



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 02:46 PM JST

PDB ID : 5XFA
Title : Crystal structure of NAD⁺-reducing [NiFe]-hydrogenase in the H₂-reduced state
Authors : Shomura, Y.; Taketa, M.; Nakashima, H.; Tai, H.; Nakagawa, H.; Ikeda, Y.; Ishii, M.; Igarashi, Y.; Nishihara, H.; Yoon, K.S.; Ogo, S.; Hirota, S.; Higuchi, Y.
Deposited on : 2017-04-09
Resolution : 2.70 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

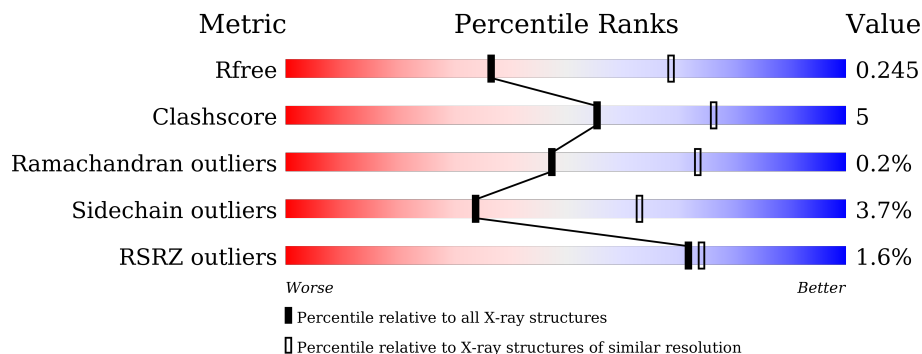
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



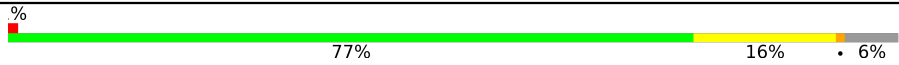


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. 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	591	 4% (poor fit), 86% (0-3 outliers), 11% (1-2 outliers), 0% (3+ outliers), 0% (not modelled)
1	E	591	 3% (poor fit), 86% (0-3 outliers), 10% (1-2 outliers), 0% (3+ outliers), 0% (not modelled)
2	B	242	 0% (poor fit), 90% (0-3 outliers), 7% (1-2 outliers), 0% (3+ outliers), 0% (not modelled)
2	F	242	 0% (poor fit), 88% (0-3 outliers), 9% (1-2 outliers), 0% (3+ outliers), 0% (not modelled)
3	C	189	 0% (poor fit), 80% (0-3 outliers), 13% (1-2 outliers), 6% (3+ outliers), 0% (not modelled)

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Mol	Chain	Length	Quality of chain
3	G	189	 <p>% 77% 16% • 6%</p>
4	D	468	 <p>81% 14% • •</p>
4	H	468	 <p>% 79% 16% • •</p>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 22444 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 NAD-reducing hydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	581	Total	C	N	O	S	0	2	0
			4450	2832	795	806	17			
1	E	571	Total	C	N	O	S	0	0	0
			4360	2776	782	785	17			

- Molecule 2 is a protein called NAD-reducing hydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	234	Total	C	N	O	S	0	0	0
			1769	1103	326	325	15			
2	F	234	Total	C	N	O	S	0	0	0
			1769	1103	326	325	15			

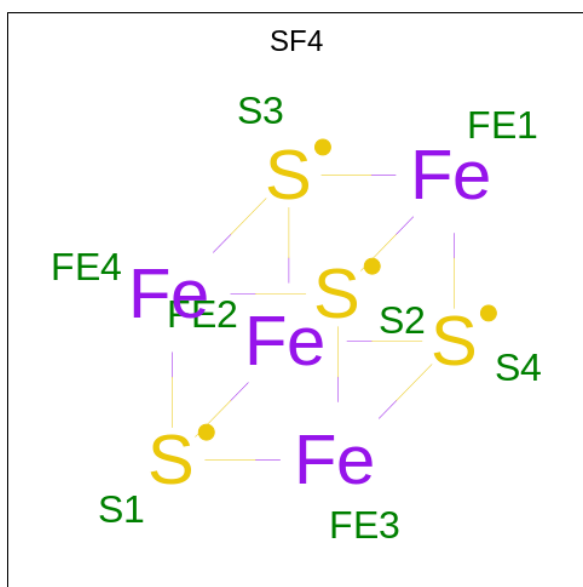
- Molecule 3 is a protein called NAD-reducing hydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	178	Total	C	N	O	S	0	0	0
			1404	894	253	250	7			
3	G	178	Total	C	N	O	S	0	0	0
			1404	894	253	250	7			

- Molecule 4 is a protein called NAD-reducing hydrogenase.

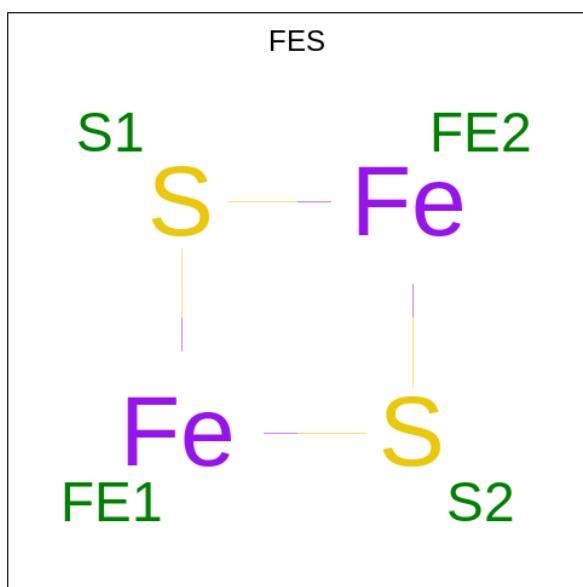
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	452	Total	C	N	O	S	0	0	0
			3538	2241	645	637	15			
4	H	451	Total	C	N	O	S	0	0	0
			3533	2238	644	636	15			

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



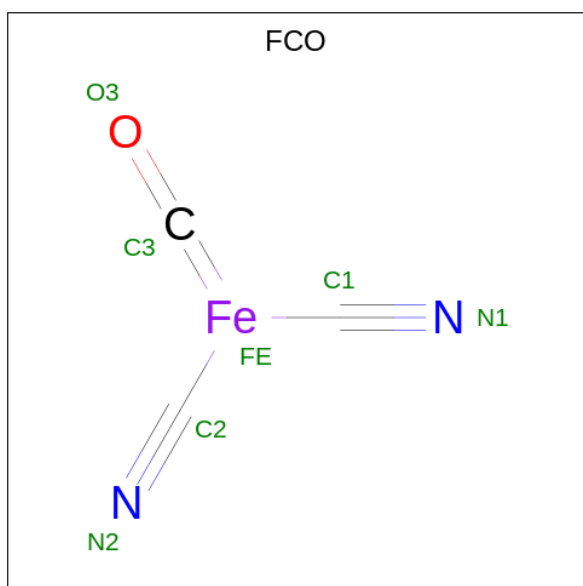
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Fe S	0	0
			8	4 4		
5	B	1	Total	Fe S	0	0
			8	4 4		
5	B	1	Total	Fe S	0	0
			8	4 4		
5	C	1	Total	Fe S	0	0
			8	4 4		
5	E	1	Total	Fe S	0	0
			8	4 4		
5	F	1	Total	Fe S	0	0
			8	4 4		
5	F	1	Total	Fe S	0	0
			8	4 4		
5	G	1	Total	Fe S	0	0
			8	4 4		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
6	B	1	4	2	2	0	0
6	F	1	4	2	2	0	0

- Molecule 7 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
7	D	1	7	3	1	2	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	H	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 8 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Ni	0	0
			1	1		
8	H	1	Total	Ni	0	0
			1	1		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Mg	0	0
			1	1		
9	H	1	Total	Mg	0	0
			1	1		

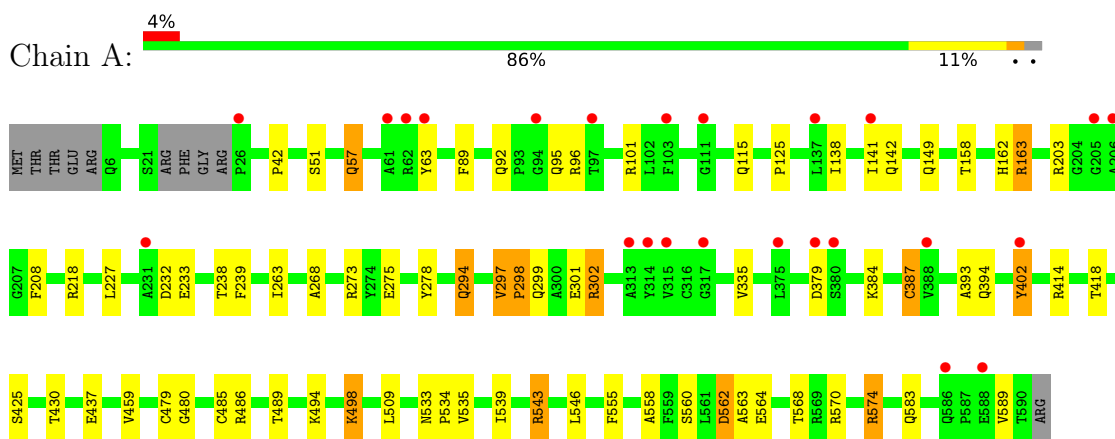
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	18	Total	O	0	0
			18	18		
10	B	15	Total	O	0	0
			15	15		
10	C	9	Total	O	0	0
			9	9		
10	D	40	Total	O	0	0
			40	40		
10	E	2	Total	O	0	0
			2	2		
10	F	3	Total	O	0	0
			3	3		
10	G	6	Total	O	0	0
			6	6		
10	H	34	Total	O	0	0
			34	34		

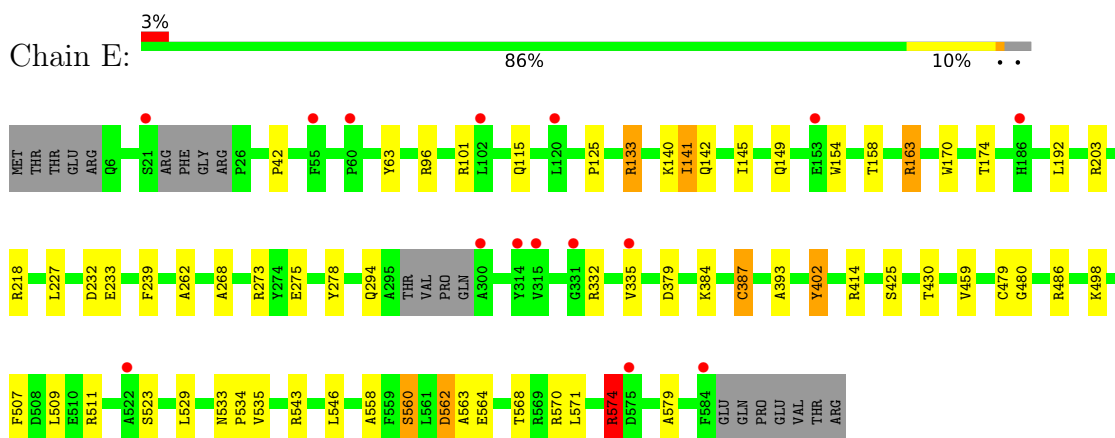
3 Residue-property plots [i](#)

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.

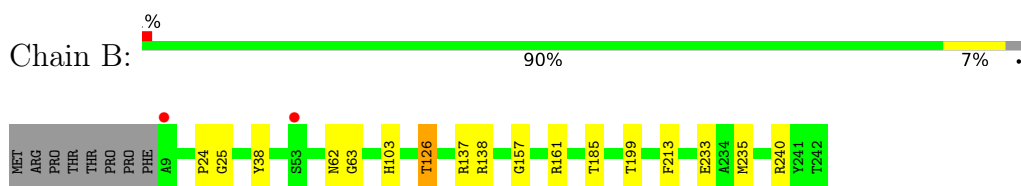
- Molecule 1: NAD-reducing hydrogenase




- Molecule 1: NAD-reducing hydrogenase



- Molecule 2: NAD-reducing hydrogenase




- Molecule 2: NAD-reducing hydrogenase

Chain F:  88% 9%




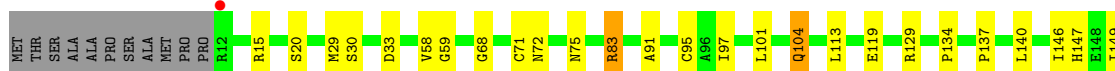
- Molecule 3: NAD-reducing hydrogenase

Chain C:  80% 13% 6%




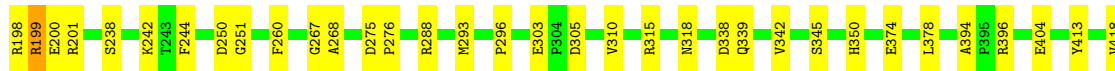
- Molecule 3: NAD-reducing hydrogenase

Chain G:  77% 16% 6%




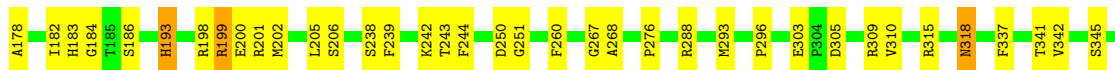
- Molecule 4: NAD-reducing hydrogenase

Chain D:  81% 14%



- Molecule 4: NAD-reducing hydrogenase

Chain H:  79% 16%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.75Å 192.47Å 130.82Å 90.00° 105.08° 90.00°	Depositor
Resolution (Å)	96.24 – 2.70 96.23 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (96.24-2.70) 99.2 (96.23-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.195 , 0.245 0.199 , 0.245	Depositor DCC
R_{free} test set	4300 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtrriage
Anisotropy	0.175	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22444	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: FES, NI, SF4, MG, FCO

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	0.45	0/4577	0.66	5/6252 (0.1%)
1	E	0.44	0/4478	0.64	1/6113 (0.0%)
2	B	0.54	0/1808	0.72	0/2450
2	F	0.53	0/1808	0.71	0/2450
3	C	0.51	0/1440	0.70	0/1966
3	G	0.46	0/1440	0.66	0/1966
4	D	0.53	0/3619	0.73	0/4912
4	H	0.46	0/3614	0.71	2/4905 (0.0%)
All	All	0.48	0/22784	0.69	8/31014 (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
3	C	0	1
4	H	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	PRO	CB-CA-C	-6.85	94.89	112.00
4	H	337	PHE	CB-CA-C	-6.25	97.90	110.40
1	A	297	VAL	CB-CA-C	6.18	123.14	111.40
1	A	298	PRO	N-CA-C	5.94	127.54	112.10
1	A	294	GLN	CB-CA-C	-5.73	98.95	110.40
4	H	337	PHE	N-CA-C	5.69	126.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	574	ARG	CG-CD-NE	5.18	122.67	111.80
1	A	302	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	58	VAL	Peptide
4	H	54	ILE	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	4450	0	4364	42	0
1	E	4360	0	4275	35	0
2	B	1769	0	1739	11	0
2	F	1769	0	1739	18	0
3	C	1404	0	1392	20	0
3	G	1404	0	1392	23	0
4	D	3538	0	3497	48	0
4	H	3533	0	3492	52	0
5	A	8	0	0	0	0
5	B	16	0	0	1	0
5	C	8	0	0	0	0
5	E	8	0	0	0	0
5	F	16	0	0	0	0
5	G	8	0	0	0	0
6	B	4	0	0	0	0
6	F	4	0	0	1	0
7	D	7	0	0	1	0
7	H	7	0	0	0	0
8	D	1	0	0	0	0
8	H	1	0	0	0	0
9	D	1	0	0	0	0
9	H	1	0	0	0	0
10	A	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	15	0	0	1	0
10	C	9	0	0	1	0
10	D	40	0	0	3	0
10	E	2	0	0	0	0
10	F	3	0	0	1	0
10	G	6	0	0	0	0
10	H	34	0	0	4	0
All	All	22444	0	21890	227	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 5.

All (227) 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:485:CYS:O	1:A:489:THR:HG23	1.59	1.02
1:A:294:GLN:O	1:A:297:VAL:HG12	1.67	0.95
1:A:89:PHE:HZ	1:A:141:ILE:HD13	1.40	0.86
4:D:201:ARG:NH1	4:D:374:GLU:OE2	2.09	0.84
4:H:201:ARG:NH1	4:H:374:GLU:OE2	2.11	0.83
2:F:126:THR:HG23	3:G:155:TYR:HB2	1.63	0.79
1:A:494:LYS:O	1:A:498:LYS:HD2	1.84	0.77
1:A:89:PHE:CZ	1:A:141:ILE:HD13	2.21	0.74
4:D:303:GLU:OE2	10:D:601:HOH:O	2.07	0.73
3:C:137:PRO:HD3	4:D:55:VAL:HG22	1.71	0.73
2:B:126:THR:HG23	3:C:155:TYR:HB2	1.72	0.72
1:A:539:ILE:O	1:A:543:ARG:HD3	1.90	0.71
1:A:574:ARG:CZ	3:C:134:PRO:HA	2.20	0.71
2:F:233:GLU:OE2	2:F:233:GLU:N	2.26	0.67
4:H:54:ILE:HD12	4:H:463:LEU:HD22	1.77	0.67
3:G:71:CYS:H	3:G:75:ASN:HD22	1.43	0.66
1:A:138:ILE:O	1:A:141:ILE:CD1	2.44	0.66
1:A:138:ILE:O	1:A:141:ILE:HD12	1.96	0.65
1:E:560:SER:HB2	1:E:563:ALA:HB3	1.78	0.65
2:B:103:HIS:HA	5:B:301:SF4:S3	2.35	0.65
4:D:315:ARG:NH2	4:D:394:ALA:O	2.28	0.65
4:D:54:ILE:HD12	4:D:463:LEU:HD22	1.79	0.64
3:G:91:ALA:HB2	3:G:146:ILE:HD11	1.80	0.64
3:C:91:ALA:HB2	3:C:146:ILE:HD11	1.80	0.64
4:H:353:ARG:HD2	10:H:604:HOH:O	1.98	0.63
4:D:79:LEU:HD12	4:D:87:HIS:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:267:GLY:N	4:H:268:ALA:HB3	2.13	0.63
4:H:315:ARG:NH2	4:H:394:ALA:O	2.31	0.62
4:D:83:CYS:HB2	4:D:119:GLN:NE2	2.15	0.61
4:H:418:VAL:HG11	4:H:465:CYS:HB3	1.81	0.61
4:D:442:VAL:HB	4:D:443:THR:HA	1.83	0.61
4:H:442:VAL:HB	4:H:443:THR:HA	1.83	0.61
1:A:92:GLN:H	1:A:95:GLN:HE21	1.49	0.61
2:F:62:ASN:N	2:F:63:GLY:HA2	2.16	0.60
4:D:32:GLU:HG3	4:D:462:CYS:HA	1.83	0.60
4:D:418:VAL:HG11	4:D:465:CYS:HB3	1.83	0.60
1:E:507:PHE:CE2	1:E:511:ARG:HD3	2.36	0.60
4:H:83:CYS:HB2	4:H:119:GLN:NE2	2.16	0.60
1:A:498:LYS:HE2	1:A:558:ALA:HB1	1.83	0.59
4:H:205:LEU:HD22	10:H:601:HOH:O	2.02	0.59
3:G:20:SER:O	4:H:34:HIS:CE1	2.55	0.59
4:D:267:GLY:N	4:D:268:ALA:HB3	2.18	0.58
3:G:137:PRO:HD3	4:H:55:VAL:HG22	1.85	0.58
4:H:267:GLY:CA	4:H:268:ALA:HB3	2.33	0.58
3:C:183:TYR:HB3	3:C:184:PRO:HD3	1.86	0.58
4:D:267:GLY:CA	4:D:268:ALA:HB3	2.34	0.58
3:G:183:TYR:HB3	3:G:184:PRO:HD3	1.86	0.58
2:B:62:ASN:N	2:B:63:GLY:HA2	2.19	0.57
1:E:560:SER:HB2	1:E:563:ALA:CB	2.34	0.57
2:F:204:ARG:NH1	10:F:402:HOH:O	2.37	0.57
4:D:288:ARG:NH2	4:D:303:GLU:OE1	2.38	0.56
1:E:574:ARG:NH2	3:G:134:PRO:HA	2.21	0.56
1:A:560:SER:O	1:A:563:ALA:HB3	2.07	0.55
1:A:218:ARG:HD3	1:A:263:ILE:HA	1.88	0.55
4:H:309:ARG:HB3	4:H:426:VAL:HG21	1.89	0.54
1:E:233:GLU:O	1:E:273:ARG:NH1	2.39	0.54
1:E:140:LYS:HD3	1:E:145:ILE:HD13	1.89	0.54
1:A:297:VAL:HG13	1:A:302:ARG:HB3	1.90	0.53
1:A:233:GLU:OE1	1:A:238:THR:HG22	2.07	0.53
1:E:63:TYR:CD2	1:E:141:ILE:HG23	2.42	0.53
4:H:288:ARG:NH2	4:H:303:GLU:OE1	2.41	0.53
4:D:79:LEU:HD13	4:D:468:HIS:HB3	1.91	0.52
1:E:393:ALA:HB3	1:E:414:ARG:HB2	1.91	0.52
4:H:250:ASP:N	4:H:251:GLY:HA2	2.25	0.52
2:F:110:LYS:NZ	2:F:212:ASN:OD1	2.40	0.52
1:A:42:PRO:HB2	2:B:185:THR:HB	1.92	0.52
3:C:175:VAL:HG12	3:C:175:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:250:ASP:N	4:D:251:GLY:HA2	2.25	0.51
1:A:51:SER:HA	1:A:57[B]:GLN:NE2	2.26	0.51
3:G:175:VAL:O	3:G:175:VAL:HG12	2.11	0.51
2:F:127:ALA:HB1	3:G:97:ILE:HG23	1.92	0.50
3:C:165:VAL:HG23	3:C:185:THR:HB	1.93	0.50
4:H:178:ALA:HB1	4:H:184:GLY:HA3	1.92	0.50
1:E:218:ARG:HD2	1:E:262:ALA:O	2.12	0.50
4:D:296:PRO:HG2	4:D:422:HIS:HA	1.93	0.50
1:E:227:LEU:O	1:E:268:ALA:HA	2.12	0.49
3:G:165:VAL:HG23	3:G:185:THR:HB	1.93	0.49
4:D:342:VAL:HA	4:D:345:SER:HB2	1.93	0.49
4:H:202:MET:HE1	10:H:601:HOH:O	2.11	0.49
1:A:393:ALA:HB3	1:A:414:ARG:HB2	1.94	0.49
4:H:342:VAL:HA	4:H:345:SER:HB2	1.94	0.49
1:A:138:ILE:O	1:A:141:ILE:HD11	2.13	0.49
1:E:459:VAL:HG12	1:E:459:VAL:O	2.13	0.49
1:A:459:VAL:HG12	1:A:459:VAL:O	2.13	0.48
4:H:199:ARG:HG3	4:H:200:GLU:N	2.28	0.48
2:B:157:GLY:O	2:B:161:ARG:HG3	2.14	0.48
1:E:523:SER:HB2	1:E:529:LEU:HD23	1.94	0.48
1:E:42:PRO:HB2	2:F:185:THR:HB	1.94	0.48
4:D:132:ALA:HB1	4:D:350:HIS:HE1	1.78	0.48
4:D:178:ALA:HB1	4:D:184:GLY:HA3	1.95	0.48
1:A:480:GLY:O	1:A:486:ARG:HD3	2.13	0.48
1:E:140:LYS:O	1:E:145:ILE:HD12	2.13	0.48
4:H:87:HIS:HE1	4:H:465:CYS:SG	2.37	0.48
4:H:296:PRO:HG2	4:H:422:HIS:HA	1.95	0.47
4:D:242:LYS:HG3	10:D:604:HOH:O	2.13	0.47
4:D:199:ARG:HG3	4:D:200:GLU:N	2.30	0.47
1:E:498:LYS:HE3	1:E:558:ALA:HA	1.96	0.47
3:G:119:GLU:HG2	3:G:129:ARG:HA	1.96	0.47
1:A:562:ASP:HA	1:A:563:ALA:C	2.34	0.47
2:B:38:TYR:CD2	2:B:233:GLU:HG2	2.49	0.47
3:C:20:SER:O	4:D:34:HIS:CE1	2.67	0.47
4:D:83:CYS:HA	4:D:119:GLN:HE21	1.80	0.47
1:A:275:GLU:OE1	1:A:275:GLU:N	2.43	0.47
3:C:119:GLU:HG2	3:C:129:ARG:HA	1.95	0.47
1:A:227:LEU:O	1:A:268:ALA:HA	2.15	0.47
2:B:199:THR:HB	4:H:206:SER:HB3	1.97	0.47
1:E:332:ARG:NH2	2:F:175:GLY:O	2.47	0.47
1:E:480:GLY:O	1:E:486:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:ARG:HD3	10:D:618:HOH:O	2.14	0.47
4:D:83:CYS:CB	4:D:119:GLN:NE2	2.79	0.46
3:G:29:MET:HA	3:G:29:MET:CE	2.45	0.46
4:D:83:CYS:CB	4:D:119:GLN:HE21	2.29	0.46
4:D:442:VAL:CB	4:D:443:THR:HA	2.45	0.46
1:A:239:PHE:CE2	1:A:387:CYS:HB2	2.49	0.46
4:D:260:PHE:CE2	4:D:276:PRO:HA	2.51	0.46
1:E:562:ASP:HA	1:E:564:GLU:N	2.31	0.46
1:A:533:ASN:HB2	1:A:534:PRO:HD3	1.98	0.46
1:A:555:PHE:HB2	3:C:151:ARG:HG3	1.97	0.46
4:H:244:PHE:HB3	4:H:310:VAL:HG12	1.98	0.45
4:D:86:SER:OG	4:D:119:GLN:NE2	2.44	0.45
4:H:83:CYS:HA	4:H:119:GLN:HE21	1.82	0.45
1:A:562:ASP:HA	1:A:564:GLU:N	2.31	0.45
4:H:132:ALA:HB1	4:H:350:HIS:HE1	1.82	0.45
1:A:138:ILE:HA	1:A:141:ILE:HD11	1.98	0.45
1:E:115:GLN:NE2	1:E:158:THR:O	2.50	0.45
1:E:275:GLU:OE1	1:E:275:GLU:N	2.46	0.45
2:F:126:THR:CG2	3:G:155:TYR:HB2	2.41	0.45
3:C:72:ASN:HA	3:C:140:LEU:HD13	1.99	0.45
4:H:260:PHE:CE2	4:H:276:PRO:HA	2.52	0.45
1:A:125:PRO:HG3	1:A:278:TYR:CE1	2.52	0.45
4:D:396:ARG:HD2	7:D:501:FCO:N2	2.32	0.45
2:F:24:PRO:HA	2:F:25:GLY:HA2	1.80	0.45
4:D:396:ARG:CD	4:D:462:CYS:HB2	2.47	0.44
3:C:67:GLU:HB2	10:C:306:HOH:O	2.16	0.44
2:F:157:GLY:O	2:F:161:ARG:HG3	2.17	0.44
1:E:239:PHE:CE2	1:E:387:CYS:HB2	2.52	0.44
4:H:83:CYS:CB	4:H:119:GLN:HE21	2.30	0.44
4:D:244:PHE:HB3	4:D:310:VAL:HG12	1.98	0.44
1:E:562:ASP:HA	1:E:563:ALA:C	2.38	0.44
4:H:182:ILE:O	4:H:183:HIS:HB2	2.18	0.44
4:H:404:GLU:HB2	4:H:413:TYR:HB3	1.99	0.44
4:D:199:ARG:NH2	2:F:204:ARG:O	2.51	0.44
4:H:396:ARG:CD	4:H:462:CYS:HB2	2.48	0.44
1:E:125:PRO:HG3	1:E:278:TYR:CE1	2.53	0.43
1:E:384:LYS:HD3	1:E:402:TYR:CZ	2.53	0.43
1:A:115:GLN:NE2	1:A:158:THR:O	2.51	0.43
4:H:83:CYS:CB	4:H:119:GLN:NE2	2.80	0.43
1:A:384:LYS:HD3	1:A:402:TYR:CZ	2.53	0.43
1:A:574:ARG:NH2	3:C:134:PRO:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:378:LEU:HD12	4:D:378:LEU:N	2.34	0.43
1:E:101:ARG:NH1	1:E:142:GLN:HA	2.34	0.43
4:H:79:LEU:HD13	4:H:468:HIS:HB3	2.00	0.43
4:H:83:CYS:HB2	4:H:119:GLN:HE22	1.84	0.43
3:C:29:MET:HA	3:C:29:MET:CE	2.49	0.43
3:G:29:MET:HA	3:G:29:MET:HE2	2.00	0.43
3:G:72:ASN:HA	3:G:140:LEU:HD13	1.99	0.43
4:H:186:SER:HA	4:H:193:HIS:CE1	2.53	0.43
4:D:83:CYS:HB2	4:D:119:GLN:HE22	1.82	0.43
4:D:182:ILE:O	4:D:183:HIS:HB2	2.18	0.43
1:E:133:ARG:CZ	1:E:154:TRP:CD1	3.02	0.43
3:G:113:LEU:HD22	4:H:62:ALA:CB	2.49	0.43
1:E:509:LEU:HD21	1:E:546:LEU:HD21	2.00	0.43
4:H:378:LEU:N	4:H:378:LEU:HD12	2.34	0.43
3:C:83:ARG:HA	3:C:83:ARG:HD3	1.85	0.43
4:D:404:GLU:HB2	4:D:413:TYR:HB3	2.00	0.43
4:H:243:THR:OG1	4:H:318:ASN:ND2	2.52	0.42
3:C:29:MET:HA	3:C:29:MET:HE2	2.01	0.42
4:D:32:GLU:HG2	4:D:462:CYS:SG	2.59	0.42
1:E:533:ASN:HB2	1:E:534:PRO:HD3	2.01	0.42
1:A:562:ASP:OD1	1:A:562:ASP:N	2.53	0.42
2:F:52:GLY:HA2	6:F:303:FES:S1	2.59	0.42
1:A:162:HIS:CD2	1:A:394:GLN:HB2	2.54	0.42
1:A:101:ARG:NH1	1:A:142:GLN:HA	2.35	0.42
4:D:448:LEU:O	4:D:451:HIS:HB2	2.19	0.42
1:E:232:ASP:HA	1:E:273:ARG:HB3	2.01	0.42
4:H:54:ILE:HG13	4:H:293:MET:SD	2.60	0.42
1:E:574:ARG:HH11	1:E:574:ARG:CG	2.33	0.42
3:G:83:ARG:HD3	3:G:83:ARG:O	2.19	0.42
3:C:68:GLY:HA2	3:C:95:CYS:HB3	2.02	0.42
1:E:133:ARG:CZ	1:E:154:TRP:HD1	2.32	0.42
3:G:149:ILE:HG22	3:G:150:VAL:HG13	2.02	0.42
2:B:24:PRO:HA	2:B:25:GLY:HA2	1.80	0.42
4:D:242:LYS:NZ	4:D:305:ASP:O	2.52	0.42
4:H:86:SER:OG	4:H:119:GLN:NE2	2.46	0.42
4:H:140:PHE:CD1	4:H:140:PHE:N	2.87	0.42
4:H:239:PHE:CE1	4:H:426:VAL:CG1	3.03	0.42
1:A:297:VAL:HA	1:A:298:PRO:HD2	1.69	0.41
4:D:186:SER:HA	4:D:193:HIS:CE1	2.55	0.41
4:D:338:ASP:N	4:D:339:GLN:HA	2.35	0.41
1:E:574:ARG:HH11	1:E:574:ARG:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:574:ARG:NH1	1:E:579:ALA:HB2	2.35	0.41
2:F:235:MET:O	2:F:240:ARG:NH1	2.53	0.41
1:A:63:TYR:CD2	1:A:141:ILE:HG22	2.55	0.41
2:F:225:ARG:O	2:F:226:ARG:C	2.58	0.41
2:B:235:MET:O	2:B:240:ARG:NH1	2.53	0.41
4:D:79:LEU:CD1	4:D:468:HIS:HB3	2.48	0.41
4:D:275:ASP:HA	4:D:276:PRO:HD2	1.97	0.41
4:H:442:VAL:CB	4:H:443:THR:HA	2.45	0.41
1:A:509:LEU:HD21	1:A:546:LEU:HD21	2.02	0.41
4:H:202:MET:CE	10:H:601:HOH:O	2.67	0.41
4:D:140:PHE:N	4:D:140:PHE:CD1	2.89	0.41
4:D:450:ASN:O	4:D:454:VAL:HG23	2.20	0.41
3:G:58:VAL:HG22	3:G:59:GLY:N	2.35	0.41
4:H:448:LEU:O	4:H:451:HIS:HB2	2.19	0.41
1:A:294:GLN:HB3	1:A:297:VAL:CG1	2.51	0.41
3:G:30:SER:O	3:G:33:ASP:HB2	2.20	0.41
1:A:232:ASP:HA	1:A:273:ARG:HB3	2.02	0.41
2:B:213:PHE:CG	4:H:198:ARG:HG2	2.56	0.41
2:F:139:ILE:HD11	4:H:67:ARG:NH1	2.36	0.41
3:G:113:LEU:HD22	4:H:62:ALA:HB3	2.03	0.41
4:H:418:VAL:CG1	4:H:465:CYS:HB3	2.51	0.41
3:C:83:ARG:HD3	3:C:83:ARG:O	2.20	0.41
4:D:198:ARG:HG2	2:F:213:PHE:CG	2.56	0.41
1:E:170:TRP:O	1:E:174:THR:OG1	2.39	0.40
4:H:242:LYS:NZ	4:H:305:ASP:O	2.53	0.40
4:H:450:ASN:O	4:H:454:VAL:HG23	2.21	0.40
3:C:104:GLN:HE21	3:C:104:GLN:HA	1.85	0.40
1:E:192:LEU:HD22	1:E:218:ARG:NE	2.37	0.40
3:G:68:GLY:HA2	3:G:95:CYS:HB3	2.04	0.40
3:G:104:GLN:HA	3:G:104:GLN:HE21	1.86	0.40
2:F:161:ARG:HG3	2:F:161:ARG:HH11	1.86	0.40
1:A:297:VAL:CG2	1:A:301:GLU:HB3	2.52	0.40
4:D:54:ILE:HG13	4:D:293:MET:SD	2.61	0.40
2:B:235:MET:HA	10:B:411:HOH:O	2.21	0.40
4:D:459:PHE:O	4:D:460:ASP:C	2.60	0.40
4:H:19:ALA:HB1	4:H:40:TRP:HB3	2.03	0.40
4:H:140:PHE:CE2	4:H:454:VAL:HG11	2.57	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	579/591 (98%)	547 (94%)	29 (5%)	3 (0%)	29	54
1	E	565/591 (96%)	534 (94%)	27 (5%)	4 (1%)	22	46
2	B	232/242 (96%)	216 (93%)	16 (7%)	0	100	100
2	F	232/242 (96%)	217 (94%)	15 (6%)	0	100	100
3	C	176/189 (93%)	164 (93%)	12 (7%)	0	100	100
3	G	176/189 (93%)	165 (94%)	11 (6%)	0	100	100
4	D	450/468 (96%)	417 (93%)	33 (7%)	0	100	100
4	H	449/468 (96%)	417 (93%)	32 (7%)	0	100	100
All	All	2859/2980 (96%)	2677 (94%)	175 (6%)	7 (0%)	47	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	GLN
1	A	562	ASP
1	A	163	ARG
1	E	163	ARG
1	E	294	GLN
1	E	562	ASP
1	E	560	SER

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	448/455 (98%)	424 (95%)	24 (5%)	22	47
1	E	436/455 (96%)	417 (96%)	19 (4%)	28	56
2	B	184/192 (96%)	181 (98%)	3 (2%)	62	85
2	F	184/192 (96%)	182 (99%)	2 (1%)	73	90
3	C	149/157 (95%)	144 (97%)	5 (3%)	37	66
3	G	149/157 (95%)	144 (97%)	5 (3%)	37	66
4	D	363/377 (96%)	350 (96%)	13 (4%)	35	64
4	H	363/377 (96%)	348 (96%)	15 (4%)	30	59
All	All	2276/2362 (96%)	2190 (96%)	86 (4%)	34	62

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57[A]	GLN
1	A	57[B]	GLN
1	A	96	ARG
1	A	149	GLN
1	A	163	ARG
1	A	203	ARG
1	A	208	PHE
1	A	335	VAL
1	A	379	ASP
1	A	387	CYS
1	A	402	TYR
1	A	418	THR
1	A	425	SER
1	A	430	THR
1	A	437	GLU
1	A	479	CYS
1	A	498	LYS
1	A	535	VAL
1	A	543	ARG
1	A	568	THR
1	A	570	ARG
1	A	574	ARG
1	A	583	GLN
1	A	589	VAL
2	B	126	THR
2	B	137	ARG
2	B	138	ARG

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Mol	Chain	Res	Type
3	C	15	ARG
3	C	83	ARG
3	C	101	LEU
3	C	104	GLN
3	C	147	HIS
4	D	32	GLU
4	D	47	VAL
4	D	55	VAL
4	D	63	PHE
4	D	75	VAL
4	D	137	LEU
4	D	143	ASP
4	D	172	GLU
4	D	193	HIS
4	D	199	ARG
4	D	238	SER
4	D	318	ASN
4	D	419	SER
1	E	96	ARG
1	E	133	ARG
1	E	141	ILE
1	E	149	GLN
1	E	163	ARG
1	E	203	ARG
1	E	335	VAL
1	E	379	ASP
1	E	387	CYS
1	E	402	TYR
1	E	425	SER
1	E	430	THR
1	E	479	CYS
1	E	535	VAL
1	E	543	ARG
1	E	568	THR
1	E	570	ARG
1	E	571	LEU
1	E	574	ARG
2	F	126	THR
2	F	137	ARG
3	G	15	ARG
3	G	83	ARG
3	G	101	LEU

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Mol	Chain	Res	Type
3	G	104	GLN
3	G	147	HIS
4	H	21	ARG
4	H	47	VAL
4	H	55	VAL
4	H	63	PHE
4	H	75	VAL
4	H	131	LEU
4	H	137	LEU
4	H	143	ASP
4	H	172	GLU
4	H	193	HIS
4	H	199	ARG
4	H	238	SER
4	H	318	ASN
4	H	341	THR
4	H	381	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	95	GLN
1	A	549	GLN
1	A	553	HIS
2	B	66	GLN
3	C	104	GLN
3	C	147	HIS
4	D	119	GLN
4	D	281	GLN
4	D	318	ASN
4	D	450	ASN
1	E	83	ASN
1	E	164	HIS
1	E	294	GLN
1	E	549	GLN
1	E	551	GLN
1	E	553	HIS
2	F	66	GLN
3	G	75	ASN
3	G	104	GLN
3	G	147	HIS

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Mol	Chain	Res	Type
4	H	87	HIS
4	H	119	GLN
4	H	281	GLN
4	H	318	ASN
4	H	450	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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
5	SF4	B	301	2	0,12,12	-	-	-		
5	SF4	F	301	2	0,12,12	-	-	-		
5	SF4	G	201	3,10	0,12,12	-	-	-		
6	FES	B	303	2	0,4,4	-	-	-		
5	SF4	B	302	2	0,12,12	-	-	-		
5	SF4	E	601	1	0,12,12	-	-	-		
5	SF4	C	201	3	0,12,12	-	-	-		
6	FES	F	303	2	0,4,4	-	-	-		
5	SF4	A	601	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SF4	F	302	2	0,12,12	-	-	-		
7	FCO	D	501	4	0,6,6	-	-	-		
7	FCO	H	501	4	0,6,6	-	-	-		

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
5	SF4	B	301	2	-	-	0/6/5/5
5	SF4	F	301	2	-	-	0/6/5/5
5	SF4	G	201	3,10	-	-	0/6/5/5
6	FES	B	303	2	-	-	0/1/1/1
5	SF4	B	302	2	-	-	0/6/5/5
5	SF4	E	601	1	-	-	0/6/5/5
5	SF4	C	201	3	-	-	0/6/5/5
6	FES	F	303	2	-	-	0/1/1/1
5	SF4	A	601	1	-	-	0/6/5/5
5	SF4	F	302	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
5	B	301	SF4	1	0
6	F	303	FES	1	0
7	D	501	FCO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	581/591 (98%)	0.23	24 (4%) 37 36	34, 73, 118, 152	0
1	E	571/591 (96%)	0.22	15 (2%) 56 57	41, 72, 106, 133	0
2	B	234/242 (96%)	-0.09	2 (0%) 84 85	30, 53, 86, 112	0
2	F	234/242 (96%)	-0.15	0 100 100	35, 52, 82, 116	0
3	C	178/189 (94%)	-0.13	0 100 100	26, 52, 83, 110	0
3	G	178/189 (94%)	0.05	1 (0%) 89 91	41, 67, 90, 110	0
4	D	452/468 (96%)	-0.11	1 (0%) 95 96	29, 51, 81, 121	0
4	H	451/468 (96%)	0.02	3 (0%) 87 89	36, 65, 103, 135	0
All	All	2879/2980 (96%)	0.05	46 (1%) 72 74	26, 63, 104, 152	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	300	ALA	9.7
1	A	314	TYR	7.1
1	A	205	GLY	5.2
1	A	402	TYR	4.1
3	G	12	ARG	4.0
1	A	313	ALA	3.9
1	A	379	ASP	3.7
1	E	314	TYR	3.5
1	A	26	PRO	3.4
1	E	21	SER	3.4
1	A	141	ILE	3.2
1	E	186	HIS	3.1
1	A	63	TYR	3.0
1	A	94	GLY	3.0
1	A	61	ALA	3.0
4	H	44	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	584	PHE	2.8
1	E	102	LEU	2.8
1	E	315	VAL	2.8
1	A	586	GLN	2.7
1	A	206	ALA	2.6
1	A	111	GLY	2.6
1	E	153	GLU	2.6
1	A	103	PHE	2.6
1	E	120	LEU	2.6
1	A	380	SER	2.6
1	E	331	GLY	2.5
1	A	375	LEU	2.5
1	E	60	PRO	2.4
1	A	315	VAL	2.3
1	E	55	PHE	2.3
1	E	522	ALA	2.2
1	A	317	GLY	2.2
1	A	137	LEU	2.2
1	E	335	VAL	2.1
4	D	459	PHE	2.1
1	E	575	ASP	2.1
1	A	231	ALA	2.1
1	A	388	VAL	2.1
1	A	588	GLU	2.1
4	H	400	ILE	2.1
2	B	9	ALA	2.0
4	H	19	ALA	2.0
1	A	97	THR	2.0
2	B	53	SER	2.0
1	A	62	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	MG	H	503	1/1	0.91	0.10	52,52,52,52	0
9	MG	D	503	1/1	0.93	0.10	31,31,31,31	0
5	SF4	B	302	8/8	0.99	0.12	23,27,30,31	0
5	SF4	C	201	8/8	0.99	0.11	20,23,27,27	0
5	SF4	E	601	8/8	0.99	0.11	32,36,38,40	0
5	SF4	F	302	8/8	0.99	0.13	34,39,42,46	0
5	SF4	G	201	8/8	0.99	0.11	29,32,34,36	0
6	FES	B	303	4/4	0.99	0.14	39,40,44,49	0
6	FES	F	303	4/4	0.99	0.12	37,41,42,45	0
7	FCO	D	501	7/7	0.99	0.19	44,51,55,59	0
7	FCO	H	501	7/7	0.99	0.23	45,46,54,65	0
8	NI	D	502	1/1	0.99	0.12	50,50,50,50	0
8	NI	H	502	1/1	0.99	0.12	63,63,63,63	0
5	SF4	A	601	8/8	0.99	0.12	34,41,41,43	0
5	SF4	B	301	8/8	0.99	0.12	24,26,30,30	0
5	SF4	F	301	8/8	1.00	0.14	40,43,44,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.