



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 06:46 PM BST

PDB ID : 4C3O
Title : Structure and function of an oxygen tolerant NiFe hydrogenase from Salmonella
Authors : Bowman, L.; Flanagan, L.; Fyfe, P.K.; Parkin, A.; Hunter, W.N.; Sargent, F.
Deposited on : 2013-08-26
Resolution : 3.20 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 ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

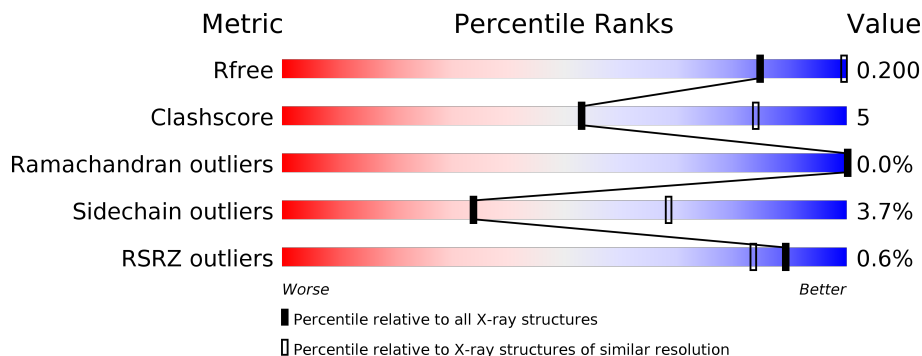
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 $\leq 5\%$. 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	585	 % 84% 15% •
1	C	585	 83% 15% •
1	E	585	 % 85% 13% •
2	B	279	 85% 8% • 6%
2	D	279	 % 81% 13% 6%
2	F	279	 82% 12% 6%

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 20051 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 HYDROGENASE-1 LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	583	4579	2917	802	840	20	0	0	0
1	C	583	4579	2917	802	840	20	0	0	0
1	E	583	4572	2911	802	839	20	0	0	0

- Molecule 2 is a protein called HYDROGENASE-1 SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	263	2037	1296	351	370	20	0	0	0
2	D	262	2028	1290	349	369	20	0	0	0
2	F	263	2033	1293	350	370	20	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

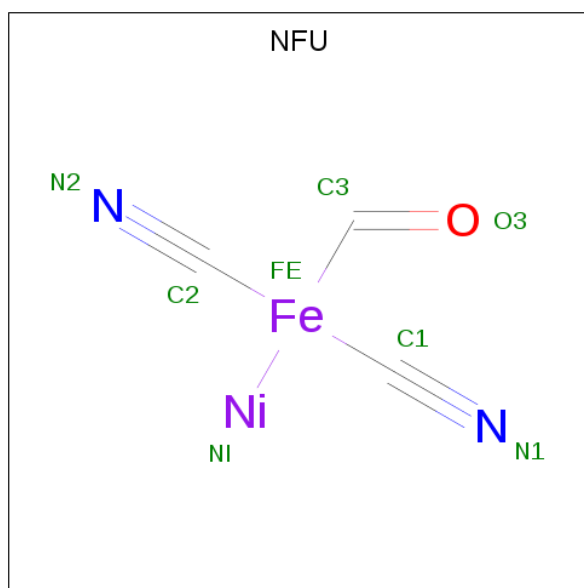
Chain	Residue	Modelled	Actual	Comment	Reference
B	270	SER	-	expression tag	UNP Q8ZPG9
B	271	ARG	-	expression tag	UNP Q8ZPG9
B	272	SER	-	expression tag	UNP Q8ZPG9
B	273	HIS	-	expression tag	UNP Q8ZPG9
B	274	HIS	-	expression tag	UNP Q8ZPG9
B	275	HIS	-	expression tag	UNP Q8ZPG9
B	276	HIS	-	expression tag	UNP Q8ZPG9
B	277	HIS	-	expression tag	UNP Q8ZPG9
B	278	HIS	-	expression tag	UNP Q8ZPG9
B	279	HIS	-	expression tag	UNP Q8ZPG9
D	270	SER	-	expression tag	UNP Q8ZPG9
D	271	ARG	-	expression tag	UNP Q8ZPG9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	272	SER	-	expression tag	UNP Q8ZPG9
D	273	HIS	-	expression tag	UNP Q8ZPG9
D	274	HIS	-	expression tag	UNP Q8ZPG9
D	275	HIS	-	expression tag	UNP Q8ZPG9
D	276	HIS	-	expression tag	UNP Q8ZPG9
D	277	HIS	-	expression tag	UNP Q8ZPG9
D	278	HIS	-	expression tag	UNP Q8ZPG9
D	279	HIS	-	expression tag	UNP Q8ZPG9
F	270	SER	-	expression tag	UNP Q8ZPG9
F	271	ARG	-	expression tag	UNP Q8ZPG9
F	272	SER	-	expression tag	UNP Q8ZPG9
F	273	HIS	-	expression tag	UNP Q8ZPG9
F	274	HIS	-	expression tag	UNP Q8ZPG9
F	275	HIS	-	expression tag	UNP Q8ZPG9
F	276	HIS	-	expression tag	UNP Q8ZPG9
F	277	HIS	-	expression tag	UNP Q8ZPG9
F	278	HIS	-	expression tag	UNP Q8ZPG9
F	279	HIS	-	expression tag	UNP Q8ZPG9

- Molecule 3 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (three-letter code: NFU) (formula: C₃HFeN₂NiO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Fe	N	Ni			O
3	A	1	8	3	1	2	1	1	0	0
3	C	1	8	3	1	2	1	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	E	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		

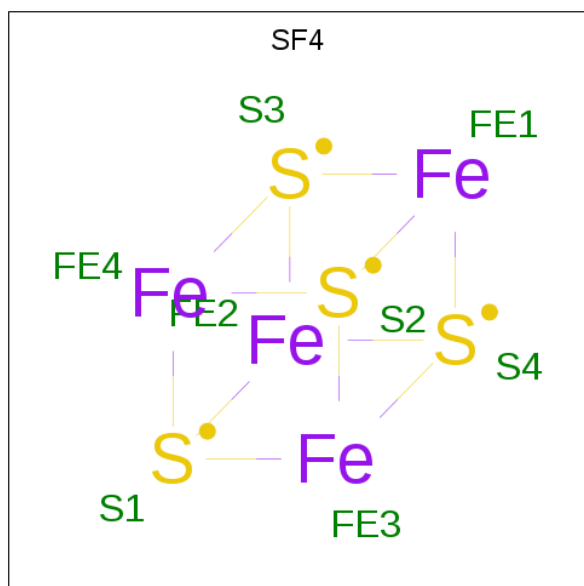
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Cl	0	0
			4	4		
4	E	2	Total	Cl	0	0
			2	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



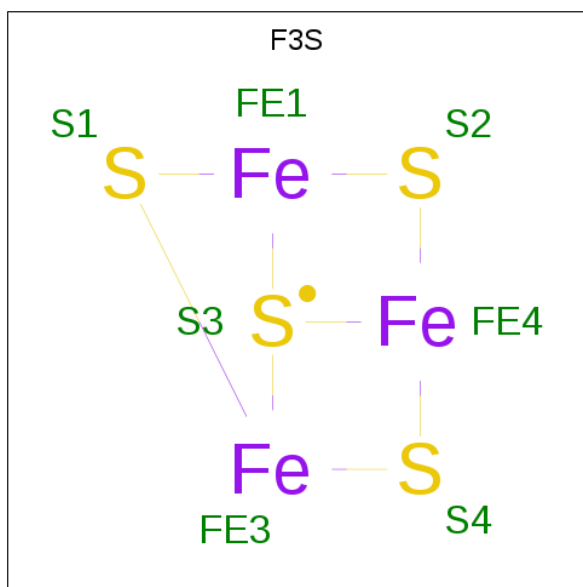
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
6	B	1	Total	Fe	S	0	0
			8	4	4		

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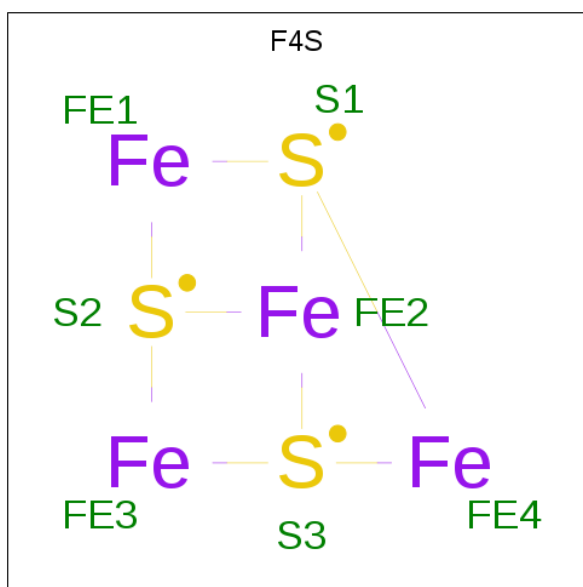
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	Fe	S	0	0
			8	4	4		
6	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



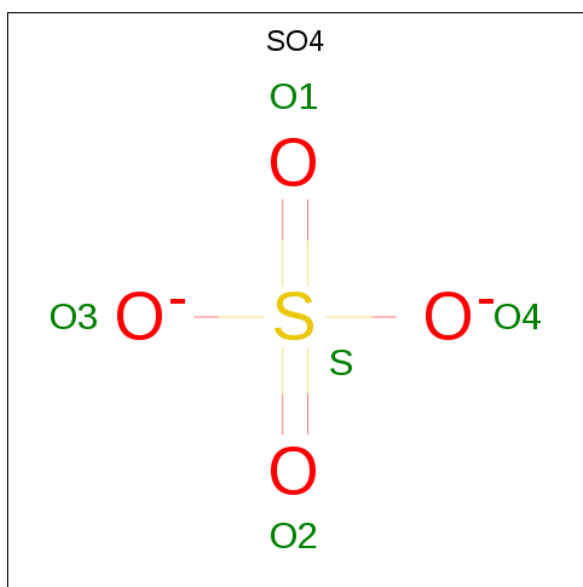
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			7	3	4		
7	D	1	Total	Fe	S	0	0
			7	3	4		
7	F	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 8 is FE4-S3 CLUSTER (three-letter code: F4S) (formula: Fe₄S₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	4	3		
8	D	1	Total	Fe	S	0	0
			7	4	3		
8	F	1	Total	Fe	S	0	0
			7	4	3		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	O	S	0	0
			5	4	1		

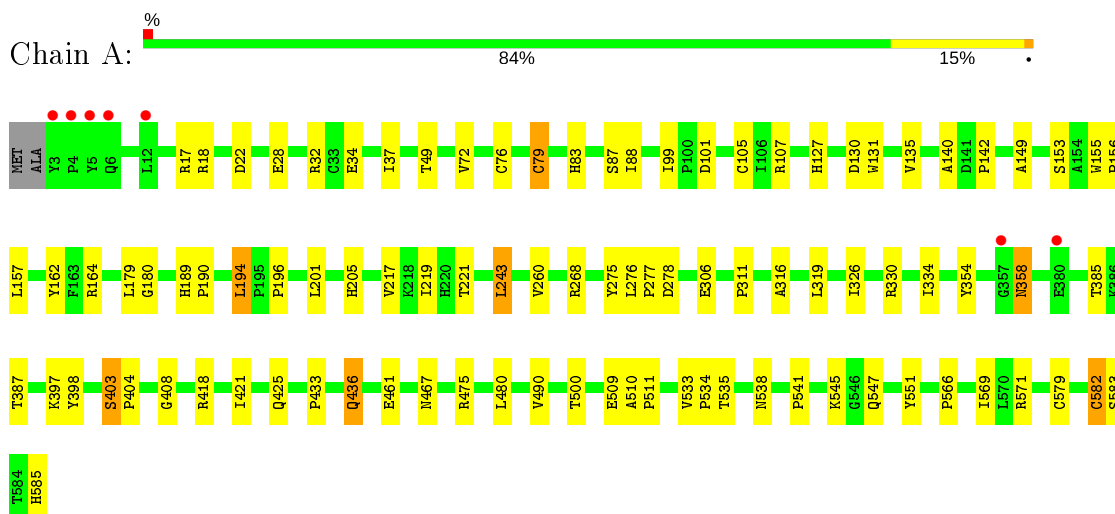
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	32	Total	O	0	0
			32	32		
10	B	10	Total	O	0	0
			10	10		
10	C	26	Total	O	0	0
			26	26		
10	D	9	Total	O	0	0
			9	9		
10	E	25	Total	O	0	0
			25	25		
10	F	12	Total	O	0	0
			12	12		

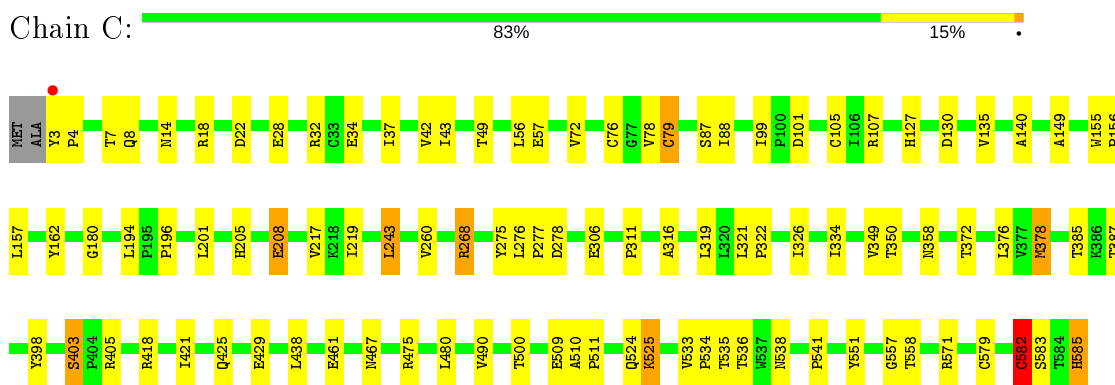
3 Residue-property plots [i](#)

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.

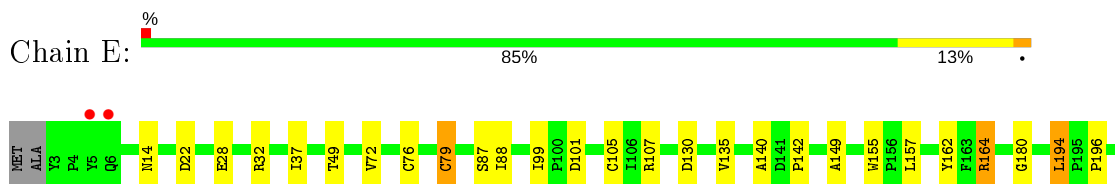
- Molecule 1: HYDROGENASE-1 LARGE SUBUNIT

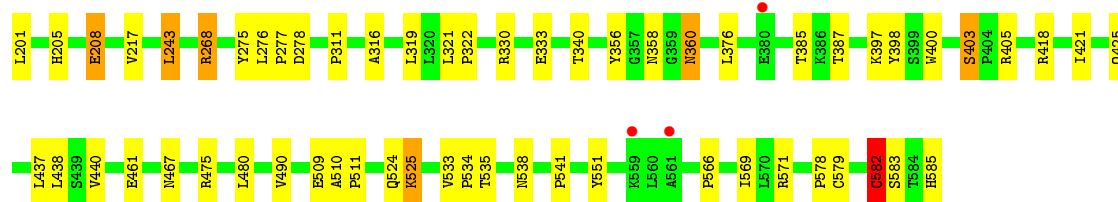


- Molecule 1: HYDROGENASE-1 LARGE SUBUNIT



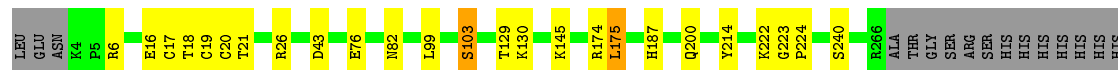
- Molecule 1: HYDROGENASE-1 LARGE SUBUNIT





● Molecule 2: HYDROGENASE-1 SMALL SUBUNIT

Chain B: 85% 8% 6%



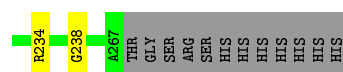
● Molecule 2: HYDROGENASE-1 SMALL SUBUNIT

Chain D: 81% 13% 6%



● Molecule 2: HYDROGENASE-1 SMALL SUBUNIT

Chain F: 82% 12% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.46Å 122.21Å 227.82Å 90.00° 95.56° 90.00°	Depositor
Resolution (Å)	29.52 – 3.20 29.50 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.52-3.20) 99.6 (29.50-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.18Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.158 , 0.205 0.160 , 0.200	Depositor DCC
R_{free} test set	2643 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	83.4	Xtrriage
Anisotropy	0.317	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20051	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: F4S, CL, SF4, MG, NFU, F3S, SO4

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	0.54	1/4706 (0.0%)	0.75	1/6413 (0.0%)
1	C	0.54	1/4706 (0.0%)	0.76	5/6413 (0.1%)
1	E	0.54	1/4698 (0.0%)	0.75	4/6402 (0.1%)
2	B	0.59	0/2093	0.75	1/2840 (0.0%)
2	D	0.57	0/2084	0.75	2/2828 (0.1%)
2	F	0.58	0/2089	0.74	1/2835 (0.0%)
All	All	0.55	3/20376 (0.0%)	0.75	14/27731 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	79	CYS	CA-CB	6.17	1.67	1.53
1	A	79	CYS	CA-CB	5.71	1.66	1.53
1	E	79	CYS	CA-CB	5.45	1.66	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	582	CYS	CB-CA-C	6.92	124.23	110.40
1	A	582	CYS	CB-CA-C	6.81	124.02	110.40
2	B	6	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	582	CYS	CB-CA-C	6.43	123.27	110.40
2	D	6	ARG	NE-CZ-NH1	6.15	123.37	120.30
2	F	6	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	C	268	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	405	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	405	ARG	NE-CZ-NH2	-5.37	117.61	120.30
2	D	174	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	E	268	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	405	ARG	NE-CZ-NH1	5.26	122.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	268	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	378	MET	N-CA-C	5.13	124.86	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4579	0	4471	68	1
1	C	4579	0	4471	55	1
1	E	4572	0	4464	46	0
2	B	2037	0	1980	17	0
2	D	2028	0	1968	22	0
2	F	2033	0	1973	21	0
3	A	8	0	0	1	0
3	C	8	0	0	0	0
3	E	8	0	0	0	0
4	A	4	0	0	0	0
4	E	2	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
6	B	8	0	0	0	0
6	D	8	0	0	1	0
6	F	8	0	0	1	0
7	B	7	0	0	0	0
7	D	7	0	0	0	0
7	F	7	0	0	0	0
8	B	7	0	0	0	0
8	D	7	0	0	0	0
8	F	7	0	0	0	0
9	B	5	0	0	0	0
9	F	5	0	0	0	0
10	A	32	0	0	3	0
10	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	26	0	0	3	0
10	D	9	0	0	3	0
10	E	25	0	0	1	0
10	F	12	0	0	4	0
All	All	20051	0	19327	213	1

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 5.

All (213) 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:579:CYS:SG	1:C:582:CYS:HB2	2.13	0.87
1:E:579:CYS:SG	1:E:582:CYS:HB2	2.14	0.87
1:C:418:ARG:NH2	1:C:510:ALA:O	2.18	0.77
10:A:2002:HOH:O	2:B:129:THR:HG22	1.85	0.76
1:E:418:ARG:NH2	1:E:510:ALA:O	2.18	0.76
1:C:162:TYR:OH	1:C:208:GLU:OE1	2.04	0.75
1:A:418:ARG:NH2	1:A:510:ALA:O	2.19	0.75
1:E:162:TYR:OH	1:E:208:GLU:OE1	2.06	0.73
1:A:131:TRP:O	1:A:194:LEU:HD21	1.89	0.73
1:A:533:VAL:HG12	1:A:534:PRO:HD2	1.73	0.69
1:A:76:CYS:HB3	1:A:79:CYS:SG	2.34	0.67
2:B:174:ARG:HG3	2:B:175:LEU:HD13	1.76	0.67
1:E:76:CYS:HB3	1:E:79:CYS:SG	2.35	0.67
1:C:7:THR:HB	1:C:8:GLN:HG3	1.77	0.66
2:D:204:ALA:HB2	10:D:2008:HOH:O	1.94	0.66
1:C:76:CYS:HB3	1:C:79:CYS:SG	2.35	0.65
1:C:524:GLN:O	1:C:525:LYS:HE3	1.98	0.63
2:D:18:THR:O	2:D:18:THR:HG22	1.99	0.63
1:E:356:TYR:O	1:E:360:ASN:ND2	2.32	0.63
1:E:524:GLN:O	1:E:525:LYS:HE3	1.99	0.63
2:B:18:THR:HG22	2:B:18:THR:O	2.00	0.62
2:F:18:THR:HG22	2:F:18:THR:O	1.98	0.62
2:D:204:ALA:CB	10:D:2008:HOH:O	2.49	0.61
1:A:490:VAL:HG12	1:A:490:VAL:O	2.00	0.61
1:A:76:CYS:HA	2:B:17:CYS:HB2	1.82	0.60
10:C:2011:HOH:O	2:D:49:MET:HE3	2.02	0.60
1:E:105:CYS:SG	1:E:475:ARG:HD3	2.44	0.58
2:B:223:GLY:N	2:B:224:PRO:HD2	2.18	0.58
1:C:105:CYS:SG	1:C:475:ARG:HD3	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PRO:HG2	1:A:164:ARG:HG3	1.84	0.57
1:A:49:THR:HG23	1:A:398:TYR:O	2.04	0.57
1:A:131:TRP:O	1:A:194:LEU:CD2	2.53	0.57
1:E:49:THR:HG23	1:E:398:TYR:O	2.05	0.56
1:C:536:THR:HG21	10:C:2019:HOH:O	2.05	0.56
1:C:49:THR:HG23	1:C:398:TYR:O	2.05	0.56
1:E:76:CYS:HA	2:F:17:CYS:HB2	1.87	0.56
1:E:142:PRO:HG2	1:E:164:ARG:HG3	1.89	0.55
1:A:162:TYR:HB2	1:C:156:PRO:HB3	1.88	0.55
2:F:17:CYS:SG	2:F:19:CYS:HB3	2.46	0.55
2:B:17:CYS:SG	2:B:19:CYS:HB3	2.47	0.55
1:A:105:CYS:SG	1:A:475:ARG:HD3	2.47	0.55
1:C:418:ARG:NH1	1:C:461:GLU:OE1	2.40	0.54
1:A:418:ARG:NH1	1:A:461:GLU:OE1	2.41	0.54
1:C:76:CYS:HA	2:D:17:CYS:HB2	1.88	0.54
1:A:500:THR:HG22	10:A:2034:HOH:O	2.08	0.54
1:E:194:LEU:H	1:E:194:LEU:HD23	1.71	0.54
1:C:217:VAL:HG21	2:D:26:ARG:HD2	1.90	0.53
2:F:12:LEU:HA	10:F:2001:HOH:O	2.08	0.53
1:A:533:VAL:CG1	1:A:534:PRO:HD2	2.38	0.53
1:A:149:ALA:HB2	1:A:201:LEU:HD13	1.91	0.53
1:A:205:HIS:ND1	1:A:278:ASP:OD2	2.38	0.53
1:A:18:ARG:NH1	1:A:34:GLU:OE1	2.41	0.53
1:A:358:ASN:ND2	1:A:358:ASN:H	2.06	0.53
2:B:174:ARG:HG3	2:B:175:LEU:CD1	2.39	0.53
1:C:149:ALA:HB2	1:C:201:LEU:HD13	1.91	0.53
2:D:223:GLY:N	2:D:224:PRO:HD2	2.24	0.53
1:E:421:ILE:O	1:E:425:GLN:HG3	2.09	0.53
1:A:421:ILE:O	1:A:425:GLN:HG3	2.10	0.52
1:C:538:ASN:HB3	1:C:551:TYR:CE1	2.45	0.52
1:E:418:ARG:NH1	1:E:461:GLU:OE1	2.42	0.52
2:D:115:CYS:HB2	10:D:2002:HOH:O	2.10	0.52
2:D:234:ARG:NH1	2:D:238:GLY:O	2.42	0.52
1:C:78:VAL:HG12	2:D:22:GLU:CG	2.39	0.52
1:A:433:PRO:HA	1:A:436:GLN:HG2	1.91	0.52
1:A:76:CYS:CB	1:A:79:CYS:SG	2.96	0.52
1:C:76:CYS:CB	1:C:79:CYS:SG	2.97	0.52
1:E:538:ASN:HB3	1:E:551:TYR:CE1	2.45	0.52
2:F:187:HIS:HB3	2:F:224:PRO:HA	1.91	0.52
1:A:538:ASN:HB3	1:A:551:TYR:CE1	2.45	0.51
1:C:18:ARG:NH1	1:C:34:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:TRP:CZ2	1:C:157:LEU:HD12	2.45	0.51
1:C:88:ILE:HD12	1:C:107:ARG:CZ	2.40	0.51
1:A:243:LEU:HD11	1:A:480:LEU:HD13	1.91	0.51
1:E:155:TRP:CZ2	1:E:157:LEU:HD12	2.45	0.51
2:B:223:GLY:N	2:B:224:PRO:CD	2.73	0.51
2:D:17:CYS:SG	2:D:19:CYS:HB3	2.51	0.51
1:E:268:ARG:NH2	1:E:467:ASN:OD1	2.44	0.51
2:F:223:GLY:N	2:F:224:PRO:HD2	2.26	0.51
1:E:243:LEU:HD11	1:E:480:LEU:HD13	1.92	0.50
1:A:194:LEU:HD23	1:A:194:LEU:H	1.77	0.50
1:E:149:ALA:HB2	1:E:201:LEU:HD13	1.92	0.50
1:A:88:ILE:HD12	1:A:107:ARG:CZ	2.41	0.50
1:A:142:PRO:HG2	1:A:164:ARG:CG	2.41	0.50
1:C:140:ALA:HB2	1:C:196:PRO:O	2.12	0.50
1:A:155:TRP:CZ2	1:A:157:LEU:HD12	2.45	0.50
1:C:42:VAL:HG12	1:C:557:GLY:HA2	1.94	0.50
1:C:243:LEU:HD11	1:C:480:LEU:HD13	1.94	0.50
1:E:88:ILE:HD12	1:E:107:ARG:CZ	2.42	0.50
2:F:234:ARG:NH1	2:F:238:GLY:O	2.45	0.50
1:A:408:GLY:O	1:A:547:GLN:NE2	2.44	0.50
1:C:421:ILE:O	1:C:425:GLN:HG3	2.11	0.50
1:E:76:CYS:CB	1:E:79:CYS:SG	2.96	0.49
1:E:330:ARG:NH2	1:E:333:GLU:OE2	2.45	0.49
2:F:82:ASN:ND2	2:F:130:LYS:HB2	2.26	0.49
1:E:180:GLY:HA2	2:F:43:ASP:HA	1.93	0.49
1:A:140:ALA:HB2	1:A:196:PRO:O	2.13	0.49
1:A:268:ARG:NH2	1:A:467:ASN:OD1	2.45	0.49
1:C:321:LEU:HD12	1:C:322:PRO:HD3	1.95	0.49
1:A:545:LYS:HB2	1:A:547:GLN:HG2	1.94	0.49
1:A:156:PRO:HB2	1:C:157:LEU:HD23	1.94	0.49
1:C:130:ASP:HB3	1:C:571:ARG:HG3	1.94	0.49
1:E:140:ALA:HB2	1:E:196:PRO:O	2.13	0.48
1:A:354:TYR:O	1:A:397:LYS:NZ	2.46	0.48
1:E:321:LEU:HD12	1:E:322:PRO:HD3	1.96	0.48
1:E:130:ASP:HB3	1:E:571:ARG:HG3	1.95	0.48
1:E:418:ARG:HE	1:E:509:GLU:HG3	1.79	0.48
1:A:180:GLY:HA2	2:B:43:ASP:HA	1.96	0.48
1:C:43:ILE:HD12	1:C:558:THR:OG1	2.13	0.48
1:A:142:PRO:CG	1:A:164:ARG:HG3	2.44	0.47
1:C:205:HIS:ND1	1:C:278:ASP:OD2	2.38	0.47
1:A:130:ASP:HB3	1:A:571:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ARG:NH2	1:C:467:ASN:OD1	2.47	0.47
1:A:17:ARG:HG2	1:A:18:ARG:N	2.29	0.47
2:D:187:HIS:HB3	2:D:224:PRO:HA	1.96	0.47
1:A:316:ALA:HA	1:A:319:LEU:HD12	1.97	0.47
1:C:99:ILE:O	1:C:99:ILE:HG13	2.15	0.47
2:B:99:LEU:O	2:B:103:SER:OG	2.32	0.47
1:A:566:PRO:HB2	1:A:569:ILE:HD12	1.97	0.47
1:C:316:ALA:HA	1:C:319:LEU:HD12	1.96	0.46
1:A:326:ILE:HD11	1:A:334:ILE:HG22	1.96	0.46
1:A:418:ARG:HE	1:A:509:GLU:HG3	1.80	0.46
1:A:156:PRO:HB3	1:C:162:TYR:HB2	1.96	0.46
1:E:578:PRO:HD2	10:E:2026:HOH:O	2.14	0.46
1:A:179:LEU:CD1	1:A:179:LEU:N	2.78	0.46
2:B:82:ASN:ND2	2:B:130:LYS:HB2	2.30	0.46
1:C:585:HIS:O	10:C:2001:HOH:O	2.21	0.46
1:A:510:ALA:HB1	1:A:511:PRO:HD2	1.97	0.46
1:A:28:GLU:HB3	1:A:579:CYS:HA	1.98	0.46
2:D:99:LEU:O	2:D:103:SER:OG	2.33	0.46
2:F:115:CYS:HB2	10:F:2003:HOH:O	2.14	0.46
1:C:101:ASP:HA	1:C:311:PRO:HG3	1.98	0.46
1:A:179:LEU:HD12	1:A:179:LEU:N	2.30	0.46
1:C:510:ALA:HB1	1:C:511:PRO:HD2	1.98	0.45
1:C:533:VAL:HG23	1:C:534:PRO:HD2	1.98	0.45
1:A:358:ASN:ND2	1:A:358:ASN:N	2.64	0.45
2:B:222:LYS:C	2:B:224:PRO:HD2	2.36	0.45
1:E:533:VAL:HG23	1:E:534:PRO:HD2	1.98	0.45
1:E:101:ASP:HA	1:E:311:PRO:HG3	1.98	0.45
1:A:276:LEU:HB3	1:A:277:PRO:HD3	1.99	0.45
1:C:403:SER:OG	1:C:541:PRO:HG2	2.16	0.45
1:E:566:PRO:HB2	1:E:569:ILE:HD12	1.99	0.45
1:E:400:TRP:CH2	2:F:87:PHE:CE1	3.04	0.45
1:A:533:VAL:HG12	1:A:534:PRO:CD	2.43	0.45
1:C:418:ARG:HE	1:C:509:GLU:HG3	1.81	0.45
1:E:510:ALA:HB1	1:E:511:PRO:HD2	1.99	0.45
2:D:223:GLY:N	2:D:224:PRO:CD	2.80	0.45
1:E:99:ILE:HG13	1:E:99:ILE:O	2.17	0.45
1:A:101:ASP:HA	1:A:311:PRO:HG3	1.98	0.45
1:A:72:VAL:HG21	1:A:87:SER:HB2	1.99	0.45
1:A:157:LEU:HD23	1:C:156:PRO:HB2	1.98	0.45
1:A:533:VAL:CG1	1:A:534:PRO:CD	2.95	0.44
1:E:316:ALA:HA	1:E:319:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:ASN:ND2	2:D:130:LYS:HB2	2.33	0.44
1:C:28:GLU:HB3	1:C:579:CYS:HA	1.99	0.44
1:E:535:THR:HG22	1:E:583:SER:HB3	2.00	0.44
1:A:217:VAL:HG21	2:B:26:ARG:HD2	1.99	0.44
2:B:187:HIS:HB3	2:B:224:PRO:HA	2.00	0.44
2:D:193:ARG:HA	6:D:1001:SF4:S3	2.58	0.43
1:E:28:GLU:HB3	1:E:579:CYS:HA	2.00	0.43
1:C:535:THR:HG22	1:C:583:SER:HB3	2.00	0.43
1:C:72:VAL:HG21	1:C:87:SER:HB2	1.98	0.43
1:A:403:SER:OG	1:A:541:PRO:HG2	2.17	0.43
2:F:99:LEU:O	2:F:103:SER:OG	2.34	0.43
1:A:535:THR:HG22	1:A:583:SER:HB3	2.00	0.43
1:C:276:LEU:HB3	1:C:277:PRO:HD3	1.99	0.43
1:C:57:GLU:OE1	1:C:372:THR:OG1	2.21	0.43
1:E:72:VAL:HG21	1:E:87:SER:HB2	2.00	0.43
1:E:276:LEU:HB3	1:E:277:PRO:HD3	2.00	0.43
2:B:200:GLN:HB3	2:B:214:TYR:CE2	2.53	0.43
1:C:180:GLY:HA2	2:D:43:ASP:HA	2.00	0.43
1:A:83:HIS:HB2	10:A:2006:HOH:O	2.19	0.42
1:E:437:LEU:O	1:E:440:VAL:HG12	2.19	0.42
1:A:221:THR:HG22	2:B:240:SER:HB3	2.00	0.42
1:A:511:PRO:HD2	3:A:1004:NFU:N1	2.34	0.42
1:C:88:ILE:HD12	1:C:107:ARG:NH2	2.35	0.42
2:F:82:ASN:CG	2:F:130:LYS:HB2	2.39	0.42
1:A:22:ASP:HB2	1:A:32:ARG:HG3	2.01	0.42
1:C:349:VAL:O	1:C:350:THR:C	2.57	0.42
1:E:217:VAL:HG21	2:F:26:ARG:HD2	2.01	0.42
2:D:200:GLN:HB3	2:D:214:TYR:CE2	2.55	0.42
1:A:194:LEU:N	1:A:194:LEU:HD23	2.35	0.42
1:E:418:ARG:HE	1:E:509:GLU:CG	2.33	0.42
1:A:99:ILE:O	1:A:99:ILE:HG13	2.18	0.41
1:E:22:ASP:HB2	1:E:32:ARG:HG3	2.03	0.41
2:F:191:TYR:HB3	10:F:2007:HOH:O	2.20	0.41
1:A:189:HIS:CG	1:A:190:PRO:HD2	2.55	0.41
1:A:219:ILE:HG12	1:A:260:VAL:HG13	2.02	0.41
2:B:82:ASN:CG	2:B:130:LYS:HB2	2.41	0.41
2:F:193:ARG:HA	6:F:1001:SF4:S3	2.60	0.41
1:C:306:GLU:HB2	1:C:509:GLU:CB	2.50	0.41
1:E:360:ASN:N	1:E:360:ASN:OD1	2.53	0.41
2:F:223:GLY:N	2:F:224:PRO:CD	2.83	0.41
1:C:219:ILE:HG12	1:C:260:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:202:VAL:HG22	2:D:210:ALA:N	2.35	0.41
1:E:397:LYS:HE2	1:E:397:LYS:HB2	1.89	0.41
1:C:22:ASP:HB2	1:C:32:ARG:HG3	2.02	0.41
1:C:28:GLU:HB3	1:C:579:CYS:SG	2.61	0.41
2:F:200:GLN:HB3	2:F:214:TYR:CE2	2.56	0.41
1:C:326:ILE:HD11	1:C:334:ILE:HG12	2.03	0.41
1:C:378:MET:HE3	1:C:378:MET:HB3	1.96	0.41
2:D:222:LYS:C	2:D:224:PRO:HD2	2.42	0.40
1:E:205:HIS:ND1	1:E:278:ASP:OD2	2.40	0.40
1:E:403:SER:OG	1:E:541:PRO:HG2	2.20	0.40
1:A:418:ARG:HE	1:A:509:GLU:CG	2.34	0.40
1:A:490:VAL:CG1	1:A:490:VAL:O	2.66	0.40
1:A:201:LEU:HD11	1:A:205:HIS:CE1	2.57	0.40
2:F:11:TRP:CZ2	2:F:112:TRP:CD1	3.09	0.40
1:A:306:GLU:HB2	1:A:509:GLU:CB	2.51	0.40
1:C:56:LEU:O	1:C:57:GLU:C	2.60	0.40
2:D:241:PHE:CE2	2:D:243:ILE:HB	2.57	0.40
2:F:202:VAL:HG22	2:F:210:ALA:N	2.36	0.40
2:D:188:ASP:O	2:D:189:LYS:HG2	2.21	0.40
2:F:218:LYS:HB2	10:F:2009:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:NH2	1:C:3:TYR:OH[1_655]	2.05	0.15

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	581/585 (99%)	537 (92%)	44 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	581/585 (99%)	538 (93%)	42 (7%)	1 (0%)	47	79
1	E	581/585 (99%)	535 (92%)	46 (8%)	0	100	100
2	B	261/279 (94%)	245 (94%)	16 (6%)	0	100	100
2	D	260/279 (93%)	243 (94%)	17 (6%)	0	100	100
2	F	261/279 (94%)	244 (94%)	17 (6%)	0	100	100
All	All	2525/2592 (97%)	2342 (93%)	182 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	4	PRO

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	486/487 (100%)	471 (97%)	15 (3%)	40	72
1	C	486/487 (100%)	466 (96%)	20 (4%)	30	66
1	E	485/487 (100%)	465 (96%)	20 (4%)	30	66
2	B	214/228 (94%)	207 (97%)	7 (3%)	38	71
2	D	213/228 (93%)	206 (97%)	7 (3%)	38	71
2	F	213/228 (93%)	205 (96%)	8 (4%)	33	67
All	All	2097/2145 (98%)	2020 (96%)	77 (4%)	34	68

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ILE
1	A	127	HIS
1	A	135	VAL
1	A	153	SER
1	A	194	LEU

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Mol	Chain	Res	Type
1	A	243	LEU
1	A	275	TYR
1	A	358	ASN
1	A	385	THR
1	A	387	THR
1	A	403	SER
1	A	404	PRO
1	A	436	GLN
1	A	582	CYS
1	A	585	HIS
2	B	16	GLU
2	B	20	CYS
2	B	21	THR
2	B	76	GLU
2	B	103	SER
2	B	145	LYS
2	B	175	LEU
1	C	14	ASN
1	C	37	ILE
1	C	127	HIS
1	C	135	VAL
1	C	194	LEU
1	C	208	GLU
1	C	243	LEU
1	C	275	TYR
1	C	358	ASN
1	C	376	LEU
1	C	385	THR
1	C	387	THR
1	C	403	SER
1	C	429	GLU
1	C	438	LEU
1	C	490	VAL
1	C	500	THR
1	C	525	LYS
1	C	582	CYS
1	C	585	HIS
2	D	16	GLU
2	D	20	CYS
2	D	21	THR
2	D	76	GLU
2	D	103	SER

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Mol	Chain	Res	Type
2	D	145	LYS
2	D	175	LEU
1	E	14	ASN
1	E	37	ILE
1	E	135	VAL
1	E	164	ARG
1	E	194	LEU
1	E	208	GLU
1	E	243	LEU
1	E	275	TYR
1	E	340	THR
1	E	358	ASN
1	E	360	ASN
1	E	376	LEU
1	E	385	THR
1	E	387	THR
1	E	403	SER
1	E	438	LEU
1	E	490	VAL
1	E	525	LYS
1	E	582	CYS
1	E	585	HIS
2	F	16	GLU
2	F	20	CYS
2	F	21	THR
2	F	76	GLU
2	F	103	SER
2	F	145	LYS
2	F	174	ARG
2	F	175	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	358	ASN
1	A	366	HIS
2	B	200	GLN
1	C	358	ASN
1	C	360	ASN
2	D	200	GLN
1	E	127	HIS

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Mol	Chain	Res	Type
1	E	328	ASN
1	E	358	ASN

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](#)

Of 23 ligands modelled in this entry, 9 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NFU	A	1004	1	2,7,7	1.28	0	-		
8	F4S	D	1003	2	0,9,9	0.00	-	-		
8	F4S	B	1003	2	0,9,9	0.00	-	-		
8	F4S	F	1003	2	0,9,9	0.00	-	-		
9	SO4	F	1268	-	4,4,4	0.47	0	6,6,6	0.41	0
7	F3S	B	1002	2	0,9,9	0.00	-	-		
6	SF4	D	1001	2	0,12,12	0.00	-	-		
7	F3S	F	1002	2	0,9,9	0.00	-	-		
7	F3S	D	1002	2	0,9,9	0.00	-	-		
6	SF4	B	1001	2	0,12,12	0.00	-	-		
9	SO4	B	1267	-	4,4,4	0.40	0	6,6,6	0.25	0
6	SF4	F	1001	2	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NFU	E	1004	1	2,7,7	1.39	0	-		
3	NFU	C	1004	1	2,7,7	1.58	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
8	F4S	D	1003	2	-	-	0/3/3/3
8	F4S	B	1003	2	-	-	0/3/3/3
8	F4S	F	1003	2	-	-	0/3/3/3
7	F3S	B	1002	2	-	-	0/3/3/3
6	SF4	D	1001	2	-	-	0/6/5/5
7	F3S	F	1002	2	-	-	0/3/3/3
7	F3S	D	1002	2	-	-	0/3/3/3
6	SF4	B	1001	2	-	-	0/6/5/5
6	SF4	F	1001	2	-	-	0/6/5/5

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1004	NFU	1	0
6	D	1001	SF4	1	0
6	F	1001	SF4	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, 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	583/585 (99%)	-0.45	7 (1%) 79 67	51, 86, 125, 174	0
1	C	583/585 (99%)	-0.50	1 (0%) 95 94	48, 83, 122, 161	0
1	E	583/585 (99%)	-0.40	5 (0%) 84 75	52, 97, 147, 174	0
2	B	263/279 (94%)	-0.69	0 100 100	52, 74, 101, 143	0
2	D	262/279 (93%)	-0.57	2 (0%) 86 78	56, 79, 106, 133	0
2	F	263/279 (94%)	-0.65	0 100 100	51, 79, 112, 142	0
All	All	2537/2592 (97%)	-0.51	15 (0%) 89 83	48, 84, 128, 174	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	5	TYR	4.4
1	A	5	TYR	3.4
1	E	380	GLU	3.1
1	A	3	TYR	3.0
1	E	6	GLN	2.9
2	D	260	TYR	2.8
1	A	6	GLN	2.7
1	A	12	LEU	2.5
1	A	357	GLY	2.5
1	E	559	LYS	2.3
1	A	380	GLU	2.3
2	D	65	ARG	2.3
1	E	561	ALA	2.3
1	A	4	PRO	2.1
1	C	3	TYR	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, 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(\AA^2)	Q<0.9
4	CL	A	1587	1/1	0.82	0.19	83,83,83,83	0
4	CL	E	1586	1/1	0.84	0.11	93,93,93,93	0
4	CL	A	1586	1/1	0.87	0.12	95,95,95,95	0
9	SO4	B	1267	5/5	0.92	0.18	91,121,124,126	0
5	MG	E	1005	1/1	0.95	0.21	49,49,49,49	0
4	CL	A	1588	1/1	0.96	0.10	50,50,50,50	0
9	SO4	F	1268	5/5	0.96	0.13	101,105,112,114	0
8	F4S	D	1003	7/7	0.97	0.09	80,97,112,115	0
4	CL	A	1590	1/1	0.97	0.16	52,52,52,52	0
5	MG	A	1005	1/1	0.98	0.35	56,56,56,56	0
4	CL	E	1587	1/1	0.98	0.16	51,51,51,51	0
8	F4S	B	1003	7/7	0.98	0.10	77,84,103,121	0
8	F4S	F	1003	7/7	0.98	0.10	79,94,111,123	0
5	MG	C	1586	1/1	0.98	0.18	41,41,41,41	0
3	NFU	E	1004	8/8	0.99	0.12	72,79,86,105	0
6	SF4	D	1001	8/8	0.99	0.06	64,68,75,77	0
3	NFU	A	1004	8/8	0.99	0.13	69,71,78,80	0
6	SF4	B	1001	8/8	0.99	0.06	66,73,78,79	0
6	SF4	F	1001	8/8	0.99	0.08	61,64,70,71	0
7	F3S	B	1002	7/7	1.00	0.09	51,59,66,76	0
7	F3S	F	1002	7/7	1.00	0.10	55,56,64,69	0
3	NFU	C	1004	8/8	1.00	0.10	59,68,83,93	0
7	F3S	D	1002	7/7	1.00	0.10	61,65,74,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.