Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2021 – 10:12 AM JST

PDB ID	:	7E5T
Title	:	Crystal structure of Fsa2
Authors	:	Fujiyama, K.; Kato, N.; Kinugasa, K.; Hino, T.; Takahashi, S.; Nagano, S.
Deposited on	:	2021-02-20
Resolution	:	2.17 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 (i)) were used in the production of this report:

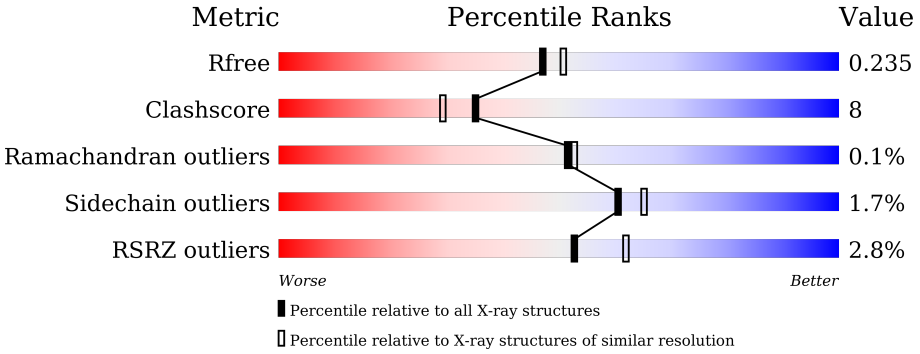
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.17 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	384	2%, 84%, 13%, •
1	B	384	2%, 81%, 15%, • •
1	C	384	5%, 77%, 19%, • •
1	D	384	3%, 78%, 18%, •
1	E	384	3%, 80%, 17%, •
1	F	384	3%, 79%, 18%, •

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Mol	Chain	Length	Quality of chain
1	G	384	3% 76% 21%
1	H	384	2% 83% 15%

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	EOH	D	402	-	-	X	-
2	EOH	D	403	-	-	X	-
2	EOH	E	401	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 24269 atoms, of which 84 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 Diels-Alderase fsa2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	374	2884	1812	491	569	12	0	1	0
1	B	370	2844	1791	483	558	12	0	0	0
1	C	373	2865	1801	486	567	11	0	0	0
1	D	369	2832	1783	479	559	11	0	0	0
1	E	372	2856	1797	485	562	12	0	0	0
1	F	374	2882	1811	489	570	12	0	1	0
1	G	374	2873	1806	487	568	12	0	0	0
1	H	374	2873	1806	487	568	12	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP A0A0E4AYE7
A	-8	GLY	-	expression tag	UNP A0A0E4AYE7
A	-7	SER	-	expression tag	UNP A0A0E4AYE7
A	-6	SER	-	expression tag	UNP A0A0E4AYE7
A	-5	HIS	-	expression tag	UNP A0A0E4AYE7
A	-4	HIS	-	expression tag	UNP A0A0E4AYE7
A	-3	HIS	-	expression tag	UNP A0A0E4AYE7
A	-2	HIS	-	expression tag	UNP A0A0E4AYE7
A	-1	HIS	-	expression tag	UNP A0A0E4AYE7
A	0	HIS	-	expression tag	UNP A0A0E4AYE7
B	-9	MET	-	initiating methionine	UNP A0A0E4AYE7
B	-8	GLY	-	expression tag	UNP A0A0E4AYE7
B	-7	SER	-	expression tag	UNP A0A0E4AYE7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	SER	-	expression tag	UNP A0A0E4AYE7
B	-5	HIS	-	expression tag	UNP A0A0E4AYE7
B	-4	HIS	-	expression tag	UNP A0A0E4AYE7
B	-3	HIS	-	expression tag	UNP A0A0E4AYE7
B	-2	HIS	-	expression tag	UNP A0A0E4AYE7
B	-1	HIS	-	expression tag	UNP A0A0E4AYE7
B	0	HIS	-	expression tag	UNP A0A0E4AYE7
C	-9	MET	-	initiating methionine	UNP A0A0E4AYE7
C	-8	GLY	-	expression tag	UNP A0A0E4AYE7
C	-7	SER	-	expression tag	UNP A0A0E4AYE7
C	-6	SER	-	expression tag	UNP A0A0E4AYE7
C	-5	HIS	-	expression tag	UNP A0A0E4AYE7
C	-4	HIS	-	expression tag	UNP A0A0E4AYE7
C	-3	HIS	-	expression tag	UNP A0A0E4AYE7
C	-2	HIS	-	expression tag	UNP A0A0E4AYE7
C	-1	HIS	-	expression tag	UNP A0A0E4AYE7
C	0	HIS	-	expression tag	UNP A0A0E4AYE7
D	-9	MET	-	initiating methionine	UNP A0A0E4AYE7
D	-8	GLY	-	expression tag	UNP A0A0E4AYE7
D	-7	SER	-	expression tag	UNP A0A0E4AYE7
D	-6	SER	-	expression tag	UNP A0A0E4AYE7
D	-5	HIS	-	expression tag	UNP A0A0E4AYE7
D	-4	HIS	-	expression tag	UNP A0A0E4AYE7
D	-3	HIS	-	expression tag	UNP A0A0E4AYE7
D	-2	HIS	-	expression tag	UNP A0A0E4AYE7
D	-1	HIS	-	expression tag	UNP A0A0E4AYE7
D	0	HIS	-	expression tag	UNP A0A0E4AYE7
E	-9	MET	-	initiating methionine	UNP A0A0E4AYE7
E	-8	GLY	-	expression tag	UNP A0A0E4AYE7
E	-7	SER	-	expression tag	UNP A0A0E4AYE7
E	-6	SER	-	expression tag	UNP A0A0E4AYE7
E	-5	HIS	-	expression tag	UNP A0A0E4AYE7
E	-4	HIS	-	expression tag	UNP A0A0E4AYE7
E	-3	HIS	-	expression tag	UNP A0A0E4AYE7
E	-2	HIS	-	expression tag	UNP A0A0E4AYE7
E	-1	HIS	-	expression tag	UNP A0A0E4AYE7
E	0	HIS	-	expression tag	UNP A0A0E4AYE7
F	-9	MET	-	initiating methionine	UNP A0A0E4AYE7
F	-8	GLY	-	expression tag	UNP A0A0E4AYE7
F	-7	SER	-	expression tag	UNP A0A0E4AYE7
F	-6	SER	-	expression tag	UNP A0A0E4AYE7
F	-5	HIS	-	expression tag	UNP A0A0E4AYE7

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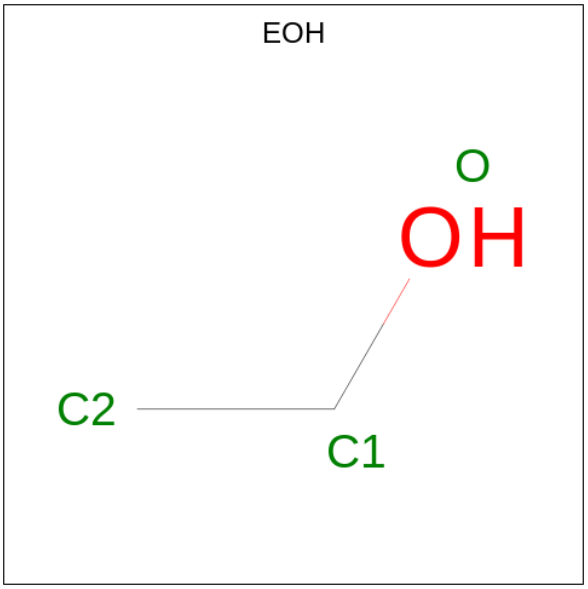
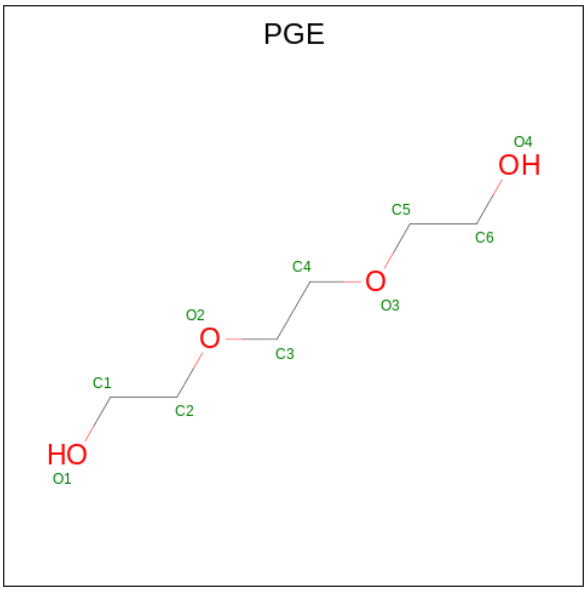
Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	HIS	-	expression tag	UNP A0A0E4AYE7
F	-3	HIS	-	expression tag	UNP A0A0E4AYE7
F	-2	HIS	-	expression tag	UNP A0A0E4AYE7
F	-1	HIS	-	expression tag	UNP A0A0E4AYE7
F	0	HIS	-	expression tag	UNP A0A0E4AYE7
G	-9	MET	-	initiating methionine	UNP A0A0E4AYE7
G	-8	GLY	-	expression tag	UNP A0A0E4AYE7
G	-7	SER	-	expression tag	UNP A0A0E4AYE7
G	-6	SER	-	expression tag	UNP A0A0E4AYE7
G	-5	HIS	-	expression tag	UNP A0A0E4AYE7
G	-4	HIS	-	expression tag	UNP A0A0E4AYE7
G	-3	HIS	-	expression tag	UNP A0A0E4AYE7
G	-2	HIS	-	expression tag	UNP A0A0E4AYE7
G	-1	HIS	-	expression tag	UNP A0A0E4AYE7
G	0	HIS	-	expression tag	UNP A0A0E4AYE7
H	-9	MET	-	initiating methionine	UNP A0A0E4AYE7
H	-8	GLY	-	expression tag	UNP A0A0E4AYE7
H	-7	SER	-	expression tag	UNP A0A0E4AYE7
H	-6	SER	-	expression tag	UNP A0A0E4AYE7
H	-5	HIS	-	expression tag	UNP A0A0E4AYE7
H	-4	HIS	-	expression tag	UNP A0A0E4AYE7
H	-3	HIS	-	expression tag	UNP A0A0E4AYE7
H	-2	HIS	-	expression tag	UNP A0A0E4AYE7
H	-1	HIS	-	expression tag	UNP A0A0E4AYE7
H	0	HIS	-	expression tag	UNP A0A0E4AYE7

- Molecule 2 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



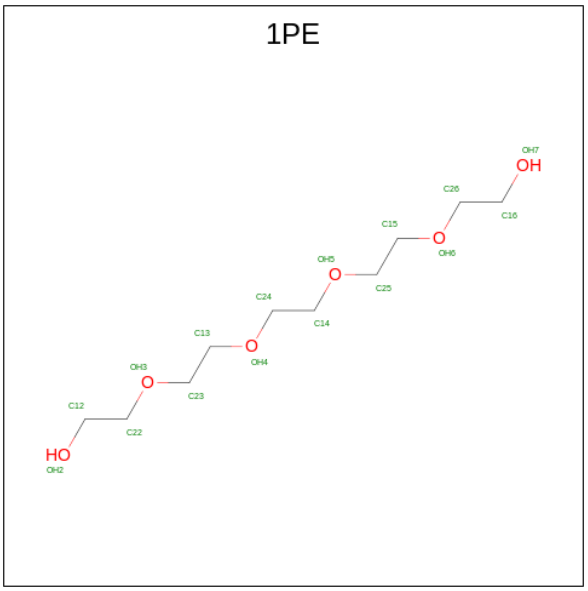
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	B	1	9	2	6	1	0	0
2	D	1	9	2	6	1	0	0
2	D	1	9	2	6	1	0	0
2	D	1	9	2	6	1	0	0
2	E	1	9	2	6	1	0	0
2	H	1	9	2	6	1	0	0
2	H	1	9	2	6	1	0	0
2	H	1	9	2	6	1	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	F	1	24	6	14	4	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	H	1	38	10	22	6	0	0

- Molecule 5 is water.

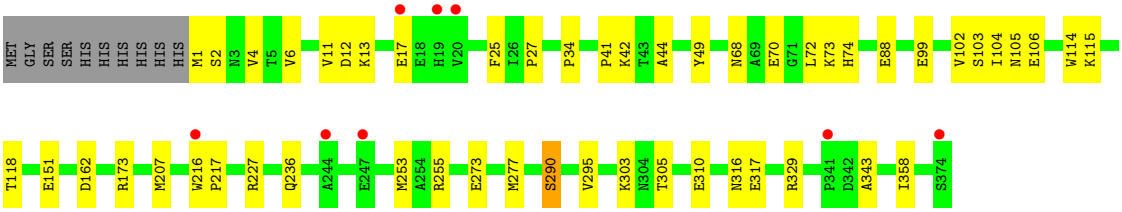
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	182	182	182	0	0
5	B	174	174	174	0	0
5	C	160	160	160	0	0
5	D	122	122	122	0	0
5	E	145	145	145	0	0
5	F	166	166	166	0	0
5	G	123	123	123	0	0
5	H	154	154	154	0	0

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.

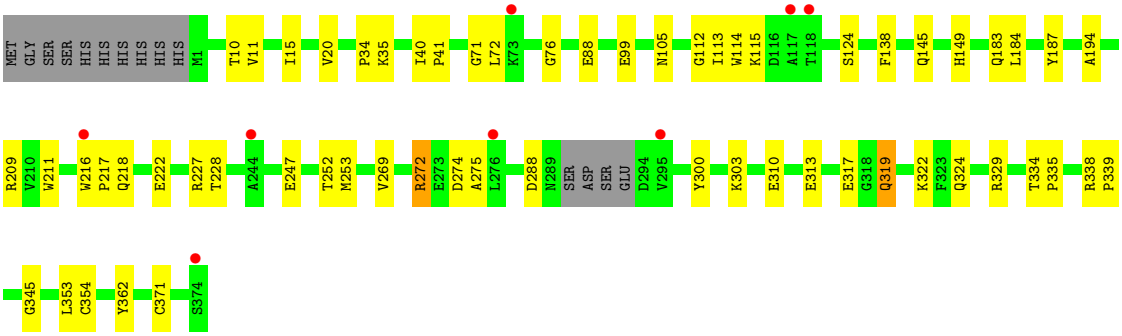
• Molecule 1: Diels-Alderase fsa2

Chain A:



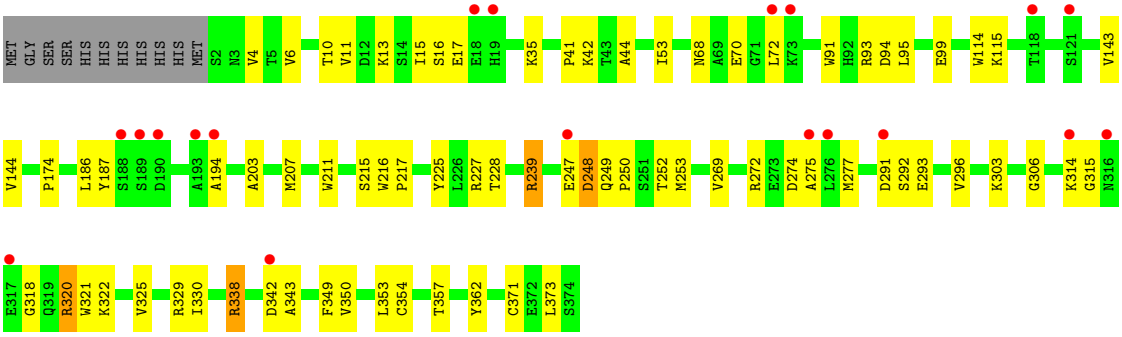
• Molecule 1: Diels-Alderase fsa2

Chain B:



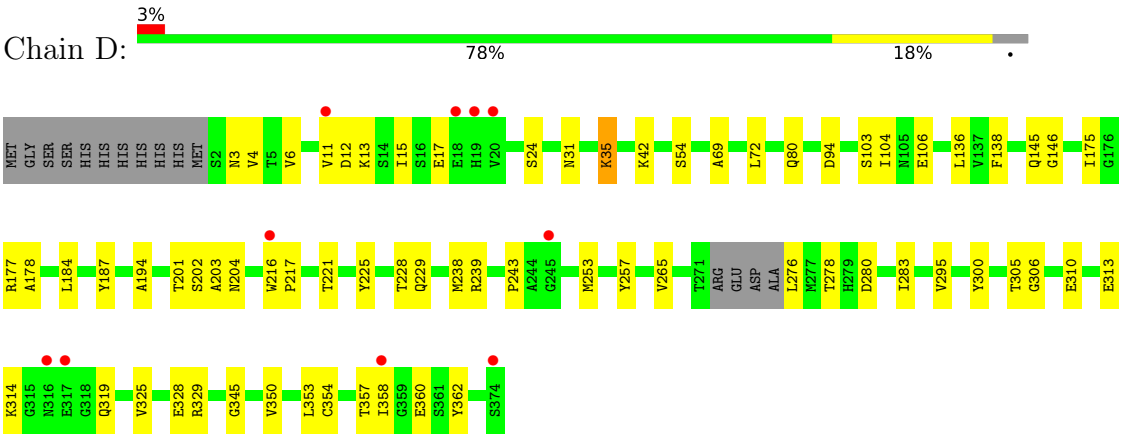
• Molecule 1: Diels-Alderase fsa2

Chain C:



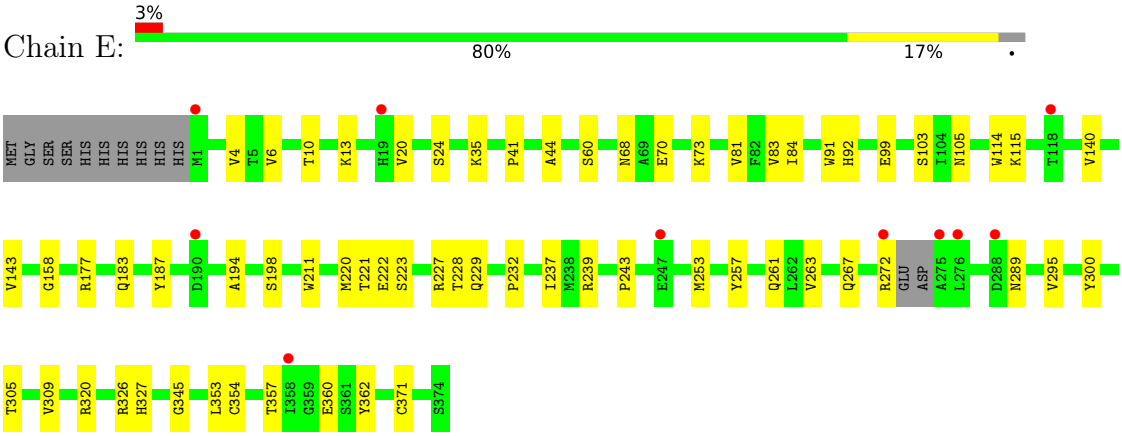
• Molecule 1: Diels-Alderase fsa2

Chain D:



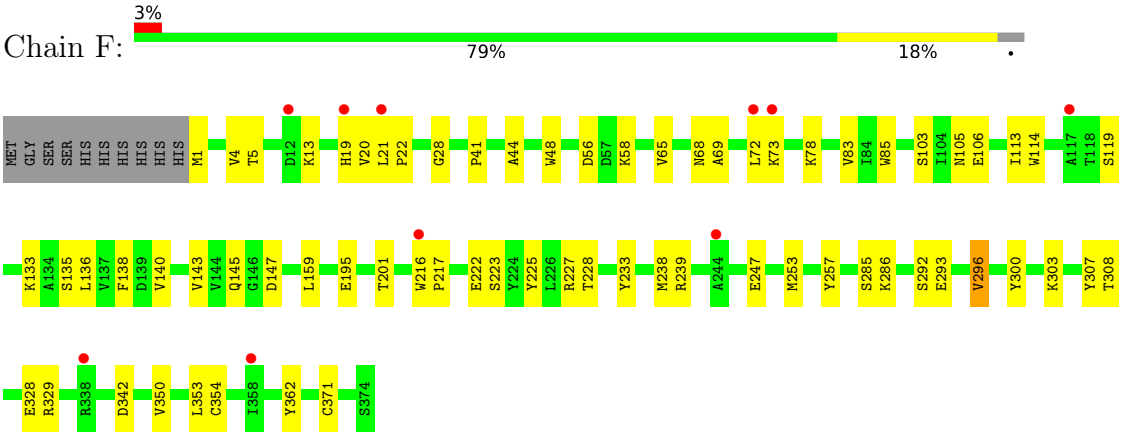
• Molecule 1: Diels-Alderase fsa2

Chain E:



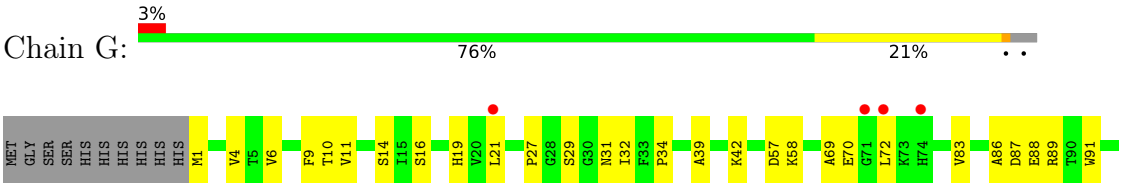
• Molecule 1: Diels-Alderase fsa2

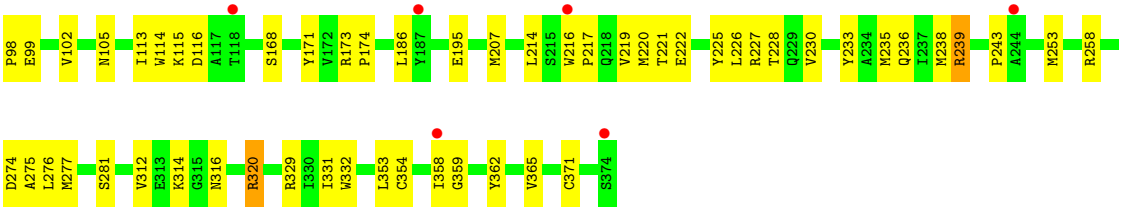
Chain F:



• Molecule 1: Diels-Alderase fsa2

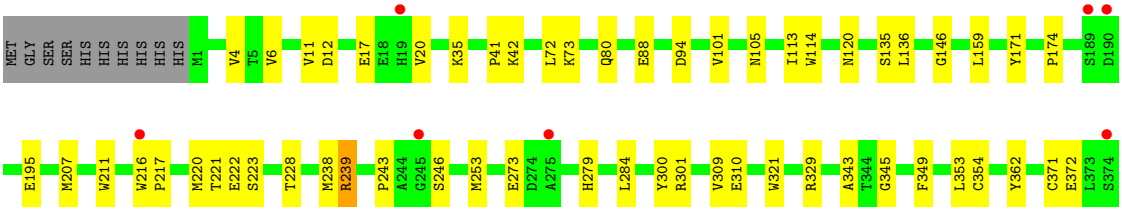
Chain G:





- Molecule 1: Diels-Alderase fsa2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	133.93Å 80.23Å 135.16Å 90.00° 108.53° 90.00°	Depositor
Resolution (Å)	45.04 – 2.17 45.14 – 2.17	Depositor EDS
% Data completeness (in resolution range)	97.6 (45.04-2.17) 97.6 (45.14-2.17)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.11.1	Depositor
R, R_{free}	0.180 , 0.235 0.180 , 0.235	Depositor DCC
R_{free} test set	7267 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24269	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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: 1PE, PGE, EOH

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	0.32	0/2953	0.54	0/4013
1	B	0.32	0/2912	0.54	0/3957
1	C	0.32	0/2934	0.53	0/3989
1	D	0.31	0/2900	0.53	0/3942
1	E	0.30	0/2924	0.53	0/3973
1	F	0.31	0/2951	0.52	0/4011
1	G	0.29	0/2942	0.51	0/3999
1	H	0.31	0/2942	0.53	0/3999
All	All	0.31	0/23458	0.53	0/31883

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	C	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	349	PHE	Peptide
1	H	349	PHE	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	2884	0	2772	37	0
1	B	2844	0	2739	39	0
1	C	2865	0	2748	60	0
1	D	2832	0	2719	49	0
1	E	2856	0	2749	46	0
1	F	2882	0	2767	51	0
1	G	2873	0	2760	58	0
1	H	2873	0	2760	39	0
2	B	3	6	6	0	0
2	D	9	18	18	4	0
2	E	3	6	6	3	0
2	H	9	18	18	0	0
3	F	10	14	14	0	0
4	H	16	22	22	1	0
5	A	182	0	0	2	0
5	B	174	0	0	3	0
5	C	160	0	0	3	0
5	D	122	0	0	1	0
5	E	145	0	0	1	0
5	F	166	0	0	2	0
5	G	123	0	0	1	0
5	H	154	0	0	1	0
All	All	24185	84	22098	368	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 8.

All (368) 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:C:143:VAL:HG12	1:C:144:VAL:HG23	1.45	0.99
1:A:295:VAL:HG21	1:A:305:THR:HB	1.45	0.99
1:B:338:ARG:HG3	1:B:339:PRO:HD2	1.53	0.91
1:H:11:VAL:HG22	1:H:72:LEU:HD13	1.52	0.91
1:G:276:LEU:HD23	1:G:316:ASN:HA	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:GLY:HA2	4:H:404:1PE:H151	1.57	0.85
1:F:72:LEU:HD12	1:F:73:LYS:HG3	1.59	0.84
1:D:4:VAL:CG2	1:D:103:SER:HB2	2.09	0.81
1:B:11:VAL:HG11	1:B:76:GLY:HA2	1.61	0.81
1:D:204:ASN:HB2	2:D:403:EOH:H22	1.62	0.80
1:C:338:ARG:H	1:C:338:ARG:HD2	1.47	0.80
1:F:72:LEU:CD1	1:F:73:LYS:HG3	2.11	0.80
1:F:1:MET:HB3	1:F:106:GLU:HG3	1.62	0.79
1:A:290:SER:HB2	1:G:27:PRO:HG2	1.64	0.78
1:H:73:LYS:HZ3	1:H:73:LYS:HB2	1.49	0.78
1:D:357:THR:HG22	1:D:360:GLU:OE2	1.84	0.78
1:F:48:TRP:HB2	1:F:65:VAL:CG1	2.14	0.77
1:E:177:ARG:HD2	2:E:401:EOH:H23	1.68	0.76
1:D:221:THR:HG23	1:D:243:PRO:HA	1.68	0.76
1:A:17:GLU:HG2	1:A:42:LYS:HE3	1.68	0.75
1:D:4:VAL:HG21	1:D:103:SER:HB2	1.68	0.75
1:E:4:VAL:HG13	1:E:6:VAL:HG23	1.68	0.74
1:E:177:ARG:HH21	2:E:401:EOH:H23	1.54	0.72
1:C:275:ALA:HA	1:C:314:LYS:HZ3	1.54	0.72
1:F:228:THR:HG21	1:F:353:LEU:HD22	1.72	0.72
1:A:11:VAL:HG22	1:A:72:LEU:HD13	1.70	0.72
1:H:301:ARG:NH2	1:H:372:GLU:OE1	2.23	0.71
1:D:4:VAL:HG23	1:D:104:ILE:O	1.89	0.71
1:A:68:ASN:OD1	1:A:70:GLU:HG2	1.90	0.71
1:G:1:MET:HG2	1:G:105:ASN:HB2	1.73	0.71
1:E:295:VAL:HG21	1:E:305:THR:HB	1.73	0.70
1:F:228:THR:HG21	1:F:353:LEU:CD2	2.22	0.70
1:C:277:MET:O	1:C:314:LYS:HE2	1.91	0.70
1:D:295:VAL:HG21	1:D:305:THR:HB	1.72	0.70
1:A:1:MET:HB3	1:C:303:LYS:HG3	1.74	0.69
1:B:11:VAL:HG11	1:B:76:GLY:CA	2.22	0.69
1:H:73:LYS:HB2	1:H:73:LYS:NZ	2.03	0.69
1:A:277:MET:CE	1:A:316:ASN:HA	2.23	0.69
1:A:12:ASP:HB3	1:A:13:LYS:HE3	1.74	0.69
1:C:249:GLN:HG3	1:C:250:PRO:HD2	1.74	0.69
1:A:295:VAL:CG2	1:A:305:THR:HB	2.21	0.68
1:F:48:TRP:O	1:F:65:VAL:HG12	1.92	0.68
1:E:295:VAL:HB	1:E:326:ARG:HD3	1.75	0.68
1:G:221:THR:HG23	1:G:243:PRO:HA	1.75	0.67
1:A:73:LYS:HE2	1:A:74:HIS:NE2	2.08	0.67
1:E:99:GLU:OE1	1:E:115:LYS:HE3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:GLU:OE1	1:D:42:LYS:HD3	1.95	0.66
1:A:358:ILE:HD12	1:A:358:ILE:O	1.94	0.66
1:B:15:ILE:HD12	1:B:72:LEU:HD22	1.79	0.65
1:B:338:ARG:HG3	1:B:339:PRO:CD	2.25	0.65
1:C:216:TRP:HE3	1:C:373:LEU:HD21	1.62	0.64
1:H:300:TYR:CD2	1:H:345:GLY:HA3	2.33	0.63
1:C:11:VAL:HG22	1:C:72:LEU:HD23	1.79	0.63
1:G:354:CYS:HA	1:G:362:TYR:O	1.98	0.63
1:E:4:VAL:HG13	1:E:6:VAL:CG2	2.28	0.63
1:F:69:ALA:HB1	1:F:72:LEU:HD23	1.80	0.63
1:F:48:TRP:HB2	1:F:65:VAL:HG13	1.79	0.63
1:C:338:ARG:HD2	1:C:338:ARG:N	2.07	0.62
1:D:280:ASP:OD1	1:D:314:LYS:HE2	1.99	0.62
1:E:68:ASN:OD1	1:E:70:GLU:HG3	1.98	0.62
1:G:274:ASP:O	1:G:320:ARG:NH2	2.31	0.62
1:D:15:ILE:HD13	1:D:69:ALA:HA	1.81	0.62
1:B:183:GLN:C	1:B:184:LEU:HD12	2.20	0.61
1:C:99:GLU:OE2	1:C:115:LYS:HE3	1.99	0.61
1:D:313:GLU:OE1	1:D:319:GLN:HG2	2.01	0.60
1:A:290:SER:HB2	1:G:27:PRO:CG	2.31	0.60
1:G:1:MET:CG	1:G:105:ASN:HB2	2.32	0.60
1:C:274:ASP:O	1:C:277:MET:HG2	2.02	0.59
1:C:354:CYS:HA	1:C:362:TYR:O	2.02	0.59
1:H:4:VAL:HG13	1:H:6:VAL:HG23	1.82	0.59
1:C:275:ALA:HA	1:C:314:LYS:NZ	2.18	0.59
1:H:20:VAL:HB	1:H:41:PRO:HD3	1.83	0.59
1:G:19:HIS:NE2	1:G:21:LEU:HD23	2.18	0.59
1:F:286:LYS:HG2	1:F:307:TYR:CE2	2.38	0.59
1:H:354:CYS:HA	1:H:362:TYR:O	2.02	0.59
1:E:272:ARG:HH12	1:H:120:ASN:HD22	1.51	0.58
1:G:58:LYS:HD2	1:G:329:ARG:NH2	2.18	0.58
1:B:272:ARG:HD2	1:B:274:ASP:OD1	2.04	0.58
1:D:228:THR:HG21	1:D:353:LEU:HD22	1.84	0.58
1:C:296:VAL:HG21	1:C:330:ILE:HG12	1.86	0.58
1:F:13:LYS:O	1:F:13:LYS:HG2	2.03	0.57
1:F:285:SER:OG	1:F:308:THR:HG22	2.03	0.57
1:E:13:LYS:O	1:E:13:LYS:HG2	2.05	0.57
1:C:10:THR:OG1	1:C:13:LYS:HB2	2.04	0.57
1:G:312:VAL:HG23	1:G:320:ARG:HG3	1.86	0.57
1:F:19:HIS:HA	1:F:41:PRO:HB3	1.87	0.57
1:C:274:ASP:OD2	1:C:277:MET:HE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLU:OE1	1:B:272:ARG:HG3	2.05	0.56
1:B:272:ARG:HB3	1:B:275:ALA:HB2	1.88	0.56
1:F:354:CYS:HA	1:F:362:TYR:O	2.05	0.56
1:D:12:ASP:OD1	1:D:13:LYS:HG3	2.06	0.56
1:G:239:ARG:C	1:G:239:ARG:HD2	2.25	0.56
5:A:472:HOH:O	1:G:314:LYS:HE2	2.04	0.56
1:D:295:VAL:CG2	1:D:305:THR:HB	2.36	0.56
1:G:99:GLU:OE1	1:G:115:LYS:HE3	2.06	0.56
1:C:343:ALA:HB1	5:C:445:HOH:O	2.06	0.56
1:G:228:THR:HG21	1:G:353:LEU:HD22	1.87	0.56
1:H:221:THR:HG23	1:H:243:PRO:HA	1.87	0.56
1:F:68:ASN:HB2	5:F:546:HOH:O	2.05	0.55
1:F:72:LEU:HD12	1:F:73:LYS:N	2.21	0.55
1:E:187:TYR:CE2	1:E:194:ALA:HB2	2.41	0.55
1:H:171:TYR:HE2	1:H:238:MET:HE3	1.71	0.55
1:G:174:PRO:HD2	1:G:207:MET:O	2.07	0.55
1:F:78:LYS:NZ	5:F:503:HOH:O	2.38	0.55
1:E:183:GLN:NE2	1:E:198:SER:OG	2.40	0.55
1:G:10:THR:HG22	1:G:99:GLU:HG2	1.88	0.55
1:A:277:MET:HE1	1:A:316:ASN:HA	1.89	0.55
1:C:272:ARG:NH2	5:C:406:HOH:O	2.40	0.54
1:H:171:TYR:CE2	1:H:238:MET:HE3	2.42	0.54
1:G:228:THR:HG21	1:G:353:LEU:CD2	2.38	0.54
1:E:35:LYS:HG3	1:E:211:TRP:CE2	2.43	0.54
1:A:118:THR:HG21	1:C:322:LYS:HE2	1.89	0.54
1:F:133:LYS:HB2	1:F:133:LYS:NZ	2.21	0.54
1:D:216:TRP:HB2	1:D:217:PRO:HD3	1.89	0.54
1:D:228:THR:HG21	1:D:353:LEU:CD2	2.38	0.54
1:A:317:GLU:OE1	1:A:317:GLU:N	2.31	0.54
1:E:357:THR:HG22	1:E:360:GLU:OE2	2.08	0.53
1:G:168:SER:CB	1:G:214:LEU:HD12	2.38	0.53
1:F:4:VAL:HG12	1:F:105:ASN:HA	1.90	0.53
1:G:11:VAL:CG2	1:G:72:LEU:HD23	2.39	0.53
1:A:4:VAL:HG23	1:A:104:ILE:O	2.08	0.53
1:G:83:VAL:HG22	1:G:91:TRP:HB3	1.91	0.53
1:C:248:ASP:OD1	1:C:248:ASP:N	2.41	0.53
1:D:201:THR:HG22	1:D:202:SER:N	2.23	0.53
1:B:310:GLU:OE2	1:B:322:LYS:NZ	2.42	0.53
1:E:4:VAL:HG23	1:E:105:ASN:HA	1.91	0.53
1:F:140:VAL:HG12	1:F:143:VAL:HB	1.91	0.53
1:G:216:TRP:HB2	1:G:217:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:TRP:CE3	1:C:373:LEU:HD21	2.43	0.53
1:E:228:THR:HG21	1:E:353:LEU:HD22	1.90	0.53
1:A:12:ASP:CB	1:A:13:LYS:HE3	2.37	0.52
1:B:99:GLU:OE1	1:B:115:LYS:HE3	2.09	0.52
1:B:218:GLN:NE2	1:C:342:ASP:OD1	2.40	0.52
1:A:2:SER:HB2	1:A:106:GLU:OE2	2.09	0.52
1:B:20:VAL:HB	1:B:41:PRO:HD3	1.92	0.52
1:C:318:GLY:O	1:C:320:ARG:NE	2.41	0.52
1:B:313:GLU:OE1	1:B:319:GLN:HG3	2.10	0.52
1:B:338:ARG:NH1	1:C:247:GLU:HG3	2.25	0.51
1:C:252:THR:HB	1:C:269:VAL:HG22	1.91	0.51
1:G:4:VAL:HG23	1:G:6:VAL:HG23	1.91	0.51
1:G:89:ARG:NH2	1:G:195:GLU:OE1	2.43	0.51
1:B:71:GLY:N	5:B:503:HOH:O	2.42	0.51
1:B:149:HIS:HD2	5:B:575:HOH:O	1.94	0.51
1:B:35:LYS:HG3	1:B:211:TRP:CE2	2.45	0.51
1:D:283:ILE:HB	1:D:310:GLU:HB3	1.92	0.51
1:F:300:TYR:O	1:F:303:LYS:NZ	2.35	0.51
1:E:20:VAL:HB	1:E:41:PRO:HD3	1.93	0.51
1:A:41:PRO:HG2	1:A:44:ALA:HB2	1.92	0.51
1:E:221:THR:HG23	1:E:243:PRO:HA	1.92	0.51
1:G:11:VAL:HG22	1:G:72:LEU:HD23	1.91	0.51
1:D:276:LEU:HD12	1:D:278:THR:HG22	1.92	0.50
1:F:72:LEU:HD11	1:F:73:LYS:HG3	1.93	0.50
1:E:300:TYR:CD2	1:E:345:GLY:HA3	2.46	0.50
1:C:247:GLU:OE1	1:C:247:GLU:HA	2.11	0.50
1:G:70:GLU:O	1:G:70:GLU:HG3	2.12	0.50
1:H:284:LEU:HD13	1:H:309:VAL:HG22	1.94	0.50
1:H:35:LYS:HG3	1:H:211:TRP:CE2	2.47	0.50
1:D:276:LEU:HD12	1:D:278:THR:CG2	2.42	0.50
1:F:41:PRO:HG2	1:F:44:ALA:HB2	1.93	0.50
1:D:4:VAL:HG22	1:D:103:SER:HB2	1.93	0.49
1:A:11:VAL:HG22	1:A:72:LEU:CD1	2.41	0.49
1:A:17:GLU:HG2	1:A:42:LYS:CE	2.41	0.49
1:B:187:TYR:CE2	1:B:194:ALA:HB2	2.46	0.49
1:C:329:ARG:HB2	1:C:350:VAL:HB	1.94	0.49
1:F:41:PRO:HG2	1:F:44:ALA:CB	2.43	0.49
1:G:34:PRO:HD3	1:G:102:VAL:HG11	1.95	0.49
1:B:11:VAL:CG1	1:B:76:GLY:HA2	2.36	0.49
1:H:73:LYS:NZ	1:H:73:LYS:CB	2.73	0.49
1:A:4:VAL:HG13	1:A:6:VAL:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:CYS:HA	1:E:362:TYR:O	2.13	0.49
1:F:20:VAL:O	1:F:22:PRO:HD3	2.12	0.49
1:H:228:THR:HG21	1:H:353:LEU:HD22	1.94	0.49
1:B:216:TRP:HB2	1:B:217:PRO:HD3	1.95	0.49
1:F:216:TRP:HB2	1:F:217:PRO:HD3	1.95	0.49
1:H:4:VAL:HG13	1:H:6:VAL:CG2	2.42	0.49
1:H:113:ILE:HG23	1:H:113:ILE:O	2.13	0.49
1:E:261:GLN:O	1:E:263:VAL:HG13	2.12	0.48
1:H:216:TRP:HB2	1:H:217:PRO:HD3	1.95	0.48
1:G:42:LYS:HA	1:G:69:ALA:HB2	1.95	0.48
1:A:343:ALA:HB1	5:A:442:HOH:O	2.13	0.48
1:C:91:TRP:CH2	1:C:144:VAL:HG22	2.48	0.48
1:G:168:SER:HB3	1:G:214:LEU:HD12	1.96	0.48
1:H:195:GLU:HA	1:H:195:GLU:OE1	2.13	0.48
1:H:220:MET:SD	1:H:223:SER:HB3	2.53	0.48
1:D:54:SER:HA	1:D:203:ALA:HA	1.96	0.48
1:D:106:GLU:HG3	5:D:587:HOH:O	2.13	0.48
1:G:222:GLU:HA	1:G:371:CYS:O	2.14	0.48
1:B:222:GLU:HA	1:B:371:CYS:O	2.13	0.48
1:E:10:THR:OG1	1:E:13:LYS:HB3	2.14	0.48
1:C:91:TRP:CZ3	1:C:186:LEU:HD22	2.49	0.48
1:F:1:MET:HB2	1:F:105:ASN:HB2	1.94	0.48
1:F:233:TYR:HA	1:F:257:TYR:O	2.14	0.47
1:B:10:THR:HG22	1:B:99:GLU:HG2	1.95	0.47
1:F:133:LYS:HB2	1:F:133:LYS:HZ3	1.78	0.47
1:C:215:SER:OG	1:C:217:PRO:HD2	2.14	0.47
1:C:291:ASP:OD1	5:C:401:HOH:O	2.20	0.47
1:D:229:GLN:H	2:D:403:EOH:H21	1.79	0.47
1:F:247:GLU:N	1:F:247:GLU:OE1	2.46	0.47
1:D:329:ARG:HB2	1:D:350:VAL:HB	1.96	0.47
1:G:276:LEU:CD2	1:G:316:ASN:HA	2.37	0.47
1:C:53:ILE:O	1:C:203:ALA:HA	2.14	0.47
1:F:56:ASP:OD2	1:F:201:THR:OG1	2.28	0.47
1:A:99:GLU:HB2	1:A:115:LYS:HG3	1.97	0.47
1:F:140:VAL:CG1	1:F:143:VAL:HB	2.45	0.47
1:C:41:PRO:HG2	1:C:44:ALA:HB2	1.97	0.47
1:F:225:TYR:HB2	1:F:238:MET:HE1	1.96	0.47
1:H:174:PRO:HG2	1:H:207:MET:HG2	1.96	0.47
1:H:243:PRO:O	1:H:246:SER:HB3	2.15	0.47
1:A:4:VAL:CG2	1:A:103:SER:HB2	2.45	0.46
1:E:41:PRO:HG2	1:E:44:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:239:ARG:HD2	1:H:239:ARG:C	2.35	0.46
1:F:113:ILE:HG23	1:F:113:ILE:O	2.15	0.46
1:E:187:TYR:CZ	1:E:194:ALA:HB2	2.51	0.46
1:G:83:VAL:HG21	1:G:186:LEU:CD1	2.45	0.46
1:A:25:PHE:O	1:A:27:PRO:HD3	2.15	0.46
1:B:334:THR:HG23	1:B:335:PRO:HD2	1.98	0.46
1:C:99:GLU:OE2	1:C:115:LYS:CE	2.64	0.46
1:C:15:ILE:HD12	1:C:72:LEU:HD21	1.96	0.46
1:E:60:SER:HB3	1:E:84:ILE:HG22	1.97	0.46
1:E:237:ILE:HD11	1:E:309:VAL:HG11	1.98	0.46
1:C:68:ASN:OD1	1:C:70:GLU:HG2	2.15	0.46
1:B:300:TYR:CD2	1:B:345:GLY:HA3	2.51	0.46
1:C:17:GLU:HG3	1:C:42:LYS:NZ	2.31	0.46
1:A:105:ASN:HB2	1:B:247:GLU:OE2	2.16	0.46
1:E:267:GLN:HG3	5:E:539:HOH:O	2.16	0.46
1:B:34:PRO:HA	1:B:209:ARG:NH2	2.31	0.45
1:F:136:LEU:N	1:F:136:LEU:HD12	2.31	0.45
1:F:296:VAL:HG11	1:F:328:GLU:O	2.17	0.45
1:G:1:MET:HG2	5:G:521:HOH:O	2.15	0.45
1:C:275:ALA:CA	1:C:314:LYS:NZ	2.79	0.45
1:F:135:SER:C	1:F:136:LEU:HD12	2.36	0.45
1:D:4:VAL:HA	2:D:402:EOH:H12	1.99	0.45
1:D:300:TYR:CD2	1:D:345:GLY:HA3	2.51	0.45
1:F:65:VAL:HG13	1:F:65:VAL:O	2.17	0.45
1:G:275:ALA:O	1:G:316:ASN:O	2.34	0.45
1:B:183:GLN:O	1:B:184:LEU:HD12	2.16	0.45
1:A:303:LYS:HA	1:A:303:LYS:HD2	1.74	0.45
1:B:88:GLU:HG2	1:B:329:ARG:HD3	1.97	0.45
1:B:113:ILE:O	1:B:113:ILE:HG23	2.17	0.45
1:C:239:ARG:HD2	1:C:239:ARG:C	2.36	0.45
1:C:306:GLY:HA3	1:C:325:VAL:O	2.16	0.45
1:F:239:ARG:HD2	1:F:239:ARG:C	2.37	0.45
1:G:331:ILE:HG22	1:G:332:TRP:HE3	1.82	0.45
1:H:80:GLN:HG2	1:H:94:ASP:OD1	2.17	0.45
1:G:230:VAL:HG21	1:G:353:LEU:HD22	1.98	0.45
1:C:187:TYR:CE2	1:C:194:ALA:HB2	2.51	0.45
1:G:58:LYS:HG2	1:G:365:VAL:HG11	1.99	0.45
1:E:222:GLU:HA	1:E:371:CYS:O	2.17	0.45
1:F:85:TRP:CZ2	1:F:195:GLU:HG2	2.52	0.45
1:G:4:VAL:HG23	1:G:6:VAL:CG2	2.48	0.44
1:G:4:VAL:HG12	1:G:105:ASN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:TRP:CD1	1:C:357:THR:HG23	2.52	0.44
1:G:228:THR:CG2	1:G:235:MET:HG2	2.47	0.44
1:H:105:ASN:HB3	5:H:589:HOH:O	2.17	0.44
1:F:20:VAL:HG12	1:F:21:LEU:N	2.32	0.44
1:F:329:ARG:HB2	1:F:350:VAL:HB	1.99	0.44
1:G:98:PRO:HD2	1:G:116:ASP:HA	2.00	0.44
1:C:16:SER:O	1:C:41:PRO:HA	2.17	0.44
1:D:306:GLY:HA3	1:D:325:VAL:O	2.17	0.44
1:G:57:ASP:HB2	1:G:86:ALA:HB1	1.99	0.44
1:D:187:TYR:CZ	1:D:194:ALA:HB2	2.53	0.44
1:E:70:GLU:HA	1:E:73:LYS:HE3	1.99	0.44
1:B:105:ASN:HB2	5:B:556:HOH:O	2.18	0.43
1:C:228:THR:HG21	1:C:353:LEU:HD22	2.00	0.43
1:D:358:ILE:O	1:D:358:ILE:HG13	2.18	0.43
1:C:91:TRP:HH2	1:C:144:VAL:CG2	2.32	0.43
1:D:31:ASN:OD1	1:D:35:LYS:NZ	2.49	0.43
1:H:88:GLU:HG2	1:H:329:ARG:HD3	1.99	0.43
1:C:174:PRO:HD2	1:C:207:MET:O	2.18	0.43
1:A:216:TRP:HB2	1:A:217:PRO:HD3	1.99	0.43
1:D:138:PHE:O	1:D:145:GLN:HA	2.19	0.43
1:G:171:TYR:CE2	1:G:238:MET:HE3	2.54	0.43
1:C:291:ASP:OD1	1:C:292:SER:N	2.51	0.43
1:E:239:ARG:HD2	1:E:239:ARG:C	2.38	0.43
1:F:72:LEU:HD12	1:F:72:LEU:C	2.38	0.43
1:C:35:LYS:HG3	1:C:211:TRP:CE2	2.54	0.43
1:B:228:THR:HG21	1:B:353:LEU:HD22	2.00	0.43
1:B:324:GLN:O	1:B:353:LEU:HA	2.18	0.43
1:C:11:VAL:CG2	1:C:72:LEU:HD23	2.47	0.43
1:D:11:VAL:HG22	1:D:72:LEU:HD13	2.01	0.43
1:D:187:TYR:CE2	1:D:194:ALA:HB2	2.53	0.43
1:F:222:GLU:HG2	1:F:223:SER:N	2.33	0.43
1:G:277:MET:CE	1:G:281:SER:HB2	2.48	0.43
1:H:135:SER:C	1:H:136:LEU:HD12	2.39	0.43
1:H:273:GLU:OE2	1:H:310:GLU:OE1	2.37	0.43
1:D:72:LEU:HD12	1:D:72:LEU:O	2.19	0.43
1:E:295:VAL:HG23	1:E:327:HIS:O	2.19	0.43
1:H:159:LEU:HD21	1:H:174:PRO:HA	2.00	0.43
1:C:91:TRP:CZ2	1:C:93:ARG:HG2	2.54	0.42
1:D:136:LEU:N	1:D:136:LEU:HD12	2.34	0.42
1:E:68:ASN:CG	1:E:70:GLU:HG3	2.39	0.42
1:F:285:SER:OG	1:F:308:THR:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:226:LEU:HD11	1:G:228:THR:HG22	2.01	0.42
1:G:87:ASP:O	1:G:88:GLU:HB2	2.19	0.42
1:G:233:TYR:CE1	1:G:258:ARG:HG3	2.54	0.42
1:A:162:ASP:O	1:A:255:ARG:NH1	2.52	0.42
1:D:80:GLN:HG2	1:D:94:ASP:OD1	2.20	0.42
1:E:220:MET:SD	1:E:223:SER:HB3	2.60	0.42
1:G:219:VAL:HG23	1:G:220:MET:HG2	2.02	0.42
1:B:138:PHE:O	1:B:145:GLN:HA	2.19	0.42
1:D:239:ARG:HD2	1:D:239:ARG:C	2.40	0.42
1:G:113:ILE:O	1:G:113:ILE:HG23	2.19	0.42
1:A:88:GLU:HG2	1:A:329:ARG:HD3	2.00	0.42
1:A:273:GLU:OE2	1:A:310:GLU:OE2	2.38	0.42
1:B:300:TYR:O	1:B:303:LYS:HE2	2.18	0.42
1:G:16:SER:HB2	1:G:39:ALA:HB1	2.00	0.42
1:D:4:VAL:HG13	1:D:6:VAL:HG23	2.02	0.42
1:F:5:THR:O	1:F:103:SER:HA	2.20	0.42
1:A:49:TYR:O	1:A:207:MET:HA	2.20	0.42
1:D:225:TYR:HB2	1:D:238:MET:CE	2.50	0.42
1:D:328:GLU:HG2	1:D:329:ARG:HG3	2.01	0.42
1:E:83:VAL:HG22	1:E:91:TRP:HB3	2.02	0.42
1:F:292:SER:O	1:F:293:GLU:HB3	2.19	0.42
1:G:32:ILE:HD11	1:G:174:PRO:HB3	2.02	0.42
1:H:136:LEU:HD12	1:H:136:LEU:N	2.34	0.42
1:E:158:GLY:HA3	1:E:257:TYR:OH	2.20	0.42
1:F:138:PHE:O	1:F:145:GLN:HA	2.20	0.42
1:C:91:TRP:CH2	1:C:144:VAL:CG2	3.03	0.41
1:D:3:ASN:O	2:D:402:EOH:H12	2.20	0.41
1:D:175:ILE:HG21	1:D:178:ALA:HB2	2.02	0.41
1:B:40:ILE:O	1:B:40:ILE:HG23	2.20	0.41
1:B:354:CYS:HA	1:B:362:TYR:O	2.19	0.41
1:C:4:VAL:HG23	1:C:6:VAL:HG23	2.01	0.41
1:D:35:LYS:HA	1:D:35:LYS:HD2	1.76	0.41
1:C:216:TRP:HZ3	1:C:371:CYS:SG	2.43	0.41
1:A:173:ARG:NH1	1:A:236:GLN:HB3	2.35	0.41
1:C:252:THR:HB	1:C:269:VAL:CG2	2.50	0.41
1:C:275:ALA:C	1:C:314:LYS:HZ1	2.24	0.41
1:E:4:VAL:HG22	1:E:103:SER:HB2	2.03	0.41
1:G:9:PHE:HA	1:G:14:SER:OG	2.20	0.41
1:B:252:THR:HB	1:B:269:VAL:CG2	2.51	0.41
1:D:146:GLY:HA3	1:D:184:LEU:HD23	2.02	0.41
1:D:177:ARG:HD3	1:D:257:TYR:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:301:ARG:HB3	1:H:343:ALA:O	2.21	0.41
1:H:310:GLU:HA	1:H:321:TRP:O	2.20	0.41
1:A:34:PRO:HD3	1:A:102:VAL:HG11	2.02	0.41
1:C:293:GLU:HG3	1:D:24:SER:HB3	2.02	0.41
1:E:272:ARG:NH1	1:H:120:ASN:HD22	2.17	0.41
1:F:58:LYS:HD2	1:F:329:ARG:NH2	2.35	0.41
1:F:222:GLU:HG3	1:F:371:CYS:O	2.21	0.41
1:E:81:VAL:O	1:E:92:HIS:HA	2.20	0.41
1:E:232:PRO:HD3	1:E:362:TYR:CE1	2.56	0.41
1:C:11:VAL:HG22	1:C:72:LEU:CD2	2.49	0.41
1:C:94:ASP:C	1:C:95:LEU:HD23	2.41	0.41
1:D:265:VAL:O	1:D:265:VAL:HG23	2.20	0.41
1:E:140:VAL:HG12	1:E:143:VAL:HB	2.02	0.41
1:E:232:PRO:HD3	1:E:362:TYR:CD1	2.56	0.41
1:E:357:THR:HG22	1:E:360:GLU:CD	2.40	0.41
1:G:29:SER:O	1:G:31:ASN:ND2	2.53	0.41
1:G:99:GLU:CD	1:G:115:LYS:HE3	2.42	0.41
1:E:295:VAL:HG23	1:E:326:ARG:HG2	2.03	0.41
1:G:173:ARG:NH1	1:G:236:GLN:HB3	2.36	0.41
1:G:312:VAL:HG23	1:G:320:ARG:CG	2.50	0.41
1:H:101:VAL:HB	1:H:113:ILE:HG22	2.03	0.41
1:B:112:GLY:O	1:B:124:SER:HA	2.21	0.40
1:E:228:THR:HG21	1:E:353:LEU:CD2	2.49	0.40
1:G:225:TYR:CD1	1:G:225:TYR:C	2.94	0.40
1:A:4:VAL:HG13	1:A:6:VAL:CG2	2.51	0.40
1:C:225:TYR:CD1	1:C:225:TYR:C	2.95	0.40
1:D:354:CYS:HA	1:D:362:TYR:O	2.21	0.40
1:H:222:GLU:HA	1:H:371:CYS:O	2.21	0.40
1:C:187:TYR:CD2	1:C:194:ALA:HB2	2.56	0.40
1:E:140:VAL:CG1	1:E:143:VAL:HB	2.51	0.40
1:F:28:GLY:HA2	1:F:159:LEU:O	2.20	0.40
1:G:358:ILE:HD12	1:G:359:GLY:N	2.36	0.40
1:H:17:GLU:OE1	1:H:42:LYS:HE2	2.21	0.40
1:H:101:VAL:HB	1:H:113:ILE:CG2	2.52	0.40
1:E:229:GLN:OE1	2:E:401:EOH:H22	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	373/384 (97%)	359 (96%)	14 (4%)	0	100	100
1	B	366/384 (95%)	355 (97%)	11 (3%)	0	100	100
1	C	371/384 (97%)	358 (96%)	12 (3%)	1 (0%)	41	37
1	D	365/384 (95%)	355 (97%)	10 (3%)	0	100	100
1	E	368/384 (96%)	354 (96%)	13 (4%)	1 (0%)	41	37
1	F	373/384 (97%)	360 (96%)	13 (4%)	0	100	100
1	G	372/384 (97%)	358 (96%)	14 (4%)	0	100	100
1	H	372/384 (97%)	360 (97%)	12 (3%)	0	100	100
All	All	2960/3072 (96%)	2859 (97%)	99 (3%)	2 (0%)	51	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	289	ASN
1	C	315	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	316/324 (98%)	312 (99%)	4 (1%)	69	74
1	B	311/324 (96%)	304 (98%)	7 (2%)	50	53
1	C	314/324 (97%)	307 (98%)	7 (2%)	52	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	311/324 (96%)	309 (99%)	2 (1%)	86	90
1	E	313/324 (97%)	308 (98%)	5 (2%)	62	67
1	F	316/324 (98%)	308 (98%)	8 (2%)	47	49
1	G	315/324 (97%)	310 (98%)	5 (2%)	62	67
1	H	315/324 (97%)	310 (98%)	5 (2%)	62	67
All	All	2511/2592 (97%)	2468 (98%)	43 (2%)	60	65

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	TRP
1	A	227	ARG
1	A	253	MET
1	A	290	SER
1	B	114	TRP
1	B	227	ARG
1	B	253	MET
1	B	272	ARG
1	B	288	ASP
1	B	317	GLU
1	B	319	GLN
1	C	114	TRP
1	C	227	ARG
1	C	239	ARG
1	C	248	ASP
1	C	253	MET
1	C	320	ARG
1	C	338	ARG
1	D	35	LYS
1	D	253	MET
1	E	24	SER
1	E	114	TRP
1	E	227	ARG
1	E	253	MET
1	E	320	ARG
1	F	83	VAL
1	F	114	TRP
1	F	119	SER
1	F	147	ASP
1	F	227	ARG

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Mol	Chain	Res	Type
1	F	253	MET
1	F	296	VAL
1	F	342	ASP
1	G	114	TRP
1	G	227	ARG
1	G	239	ARG
1	G	253	MET
1	G	320	ARG
1	H	12	ASP
1	H	114	TRP
1	H	239	ARG
1	H	253	MET
1	H	279	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	149	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)

10 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	EOH	H	402	-	2,2,2	0.48	0	1,1,1	0.38	0
2	EOH	D	401	-	2,2,2	0.52	0	1,1,1	0.29	0
2	EOH	D	402	-	2,2,2	0.50	0	1,1,1	0.38	0
2	EOH	H	401	-	2,2,2	0.48	0	1,1,1	0.33	0
4	1PE	H	404	-	15,15,15	0.51	0	14,14,14	0.37	0
2	EOH	E	401	-	2,2,2	0.50	0	1,1,1	0.32	0
2	EOH	B	401	-	2,2,2	0.50	0	1,1,1	0.45	0
2	EOH	D	403	-	2,2,2	0.53	0	1,1,1	0.22	0
2	EOH	H	403	-	2,2,2	0.50	0	1,1,1	0.36	0
3	PGE	F	401	-	9,9,9	0.33	0	8,8,8	0.25	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	1PE	H	404	-	-	5/13/13/13	-
3	PGE	F	401	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	401	PGE	O1-C1-C2-O2
4	H	404	1PE	OH4-C13-C23-OH3
3	F	401	PGE	O2-C3-C4-O3
4	H	404	1PE	OH6-C15-C25-OH5
3	F	401	PGE	O3-C5-C6-O4
4	H	404	1PE	OH5-C14-C24-OH4
4	H	404	1PE	C23-C13-OH4-C24
4	H	404	1PE	C15-C25-OH5-C14

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	402	EOH	2	0
4	H	404	1PE	1	0
2	E	401	EOH	3	0
2	D	403	EOH	2	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	374/384 (97%)	-0.12	8 (2%)	63	71	16, 26, 46, 67	0
1	B	370/384 (96%)	-0.06	8 (2%)	62	69	16, 25, 50, 62	0
1	C	373/384 (97%)	0.07	19 (5%)	28	36	16, 28, 54, 67	0
1	D	369/384 (96%)	0.07	10 (2%)	54	63	19, 31, 50, 77	0
1	E	372/384 (96%)	0.01	10 (2%)	54	63	21, 31, 52, 65	0
1	F	374/384 (97%)	-0.00	10 (2%)	54	63	18, 28, 49, 69	0
1	G	374/384 (97%)	0.08	10 (2%)	54	63	22, 35, 50, 70	0
1	H	374/384 (97%)	-0.09	7 (1%)	66	74	19, 27, 49, 60	0
All	All	2980/3072 (97%)	-0.01	82 (2%)	53	62	16, 29, 50, 77	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	374	SER	5.3
1	B	374	SER	5.0
1	F	19	HIS	4.8
1	C	19	HIS	4.8
1	A	244	ALA	4.5
1	G	21	LEU	4.5
1	B	216	TRP	4.3
1	D	317	GLU	4.3
1	E	276	LEU	4.2
1	H	189	SER	4.2
1	C	247	GLU	4.1
1	D	316	ASN	4.0
1	F	216	TRP	3.8
1	D	358	ILE	3.7
1	G	358	ILE	3.6
1	A	20	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	216	TRP	3.5
1	C	316	ASN	3.4
1	A	247	GLU	3.4
1	C	190	ASP	3.4
1	A	374	SER	3.3
1	D	19	HIS	3.3
1	C	189	SER	3.3
1	C	276	LEU	3.3
1	G	374	SER	3.3
1	D	216	TRP	3.2
1	E	247	GLU	3.2
1	F	117	ALA	3.2
1	D	245	GLY	3.1
1	B	276	LEU	3.1
1	G	71	GLY	3.1
1	E	190	ASP	3.1
1	E	275	ALA	3.1
1	H	245	GLY	3.0
1	H	216	TRP	3.0
1	E	288	ASP	2.9
1	F	244	ALA	2.9
1	D	11	VAL	2.9
1	A	19	HIS	2.9
1	E	272	ARG	2.9
1	C	193	ALA	2.8
1	A	341	PRO	2.7
1	F	72	LEU	2.7
1	C	18	GLU	2.7
1	F	73	LYS	2.7
1	B	73	LYS	2.7
1	B	118	THR	2.7
1	G	244	ALA	2.6
1	C	314	LYS	2.6
1	C	118	THR	2.6
1	E	1	MET	2.6
1	B	295	VAL	2.6
1	E	358	ILE	2.5
1	G	72	LEU	2.5
1	F	21	LEU	2.5
1	F	358	ILE	2.5
1	B	117	ALA	2.5
1	H	19	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	338	ARG	2.4
1	D	20	VAL	2.4
1	C	72	LEU	2.4
1	C	188	SER	2.3
1	H	374	SER	2.3
1	G	74	HIS	2.3
1	C	73	LYS	2.3
1	F	12	ASP	2.3
1	A	17	GLU	2.3
1	C	121	SER	2.3
1	C	291	ASP	2.2
1	G	118	THR	2.2
1	B	244	ALA	2.1
1	G	187	TYR	2.1
1	C	275	ALA	2.1
1	E	118	THR	2.1
1	E	19	HIS	2.1
1	A	216	TRP	2.1
1	H	275	ALA	2.1
1	H	190	ASP	2.1
1	C	194	ALA	2.1
1	C	317	GLU	2.0
1	D	18	GLU	2.0
1	C	342	ASP	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EOH	E	401	3/3	0.78	0.22	28,34,44,44	0
2	EOH	H	402	3/3	0.80	0.14	39,47,56,61	0
3	PGE	F	401	10/10	0.84	0.20	33,42,50,52	0
2	EOH	D	403	3/3	0.89	0.14	25,30,39,39	0
2	EOH	D	402	3/3	0.90	0.12	32,38,39,45	0
2	EOH	B	401	3/3	0.91	0.30	30,36,36,42	0
2	EOH	D	401	3/3	0.92	0.19	28,33,42,42	0
4	1PE	H	404	16/16	0.92	0.16	30,39,59,62	0
2	EOH	H	401	3/3	0.94	0.10	29,35,38,39	0
2	EOH	H	403	3/3	0.95	0.17	26,31,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.