Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:09 am BST

PDB ID	:	6BRS
Title	:	The Crystal Structure of the Ferredoxin Protease FusC in complex with Arabidopsis Ferredoxin, Ethylmercury phosphate soaked dataset
Authors	:	Grinter, R.
Deposited on	:	2017-11-30
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 ⓘ symbol.

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

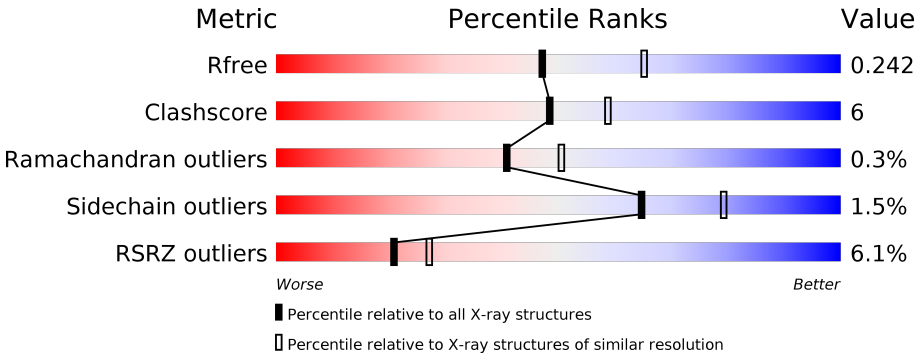
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 on 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	899	4% 85% 14%
2	C	104	3% 6% 93%
2	F	104	21% 26% 12% 61%
3	E	4	75% 25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7897 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 Putative zinc protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	896	Total	C	N	O	S	0	9	0
			7187	4513	1288	1364	22			

- Molecule 2 is a protein called Ferredoxin-2, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	41	Total	C	N	O	S	0	0	0
			315	200	43	71	1			
2	C	7	Total	C	N	O		0	0	0
			56	34	9	13				

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	95	ALA	-	expression tag	UNP P16972
F	96	ILE	-	expression tag	UNP P16972
F	97	MET	-	expression tag	UNP P16972
F	98	LEU	-	expression tag	UNP P16972
F	99	GLU	-	expression tag	UNP P16972
F	100	HIS	-	expression tag	UNP P16972
F	101	HIS	-	expression tag	UNP P16972
F	102	HIS	-	expression tag	UNP P16972
F	103	HIS	-	expression tag	UNP P16972
F	104	HIS	-	expression tag	UNP P16972
F	105	HIS	-	expression tag	UNP P16972
C	144	ALA	-	expression tag	UNP P16972
C	145	ILE	-	expression tag	UNP P16972
C	146	MET	-	expression tag	UNP P16972
C	147	LEU	-	expression tag	UNP P16972
C	148	GLU	-	expression tag	UNP P16972
C	149	HIS	-	expression tag	UNP P16972
C	150	HIS	-	expression tag	UNP P16972

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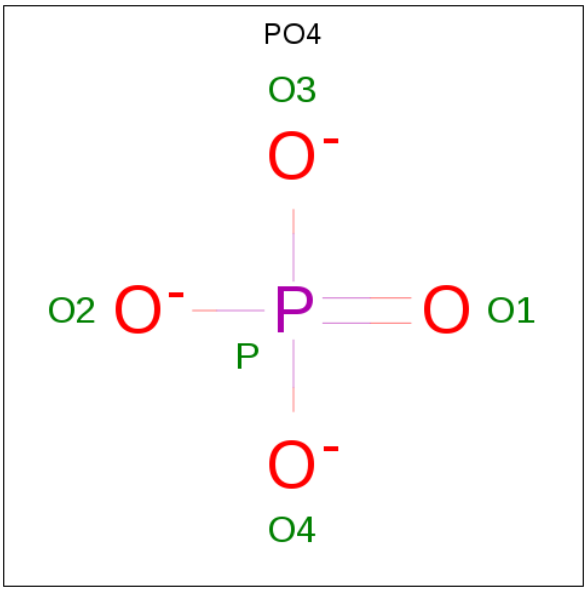
Chain	Residue	Modelled	Actual	Comment	Reference
C	151	HIS	-	expression tag	UNP P16972
C	152	HIS	-	expression tag	UNP P16972
C	153	HIS	-	expression tag	UNP P16972
C	154	HIS	-	expression tag	UNP P16972

- Molecule 3 is a protein called unidentified Ferredoxin peptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	4	Total C N O 20 12 4 4	0	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0

- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total Hg 5 5	0	0

- Molecule 6 is water.

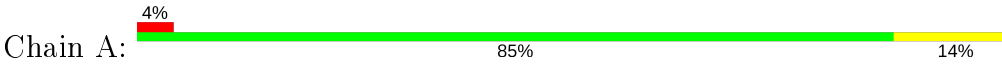
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	296	Total O 296 296	0	0
6	F	2	Total O 2 2	0	0
6	C	1	Total O 1 1	0	0

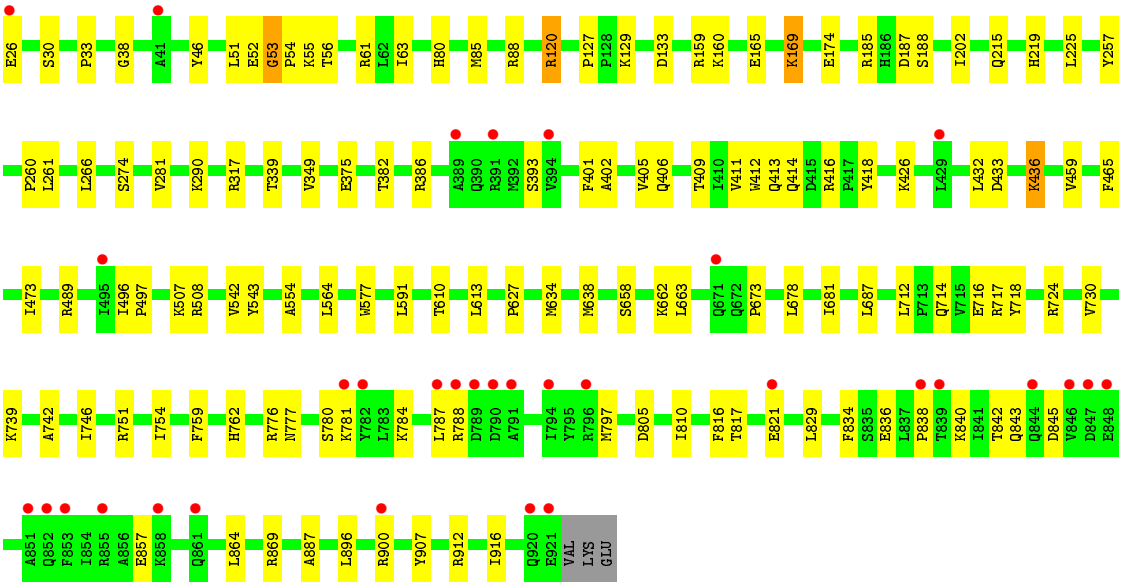
3 Residue-property plots (i)

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

- Molecule 1: Putative zinc protease

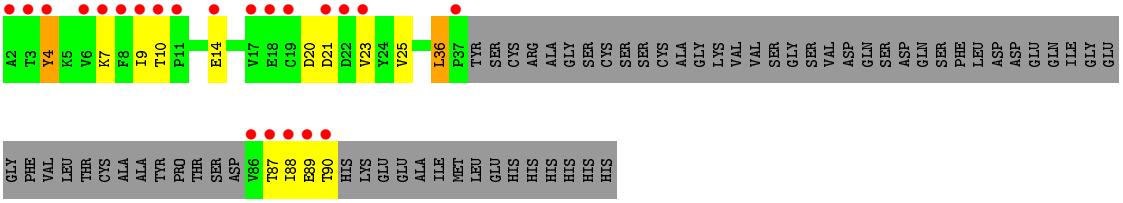
Chain A:





- Molecule 2: Ferredoxin-2, chloroplastic

Chain F:



- Molecule 2: Ferredoxin-2, chloroplastic

Chain C:

- Molecule 3: unidentified Ferredoxin peptide

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.53Å 127.37Å 132.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.65 – 2.30 41.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.65-2.30) 100.0 (41.64-2.30)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.189 , 0.242 0.189 , 0.242	Depositor DCC
R_{free} test set	3188 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7897	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: PO4, HG

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	0.44	0/7335	0.59	4/9946 (0.0%)
2	C	0.30	0/56	0.49	0/76
2	F	0.40	0/318	0.55	0/433
All	All	0.44	0/7709	0.59	4/10455 (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
2	F	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	317	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	724	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	591	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	317	ARG	NE-CZ-NH1	5.41	123.00	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	36	LEU	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	7187	0	7177	79	0
2	C	56	0	50	1	0
2	F	315	0	297	11	0
3	E	20	0	6	1	0
4	A	15	0	0	1	0
5	A	5	0	0	0	0
6	A	296	0	0	4	0
6	C	1	0	0	1	0
6	F	2	0	0	0	0
All	All	7897	0	7530	91	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 6.

All (91) 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:A:754:ILE:HD12	1:A:916:ILE:HG12	1.57	0.86
1:A:836:GLU:HB3	1:A:840:LYS:HE2	1.63	0.80
2:F:7:LYS:HZ2	2:F:87:THR:HG21	1.46	0.79
1:A:776:ARG:NH2	1:A:777:ASN:OD1	2.18	0.77
1:A:843:GLN:HB2	1:A:896:LEU:HD11	1.65	0.77
2:C:134:ASP:N	6:C:201:HOH:O	2.23	0.71
1:A:658:SER:O	1:A:662:LYS:HD3	1.93	0.68
1:A:185:ARG:NH1	4:A:1002:PO4:O1	2.27	0.67
1:A:187:ASP:OD2	6:A:1101:HOH:O	2.15	0.65
1:A:838:PRO:O	1:A:900:ARG:HD2	1.99	0.63
1:A:821:GLU:N	1:A:821:GLU:OE1	2.31	0.62
1:A:496:ILE:HD12	1:A:497:PRO:HD2	1.83	0.61
1:A:780:SER:O	1:A:784:LYS:HG3	2.00	0.61
1:A:375:GLU:OE2	6:A:1102:HOH:O	2.16	0.60
1:A:382:THR:HG23	1:A:432:LEU:HD22	1.82	0.60
2:F:7:LYS:HZ2	2:F:87:THR:CG2	2.14	0.59
1:A:507:LYS:HG3	1:A:508:ARG:O	2.03	0.59
1:A:907:TYR:HE1	1:A:912:ARG:HG3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HG2	1:A:56:THR:HG23	1.86	0.56
2:F:25:VAL:HG21	2:F:88:ILE:HD11	1.87	0.56
1:A:33:PRO:HB3	1:A:51:LEU:HD23	1.88	0.56
1:A:393:SER:HB2	1:A:426:LYS:HG2	1.89	0.55
1:A:673:PRO:HG2	1:A:678:LEU:HD13	1.89	0.55
1:A:414:GLN:NE2	1:A:416:ARG:NH1	2.55	0.54
1:A:564:LEU:HD21	1:A:638[B]:MET:SD	2.47	0.54
1:A:402:ALA:O	1:A:406:GLN:HG3	2.08	0.54
1:A:843:GLN:HB2	1:A:896:LEU:CD1	2.36	0.54
1:A:857:GLU:OE1	1:A:887:ALA:HB1	2.08	0.53
1:A:281:VAL:HG13	1:A:349:VAL:HG21	1.90	0.53
1:A:627:PRO:HG2	1:A:687:LEU:HD22	1.91	0.53
1:A:61:ARG:O	1:A:225:LEU:HD12	2.10	0.52
1:A:26:GLU:HA	1:A:54:PRO:HG3	1.92	0.52
1:A:762:HIS:NE2	6:A:1106:HOH:O	2.34	0.51
1:A:634:MET:O	1:A:638[B]:MET:HG2	2.11	0.50
1:A:38:GLY:HA3	1:A:46:TYR:CZ	2.46	0.50
1:A:759:PHE:HA	1:A:810:ILE:O	2.12	0.50
1:A:414:GLN:NE2	1:A:416:ARG:HH11	2.11	0.49
1:A:436:LYS:HG3	6:A:1261:HOH:O	2.11	0.49
1:A:842:THR:HG23	1:A:845:ASP:OD2	2.12	0.49
1:A:85:MET:HE2	1:A:88:ARG:HG3	1.95	0.48
2:F:20:ASP:HB2	2:F:23:VAL:HG23	1.95	0.48
1:A:784:LYS:HA	1:A:797:MET:HE3	1.95	0.47
1:A:290:LYS:HG2	1:A:339:THR:HA	1.97	0.47
1:A:712:LEU:HG	1:A:716:GLU:OE2	2.15	0.47
1:A:30:SER:HB3	1:A:53:GLY:H	1.79	0.46
1:A:751:ARG:HD2	1:A:817:THR:CG2	2.45	0.46
1:A:542[B]:VAL:HG23	1:A:610:THR:HG22	1.97	0.46
1:A:663:LEU:HD11	1:A:742:ALA:HB3	1.98	0.46
1:A:787:LEU:HD11	1:A:829:LEU:HB3	1.97	0.46
1:A:739:LYS:HE3	1:A:912:ARG:NH1	2.31	0.46
1:A:169:LYS:HG3	1:A:174:GLU:HG3	1.98	0.45
2:F:4:TYR:OH	2:F:21:ASP:OD2	2.33	0.45
1:A:215:GLN:O	1:A:219:HIS:NE2	2.50	0.45
1:A:266:LEU:HD11	1:A:473:ILE:HG22	1.99	0.45
1:A:386:ARG:NH2	1:A:433:ASP:OD1	2.50	0.45
2:F:7:LYS:HZ1	2:F:9:ILE:CG1	2.30	0.45
1:A:507:LYS:HA	1:A:716:GLU:OE1	2.17	0.45
1:A:784:LYS:HG2	1:A:797:MET:HE3	2.00	0.44
2:F:7:LYS:NZ	2:F:87:THR:CG2	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10:THR:HG22	2:F:90:THR:HG23	1.99	0.44
1:A:52:GLU:O	1:A:53:GLY:O	2.36	0.44
2:F:7:LYS:NZ	2:F:9:ILE:HG12	2.32	0.44
1:A:405:VAL:O	1:A:409:THR:HG23	2.18	0.44
1:A:717:ARG:HD2	1:A:718:TYR:CZ	2.53	0.44
1:A:781:LYS:HB3	1:A:781:LYS:HE2	1.70	0.44
1:A:26:GLU:CB	1:A:401:PHE:H	2.31	0.43
1:A:754:ILE:HB	1:A:816:PHE:HB2	2.00	0.43
1:A:129:LYS:HB2	1:A:133:ASP:OD2	2.18	0.43
1:A:717:ARG:HG3	1:A:717:ARG:HH11	1.83	0.43
1:A:784:LYS:HA	1:A:797:MET:CE	2.49	0.43
1:A:120[A]:ARG:NH1	1:A:413:GLN:NE2	2.67	0.43
1:A:46:TYR:HA	1:A:225:LEU:O	2.19	0.43
1:A:497:PRO:HB2	1:A:577:TRP:CE2	2.53	0.43
2:F:7:LYS:HE2	2:F:14:GLU:OE2	2.19	0.43
1:A:843:GLN:CB	1:A:896:LEU:HD11	2.42	0.42
1:A:63:ILE:HG13	1:A:412:TRP:CH2	2.54	0.42
1:A:554:ALA:HA	1:A:730:VAL:HG22	2.00	0.42
2:F:89:GLU:N	2:F:89:GLU:OE1	2.53	0.42
1:A:459:VAL:HG21	1:A:465:PHE:CD1	2.55	0.41
1:A:739:LYS:HA	1:A:912:ARG:O	2.20	0.41
1:A:842:THR:O	1:A:845:ASP:HB2	2.20	0.41
1:A:869:ARG:HD2	3:E:69:UNK:CB	2.50	0.41
1:A:613:LEU:HD23	1:A:714:GLN:HG3	2.02	0.41
1:A:127:PRO:HB2	1:A:133:ASP:HB2	2.02	0.41
1:A:681:ILE:HD12	1:A:681:ILE:HA	1.90	0.41
1:A:159:ARG:NH2	1:A:202:ILE:O	2.41	0.40
1:A:836:GLU:O	1:A:840:LYS:HG2	2.20	0.40
1:A:411:VAL:HG21	1:A:418:TYR:HB2	2.02	0.40
1:A:543:TYR:CE2	1:A:864:LEU:HD21	2.57	0.40
1:A:80:HIS:CE1	1:A:165:GLU:OE2	2.74	0.40
1:A:188:SER:HB3	1:A:260:PRO:HA	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	903/899 (100%)	887 (98%)	14 (2%)	2 (0%)	47 58
2	C	5/104 (5%)	5 (100%)	0	0	100 100
2	F	37/104 (36%)	36 (97%)	0	1 (3%)	5 3
All	All	945/1107 (85%)	928 (98%)	14 (2%)	3 (0%)	41 50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	36	LEU
1	A	53	GLY
1	A	746	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	774/769 (101%)	762 (98%)	12 (2%)	62 78
2	C	7/88 (8%)	7 (100%)	0	100 100
2	F	35/88 (40%)	34 (97%)	1 (3%)	42 58
All	All	816/945 (86%)	803 (98%)	13 (2%)	65 78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120[A]	ARG
1	A	120[B]	ARG
1	A	160	LYS
1	A	169	LYS
1	A	257	TYR
1	A	261	LEU

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Mol	Chain	Res	Type
1	A	274	SER
1	A	436	LYS
1	A	489	ARG
1	A	788	ARG
1	A	805	ASP
1	A	834	PHE
2	F	4	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	GLN
1	A	521	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PO4	A	1003	-	4,4,4	0.85	0	6,6,6	0.64	0
4	PO4	A	1002	-	4,4,4	0.78	0	6,6,6	0.72	0
4	PO4	A	1001	-	4,4,4	0.85	0	6,6,6	0.52	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	896/899 (99%)	0.21	33 (3%) 41 48	27, 47, 85, 112	0
2	C	7/104 (6%)	2.64	3 (42%) 0 0	62, 78, 107, 121	0
2	F	41/104 (39%)	2.77	22 (53%) 0 0	46, 122, 154, 158	0
3	E	0/4	-	-	-	-
All	All	944/1111 (84%)	0.34	58 (6%) 21 27	27, 48, 93, 158	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	2	ALA	10.8
2	F	4	TYR	6.8
2	F	89	GLU	6.2
2	F	9	ILE	6.2
2	F	90	THR	6.1
2	F	3	THR	6.0
2	C	139	THR	5.7
2	F	87	THR	5.6
2	F	8	PHE	5.5
2	F	88	ILE	5.5
2	F	22	ASP	5.3
2	C	140	HIS	5.3
2	F	86	VAL	5.2
2	F	10	THR	5.1
2	F	7	LYS	4.9
1	A	855	ARG	4.6
1	A	790	ASP	4.5
1	A	791	ALA	4.3
1	A	41	ALA	3.9
1	A	851	ALA	3.8
2	F	23	VAL	3.6
2	F	19	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	F	18	GLU	3.4
2	F	17	VAL	3.4
1	A	853	PHE	3.2
1	A	794	ILE	3.1
1	A	789	ASP	2.9
1	A	782	TYR	2.9
2	F	21	ASP	2.9
1	A	838	PRO	2.8
1	A	495	ILE	2.8
1	A	26	GLU	2.7
1	A	839	THR	2.7
1	A	781	LYS	2.6
1	A	788	ARG	2.6
1	A	671	GLN	2.6
2	F	6	VAL	2.6
1	A	821	GLU	2.6
1	A	847	ASP	2.5
2	F	14	GLU	2.5
1	A	394	VAL	2.4
1	A	848	GLU	2.4
1	A	846	VAL	2.4
1	A	861	GLN	2.4
1	A	858	LYS	2.3
1	A	796	ARG	2.3
1	A	921	GLU	2.3
1	A	389	ALA	2.3
1	A	852	GLN	2.3
1	A	900	ARG	2.3
2	F	37	PRO	2.2
1	A	920	GLN	2.2
1	A	391	ARG	2.2
1	A	429	LEU	2.1
1	A	844	GLN	2.1
2	C	138	GLU	2.1
2	F	11	PRO	2.1
1	A	787	LEU	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	PO4	A	1003	5/5	0.78	0.27	112,114,120,121	0
4	PO4	A	1002	5/5	0.80	0.33	112,118,121,130	0
4	PO4	A	1001	5/5	0.82	0.30	81,84,95,114	0
5	HG	A	1008	1/1	0.87	0.17	70,70,70,70	1
5	HG	A	1007	1/1	0.89	0.13	72,72,72,72	1
5	HG	A	1004	1/1	0.93	0.10	75,75,75,75	1
5	HG	A	1006	1/1	0.94	0.08	56,56,56,56	1
5	HG	A	1005	1/1	0.99	0.15	66,66,66,66	1

6.5 Other polymers (i)

There are no such residues in this entry.