	304	-	-	2/5/5/5	-
4	MRD	D	304	-	-	0/5/5/5	-
4	MRD	B	307	-	-	2/5/5/5	-
4	MRD	D	306	-	-	4/5/5/5	-
4	MRD	C	305	-	-	2/5/5/5	-
2	MPD	A	304	-	-	4/5/5/5	-
4	MRD	C	307	-	-	5/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	304	MPD	C1-C2-C3-C4
2	A	304	MPD	O2-C2-C3-C4
4	B	306	MRD	C2-C3-C4-C5
4	C	307	MRD	O2-C2-C3-C4
4	C	307	MRD	CM-C2-C3-C4
4	D	306	MRD	C2-C3-C4-C5
2	B	304	MPD	O2-C2-C3-C4
2	B	305	MPD	O2-C2-C3-C4
4	D	306	MRD	O2-C2-C3-C4
2	B	304	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	C	307	MRD	C2-C3-C4-C5
2	A	304	MPD	CM-C2-C3-C4
2	B	305	MPD	C1-C2-C3-C4
2	B	305	MPD	CM-C2-C3-C4
4	B	306	MRD	CM-C2-C3-C4
4	B	307	MRD	C1-C2-C3-C4
4	C	304	MRD	C1-C2-C3-C4
4	C	305	MRD	C1-C2-C3-C4
4	C	307	MRD	C1-C2-C3-C4
4	D	306	MRD	C1-C2-C3-C4
4	D	306	MRD	CM-C2-C3-C4
4	B	307	MRD	O2-C2-C3-C4
4	C	304	MRD	O2-C2-C3-C4
4	C	305	MRD	O2-C2-C3-C4
2	A	304	MPD	C2-C3-C4-C5
2	B	305	MPD	C2-C3-C4-C5
4	C	307	MRD	C2-C3-C4-O4

There are no ring outliers.

9 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	308	PO4	1	0
4	B	306	MRD	6	0
2	B	305	MPD	7	0
2	B	304	MPD	3	0
4	C	304	MRD	1	0
4	D	306	MRD	2	0
4	C	305	MRD	1	0
2	A	304	MPD	5	0
4	C	307	MRD	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	283/323 (87%)	-0.30	1 (0%)	92 95	10, 20, 39, 57	0
1	B	283/323 (87%)	-0.20	4 (1%)	75 80	8, 20, 41, 65	0
1	C	283/323 (87%)	-0.20	8 (2%)	53 60	10, 20, 50, 70	0
1	D	283/323 (87%)	-0.03	9 (3%)	47 54	13, 23, 62, 81	0
All	All	1132/1292 (87%)	-0.18	22 (1%)	66 73	8, 20, 47, 81	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	21	ALA	6.3
1	D	33	PHE	6.1
1	D	281	PHE	5.0
1	D	21	ALA	5.0
1	A	281	PHE	3.5
1	C	33	PHE	3.3
1	D	30	PHE	3.2
1	D	36	LEU	3.2
1	B	21	ALA	3.0
1	B	67	GLN	2.9
1	C	303	LYS	2.7
1	D	29	LEU	2.6
1	C	38	PRO	2.4
1	D	32	GLN	2.4
1	D	167	ASN	2.4
1	C	36	LEU	2.3
1	C	35	SER	2.1
1	C	67	GLN	2.1
1	C	167	ASN	2.1
1	B	167	ASN	2.1
1	B	28	SER	2.1
1	D	52	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 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MRD	D	306	8/8	0.83	0.26	59,60,65,69	0
4	MRD	C	305	8/8	0.86	0.20	56,57,58,60	0
4	MRD	B	306	8/8	0.86	0.27	58,60,62,63	0
3	PO4	B	308	5/5	0.88	0.30	37,40,46,51	0
4	MRD	C	307	8/8	0.88	0.18	31,38,40,43	0
3	PO4	A	306	5/5	0.88	0.38	69,71,71,72	0
2	MPD	B	305	8/8	0.90	0.18	33,43,49,52	0
3	PO4	D	305	5/5	0.90	0.29	60,61,65,65	0
3	PO4	A	305	5/5	0.91	0.15	56,57,62,65	0
2	MPD	A	304	8/8	0.92	0.23	23,26,29,30	0
2	MPD	B	304	8/8	0.93	0.20	14,24,28,33	0
4	MRD	B	307	8/8	0.93	0.17	48,48,50,51	0
4	MRD	C	304	8/8	0.93	0.20	12,24,32,32	0
3	PO4	C	306	5/5	0.96	0.33	47,49,51,52	0
4	MRD	D	304	8/8	0.97	0.22	21,25,27,28	0

6.5 Other polymers (i)

There are no such residues in this entry.