



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:56 PM UTC

PDB ID : 8BOQ / pdb_00008boq
Title : A. vinelandii Fe-nitrogenase FeFe protein
Authors : Trncik, C.; Detemple, F.; Einsle, O.
Deposited on : 2022-11-15
Resolution : 1.55 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

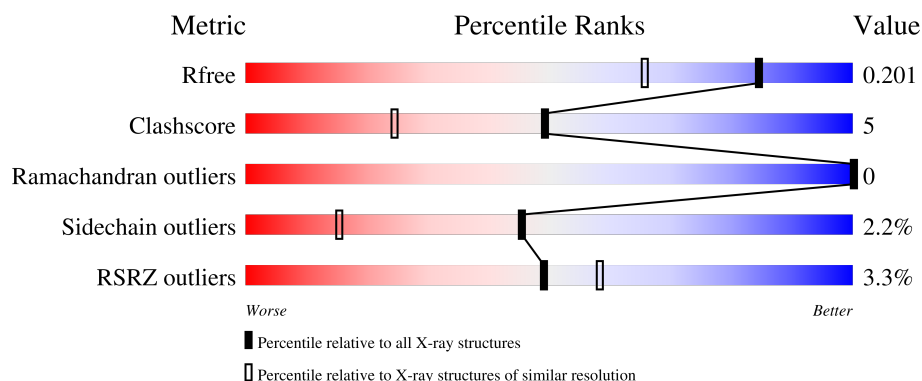
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	180053	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	515	2% 81% 18%
1	D	515	3% 85% 14%
2	B	461	89% 11%
2	E	461	% 90% 10%
3	C	119	11% 83% 16%

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Mol	Chain	Length	Quality of chain
3	F	119	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment on the left labeled '23%', a green segment in the middle labeled '87%', and a yellow segment on the right labeled '12%'. A small black dot is located at the end of the yellow segment.

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18904 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 Nitrogenase protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	4	0
			4118	2611	719	764	24			
1	D	513	Total	C	N	O	S	0	1	0
			4080	2590	710	757	23			

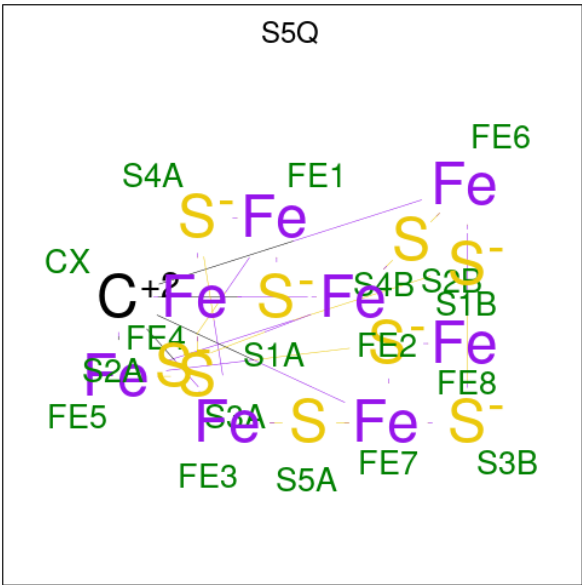
- Molecule 2 is a protein called Fe-only nitrogenase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	461	Total	C	N	O	S	0	1	0
			3604	2304	607	676	17			
2	E	461	Total	C	N	O	S	0	1	0
			3604	2304	607	676	17			

- Molecule 3 is a protein called Nitrogenase iron-iron protein delta chain.

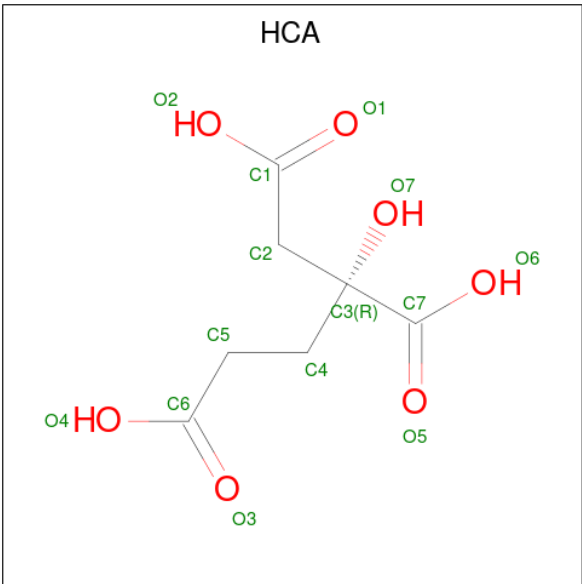
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	119	Total	C	N	O	S	0	0	0
			985	615	168	193	9			
3	F	119	Total	C	N	O	S	0	0	0
			985	615	168	193	9			

- Molecule 4 is FeFe cofactor (CCD ID: S5Q) (formula: CFe₈S₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Fe	S	0	0
			18	1	8	9		
4	D	1	Total	C	Fe	S	0	0
			18	1	8	9		

- Molecule 5 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: C₇H₁₀O₇).



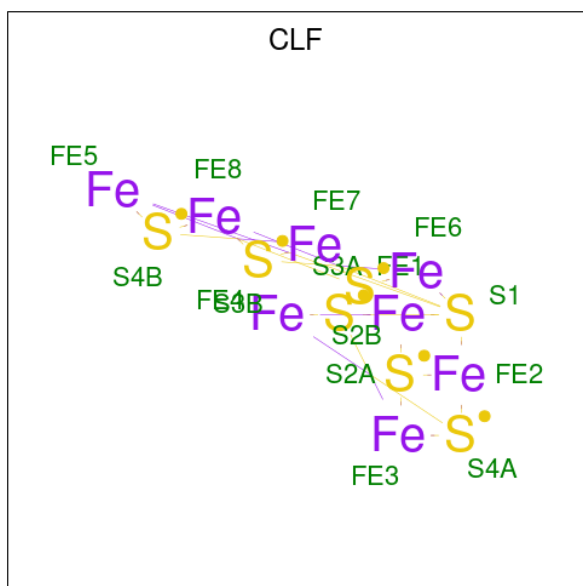
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			14	7	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			14	7	7		

- Molecule 6 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe_8S_7).

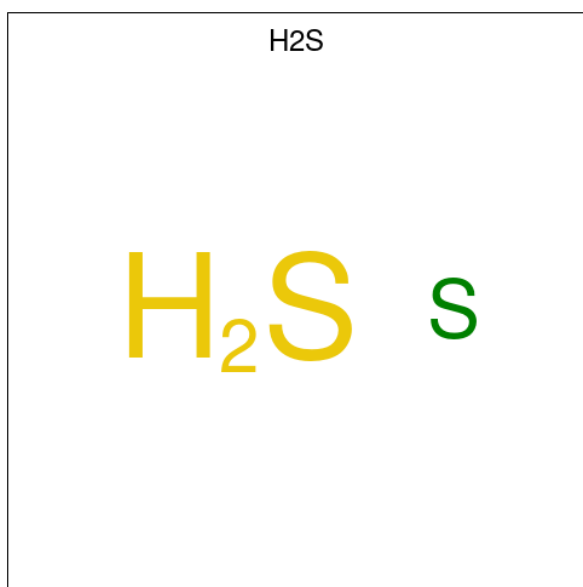


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			15	8	7		
6	E	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 7 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	D	1	Total	O	0	0
			1	1		

- Molecule 8 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H_2S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total S 1 1	0	0
8	D	1	Total S 1 1	0	0

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Mg 2 2	0	0

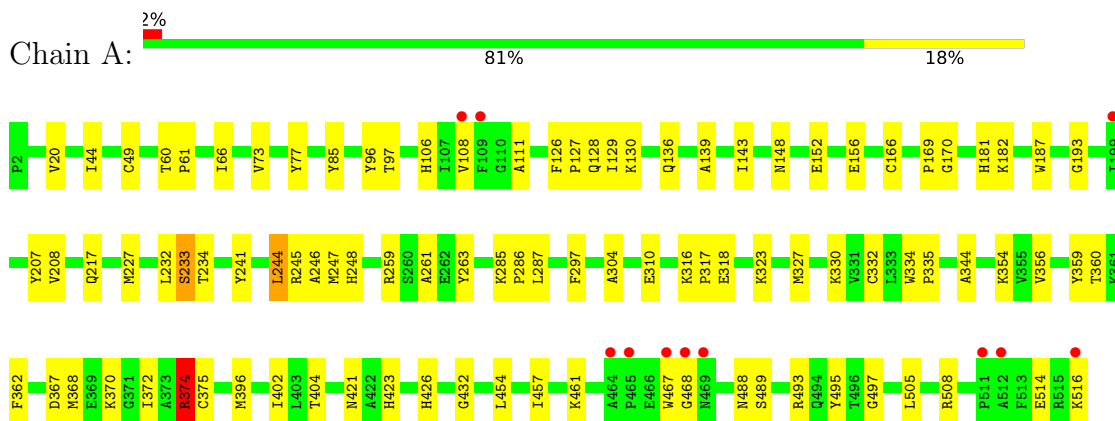
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	337	Total O 337 337	0	0
10	B	371	Total O 371 371	0	0
10	C	79	Total O 79 79	0	0
10	D	261	Total O 261 261	0	0
10	E	334	Total O 334 334	0	0
10	F	46	Total O 46 46	0	0

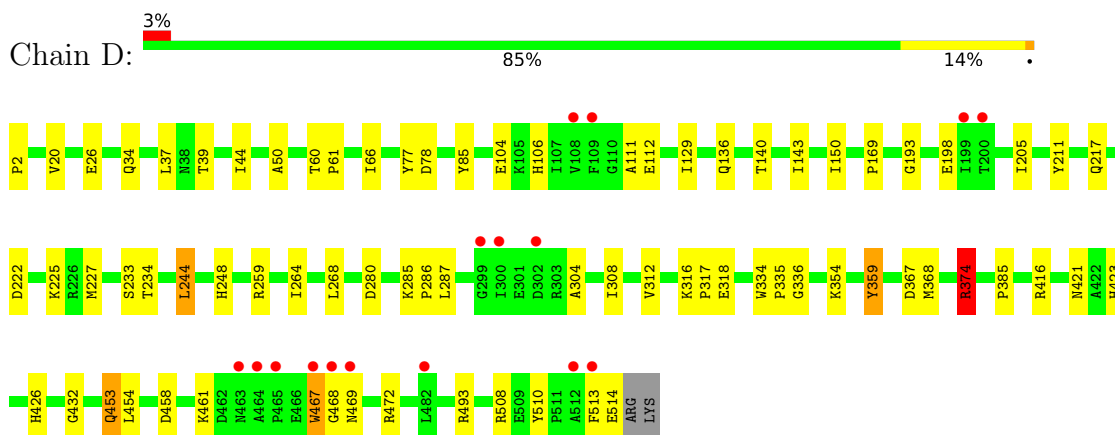
3 Residue-property plots

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.

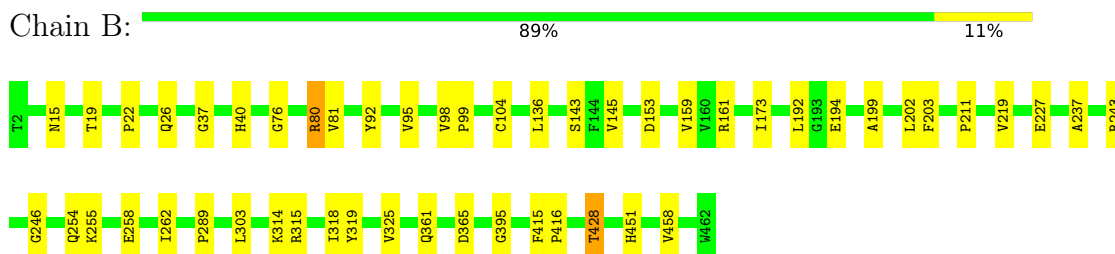
• Molecule 1: Nitrogenase protein alpha chain



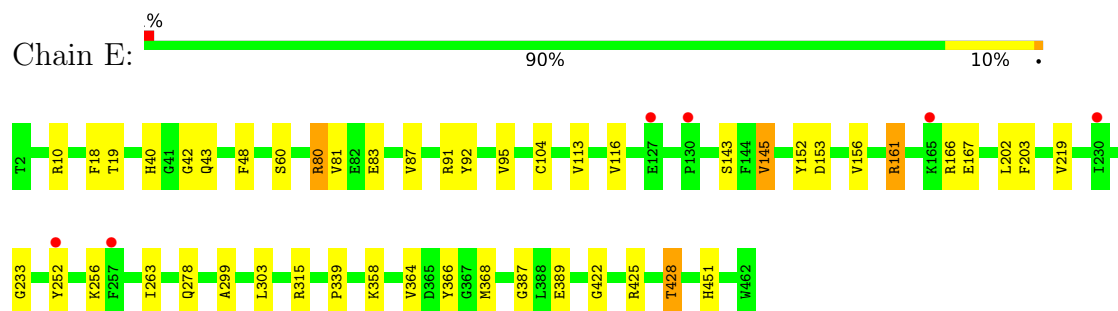
• Molecule 1: Nitrogenase protein alpha chain



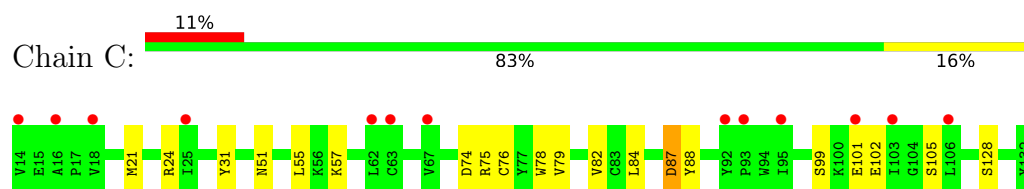
• Molecule 2: Fe-only nitrogenase, beta subunit



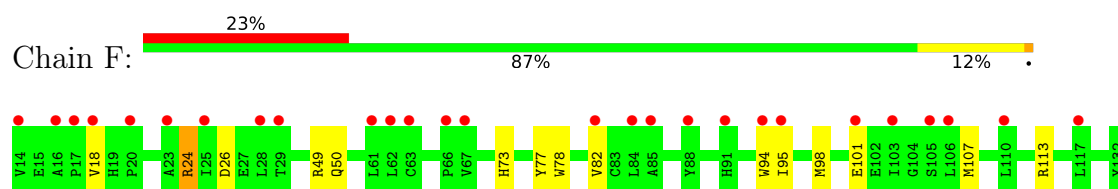
- Molecule 2: Fe-only nitrogenase, beta subunit



- Molecule 3: Nitrogenase iron-iron protein delta chain



- Molecule 3: Nitrogenase iron-iron protein delta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.97Å 151.05Å 158.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.55 20.00 – 1.55	Depositor EDS
% Data completeness (in resolution range)	91.8 (20.00-1.55) 40.2 (20.00-1.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0352, REFMAC 5.8.0352	Depositor
R, R_{free}	0.169 , 0.215 (Not available) , 0.201	Depositor DCC
R_{free} test set	7578 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18904	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H2S, O, CLF, HCA, S5Q, MG

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	0.55	0/4217	0.97	1/5695 (0.0%)
1	D	0.53	0/4179	0.96	1/5646 (0.0%)
2	B	0.56	0/3680	0.93	2/4986 (0.0%)
2	E	0.55	0/3680	0.95	2/4986 (0.0%)
3	C	0.51	0/1008	0.99	0/1362
3	F	0.46	0/1008	0.93	0/1362
All	All	0.54	0/17772	0.95	6/24037 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	3
2	B	0	4
2	E	0	3
All	All	0	11

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	76	GLY	CA-C-O	-5.67	118.31	122.23
2	E	18	PHE	CA-CB-CG	5.65	119.45	113.80
1	D	211	TYR	CB-CA-C	5.63	119.69	110.17
2	E	153	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	156	GLU	CB-CA-C	-5.49	102.02	110.81
2	B	153	ASP	CA-CB-CG	5.23	117.83	112.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	ARG	Sidechain
2	B	161	ARG	Sidechain
2	B	211	PRO	Peptide
2	B	243	ARG	Sidechain
2	B	80	ARG	Sidechain
1	D	205	ILE	Peptide
1	D	374	ARG	Sidechain
1	D	416	ARG	Sidechain
2	E	161	ARG	Sidechain
2	E	80	ARG	Sidechain
2	E	91	ARG	Sidechain

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	4118	0	4031	55	0
1	D	4080	0	3993	47	0
2	B	3604	0	3595	38	0
2	E	3604	0	3595	32	0
3	C	985	0	934	11	0
3	F	985	0	934	12	0
4	A	18	0	0	1	0
4	D	18	0	0	2	0
5	A	14	0	6	1	0
5	D	14	0	6	0	0
6	A	15	0	0	0	0
6	E	15	0	0	1	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	B	2	0	0	0	0
10	A	337	0	0	8	0
10	B	371	0	0	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	79	0	0	3	0
10	D	261	0	0	3	0
10	E	334	0	0	11	0
10	F	46	0	0	3	0
All	All	18904	0	17094	186	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 (186) 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)
3:F:98:MET:SD	10:F:236:HOH:O	2.28	0.92
1:D:368:MET:SD	10:D:952:HOH:O	2.34	0.86
1:A:166:CYS:SG	10:A:923:HOH:O	2.35	0.84
1:A:227:MET:HE3	1:A:304:ALA:HB2	1.61	0.82
1:A:310:GLU:OE2	10:A:701:HOH:O	1.97	0.81
2:E:315:ARG:NH1	2:E:389:GLU:O	2.15	0.80
1:A:360:THR:HG22	1:A:368:MET:HE2	1.64	0.79
3:C:31:TYR:OH	3:C:87:ASP:OD2	2.03	0.77
2:B:237:ALA:N	10:B:603:HOH:O	2.20	0.75
2:B:428:THR:HG21	10:B:861:HOH:O	1.86	0.73
3:F:26:ASP:OD1	3:F:113:ARG:NH2	2.21	0.72
1:D:469:ASN:HB3	10:D:893:HOH:O	1.89	0.72
1:A:468:GLY:O	10:A:703:HOH:O	2.08	0.72
1:A:148:ASN:O	1:A:152:GLU:HG2	1.90	0.71
1:D:453:GLN:HE22	1:D:472:ARG:HD2	1.56	0.71
2:E:364:VAL:HG11	2:E:368:MET:HE3	1.71	0.70
2:B:173:ILE:HA	10:B:603:HOH:O	1.91	0.70
1:D:233:SER:HB2	1:D:244:LEU:HD13	1.76	0.68
2:E:428:THR:HG23	10:E:737:HOH:O	1.93	0.67
1:D:374:ARG:HD2	10:F:210:HOH:O	1.96	0.66
2:B:318:ILE:O	10:B:601:HOH:O	2.14	0.66
1:A:514:GLU:O	10:A:704:HOH:O	2.14	0.66
3:C:101:GLU:HG3	10:C:248:HOH:O	1.97	0.65
2:E:10:ARG:O	10:E:601:HOH:O	2.14	0.64
2:B:315:ARG:HD3	10:B:925:HOH:O	1.98	0.64
1:A:233[B]:SER:HB2	1:A:244:LEU:HD13	1.78	0.64
10:B:679:HOH:O	2:E:451[A]:HIS:HE1	1.81	0.64
2:E:104:CYS:HB3	2:E:143:SER:OG	2.00	0.62
1:D:106:HIS:HB3	1:D:111:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:428:THR:HG21	10:E:794:HOH:O	2.01	0.61
1:A:421:ASN:H	1:A:426:HIS:CD2	2.20	0.60
2:E:299:ALA:O	2:E:303:LEU:HD13	2.01	0.59
1:D:453:GLN:NE2	1:D:472:ARG:HD2	2.17	0.58
1:A:285:LYS:HB3	1:A:286:PRO:HD3	1.85	0.58
2:B:246:GLY:C	10:B:612:HOH:O	2.46	0.58
1:A:97:THR:H	2:B:15:ASN:ND2	2.02	0.57
1:D:222:ASP:OD1	1:D:510:TYR:OH	2.21	0.57
3:F:49:ARG:NH1	3:F:50:GLN:OE1	2.37	0.57
1:D:513:PHE:O	1:D:514:GLU:CB	2.52	0.57
1:A:66:ILE:HG13	1:A:129:ILE:HG21	1.87	0.57
1:A:372:ILE:HA	1:A:375[B]:CYS:SG	2.45	0.57
2:B:451[A]:HIS:CE1	10:B:759:HOH:O	2.58	0.56
1:D:136:GLN:HE21	1:D:169:PRO:HD3	1.70	0.56
1:D:336:GLY:HA3	4:D:601:S5Q:S1B	2.46	0.56
1:A:193:GLY:HA2	1:A:248:HIS:CE1	2.41	0.56
1:D:513:PHE:O	1:D:514:GLU:HB2	2.06	0.56
1:D:308:ILE:O	1:D:312:VAL:HG23	2.06	0.56
1:D:421:ASN:H	1:D:426:HIS:CD2	2.23	0.55
1:D:104:GLU:HG3	2:E:145:VAL:HG12	1.88	0.55
3:F:107:MET:HA	3:F:107:MET:HE2	1.89	0.55
1:A:505:LEU:O	10:A:705:HOH:O	2.18	0.55
3:C:78:TRP:O	3:C:82:VAL:HG23	2.06	0.55
1:A:297:PHE:O	3:C:75:ARG:NH1	2.40	0.55
3:F:94:TRP:CE3	3:F:95:ILE:N	2.75	0.55
1:A:330:LYS:HD2	1:A:356:VAL:HG11	1.89	0.54
1:D:66:ILE:HG13	1:D:129:ILE:HG21	1.89	0.54
2:B:428:THR:HG23	10:B:749:HOH:O	2.07	0.54
1:D:217:GLN:HG3	1:D:234:THR:HG21	1.90	0.54
2:B:192:LEU:HD23	10:B:843:HOH:O	2.07	0.54
1:A:106:HIS:HB3	1:A:111:ALA:HB2	1.89	0.54
2:E:161:ARG:HG3	2:E:252:TYR:CE2	2.42	0.54
2:E:422:GLY:O	2:E:425:ARG:HG2	2.08	0.54
1:D:112:GLU:HB3	1:D:150:ILE:HD11	1.90	0.53
3:F:24:ARG:HD2	3:F:98:MET:HE1	1.91	0.53
1:D:285:LYS:HB3	1:D:286:PRO:HD3	1.91	0.53
1:A:488:ASN:O	1:A:489:SER:C	2.52	0.53
2:B:104:CYS:HB3	2:B:143:SER:OG	2.09	0.53
1:D:77:TYR:CD1	2:E:19:THR:HB	2.44	0.52
2:B:92:TYR:HB3	2:B:95:VAL:HG23	1.91	0.52
1:A:244:LEU:O	1:A:247:MET:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:24:ARG:HG2	3:F:24:ARG:HH11	1.72	0.52
2:E:161:ARG:HD2	10:E:660:HOH:O	2.10	0.52
2:E:256:LYS:NZ	10:E:607:HOH:O	2.41	0.52
2:B:365:ASP:O	10:B:602:HOH:O	2.19	0.52
1:A:136:GLN:HE21	1:A:169:PRO:HD3	1.74	0.51
1:A:217:GLN:HG3	1:A:234:THR:HG21	1.92	0.51
1:A:139:ALA:O	1:A:143:ILE:HG23	2.11	0.51
2:B:451[B]:HIS:HE1	10:E:760:HOH:O	1.93	0.51
1:D:2:PRO:N	1:D:26:GLU:OE1	2.43	0.51
2:B:361:GLN:HG3	10:B:712:HOH:O	2.10	0.50
2:E:428:THR:CG2	10:E:737:HOH:O	2.56	0.50
1:A:362:PHE:CZ	4:A:601:S5Q:S2B	3.05	0.50
2:B:325:VAL:HG11	10:B:601:HOH:O	2.11	0.50
2:E:166:ARG:NH1	2:E:233:GLY:O	2.38	0.50
1:D:316:LYS:N	1:D:317:PRO:CD	2.75	0.50
1:D:359:TYR:C	1:D:359:TYR:HD1	2.20	0.50
1:D:78:ASP:HB3	2:E:48:PHE:HB3	1.94	0.50
2:E:83:GLU:O	2:E:87:VAL:HG23	2.11	0.50
2:E:60:SER:HA	10:E:724:HOH:O	2.12	0.50
1:A:77:TYR:CD1	2:B:19:THR:HB	2.48	0.49
1:A:374:ARG:HD2	10:C:209:HOH:O	2.13	0.49
1:A:96:TYR:HA	2:B:15:ASN:HD21	1.78	0.48
2:B:262:ILE:HD12	2:B:262:ILE:N	2.28	0.48
1:D:61:PRO:HG3	1:D:85:TYR:CD2	2.49	0.48
1:A:181:HIS:HD2	1:A:263:TYR:CD1	2.32	0.48
2:B:22:PRO:O	2:B:26:GLN:HG3	2.13	0.48
1:D:259:ARG:CZ	1:D:259:ARG:HA	2.44	0.48
1:A:259:ARG:HD2	1:A:367:ASP:OD2	2.14	0.48
1:D:359:TYR:C	1:D:359:TYR:CD1	2.92	0.48
2:E:80:ARG:HD2	10:E:840:HOH:O	2.14	0.48
2:E:339:PRO:O	2:E:368:MET:HE2	2.14	0.47
1:A:332:CYS:HB2	1:A:402:ILE:HG22	1.97	0.47
2:E:92:TYR:HB3	2:E:95:VAL:HG23	1.95	0.47
2:E:278:GLN:NE2	10:E:606:HOH:O	2.37	0.47
1:A:423:HIS:HB3	5:A:602:HCA:O6	2.15	0.46
2:B:173:ILE:O	2:B:199:ALA:HA	2.15	0.46
1:D:193:GLY:HA2	1:D:248:HIS:CE1	2.50	0.46
2:E:387:GLY:N	10:E:608:HOH:O	2.41	0.46
1:A:97:THR:H	2:B:15:ASN:HD21	1.62	0.46
3:C:76:CYS:O	3:C:79:VAL:HG22	2.15	0.46
2:B:451[A]:HIS:HE1	10:B:759:HOH:O	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:GLU:HA	1:D:493:ARG:O	2.16	0.46
2:B:325:VAL:CG1	10:B:601:HOH:O	2.64	0.46
2:B:319:TYR:CZ	2:B:395:GLY:HA3	2.51	0.46
3:C:128:SER:HB2	10:C:240:HOH:O	2.16	0.45
1:A:130:LYS:NZ	10:A:730:HOH:O	2.49	0.45
2:B:173:ILE:HG22	10:B:603:HOH:O	2.16	0.45
2:E:113:VAL:HA	2:E:116:VAL:HG12	1.98	0.45
1:D:421:ASN:H	1:D:426:HIS:HD2	1.65	0.45
1:A:60:THR:N	1:A:61:PRO:CD	2.79	0.45
1:D:60:THR:N	1:D:61:PRO:CD	2.79	0.45
1:A:187:TRP:CZ2	1:A:244:LEU:HB3	2.52	0.45
1:A:287:LEU:HD21	1:A:432:GLY:HA2	1.98	0.45
1:A:323:LYS:HG2	1:A:327:MET:HE1	1.99	0.44
1:A:316:LYS:N	1:A:317:PRO:CD	2.81	0.44
1:A:232:LEU:HD21	1:A:246:ALA:O	2.18	0.44
2:E:40:HIS:CE1	2:E:81:VAL:HG23	2.52	0.44
1:D:227:MET:HE3	1:D:304:ALA:HB2	1.98	0.44
2:E:202:LEU:HA	2:E:203:PHE:HA	1.76	0.44
1:D:140:THR:HA	1:D:143:ILE:HG12	1.99	0.44
2:B:37:GLY:HA2	2:B:99:PRO:HD2	2.00	0.44
1:D:198:GLU:HB2	10:D:905:HOH:O	2.18	0.44
1:A:126:PHE:HA	1:A:128:GLN:HE22	1.83	0.44
1:A:404:THR:O	1:A:421:ASN:HA	2.18	0.44
3:C:84:LEU:HD11	3:C:88:TYR:CZ	2.53	0.44
1:D:225:LYS:HE3	1:D:510:TYR:CD2	2.53	0.43
1:D:458:ASP:CG	1:D:461:LYS:HG2	2.42	0.43
1:A:370:LYS:NZ	10:A:726:HOH:O	2.48	0.43
2:B:202:LEU:HA	2:B:203:PHE:HA	1.81	0.43
1:D:50:ALA:HB3	1:D:169:PRO:O	2.19	0.43
1:A:207:TYR:O	1:A:234:THR:HA	2.19	0.43
1:A:318:GLU:HA	1:A:493:ARG:O	2.19	0.43
1:D:287:LEU:HD21	1:D:432:GLY:HA2	2.01	0.42
3:C:51:ASN:O	3:C:55:LEU:HB2	2.18	0.42
1:D:259:ARG:HD2	1:D:367:ASP:OD2	2.18	0.42
1:A:127:PRO:O	1:A:130:LYS:HE2	2.18	0.42
1:A:334:TRP:N	1:A:335:PRO:CD	2.82	0.42
3:F:24:ARG:HG2	3:F:24:ARG:NH1	2.34	0.42
1:D:264:ILE:O	1:D:268:LEU:HG	2.20	0.42
1:D:334:TRP:N	1:D:335:PRO:CD	2.82	0.42
1:A:241:TYR:CE1	1:A:245:ARG:HD2	2.55	0.42
2:B:80:ARG:HD2	10:B:891:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:GLN:OE1	1:D:37:LEU:HD11	2.20	0.42
2:E:152:TYR:O	2:E:156:VAL:HG23	2.20	0.42
2:E:366:TYR:OH	2:E:368:MET:HE2	2.18	0.42
1:A:61:PRO:HG3	1:A:85:TYR:CD2	2.55	0.42
1:A:344:ALA:HB3	1:A:374:ARG:HB3	2.02	0.42
1:D:359:TYR:CG	1:D:385:PRO:HG3	2.55	0.42
1:D:467:TRP:O	1:D:468:GLY:C	2.62	0.42
2:E:364:VAL:HG21	2:E:368:MET:HE1	2.02	0.42
3:F:73:HIS:O	3:F:77:TYR:CD2	2.73	0.42
2:B:254:GLN:O	2:B:258:GLU:HA	2.20	0.41
2:B:415:PHE:HA	2:B:416:PRO:HA	1.83	0.41
3:F:78:TRP:O	3:F:82:VAL:HG23	2.19	0.41
2:B:227:GLU:HG3	10:B:849:HOH:O	2.21	0.41
3:C:99:SER:N	3:C:102:GLU:OE2	2.46	0.41
1:A:136:GLN:NE2	1:A:169:PRO:HD3	2.36	0.41
3:F:101:GLU:HG2	10:F:243:HOH:O	2.19	0.41
2:B:194:GLU:O	2:B:289:PRO:HG3	2.20	0.41
1:D:280:ASP:CG	1:D:374:ARG:HH22	2.29	0.41
2:B:98:VAL:HB	2:B:136:LEU:HD23	2.03	0.41
2:B:145:VAL:HB	10:B:704:HOH:O	2.20	0.41
2:B:428:THR:CG2	10:B:749:HOH:O	2.67	0.41
1:A:49:CYS:HB2	1:A:170:GLY:CA	2.51	0.41
1:A:396:MET:CE	10:A:845:HOH:O	2.68	0.41
1:A:495:TYR:CZ	1:A:497:GLY:HA3	2.56	0.41
3:C:21:MET:HE1	3:C:105:SER:HB3	2.02	0.41
1:D:423:HIS:HA	4:D:601:S5Q:S4B	2.61	0.41
2:E:42:GLY:HA3	6:E:501:CLF:S2A	2.60	0.40
1:A:208:VAL:HG12	1:A:261:ALA:HB1	2.04	0.40
2:B:40:HIS:CE1	2:B:81:VAL:HG23	2.56	0.40
2:B:314:LYS:HD3	10:B:714:HOH:O	2.21	0.40
3:C:57:LYS:NZ	3:C:74:ASP:OD1	2.54	0.40
1:A:457:ILE:HG21	1:A:467:TRP:HZ2	1.87	0.40
1:D:39:THR:CB	2:E:43:GLN:HE22	2.35	0.40
3:F:94:TRP:CE3	3:F:95:ILE:CA	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	517/515 (100%)	499 (96%)	18 (4%)	0	100	100
1	D	512/515 (99%)	491 (96%)	21 (4%)	0	100	100
2	B	460/461 (100%)	449 (98%)	11 (2%)	0	100	100
2	E	460/461 (100%)	449 (98%)	11 (2%)	0	100	100
3	C	117/119 (98%)	115 (98%)	2 (2%)	0	100	100
3	F	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
All	All	2183/2190 (100%)	2116 (97%)	67 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	435/431 (101%)	420 (97%)	15 (3%)	32	7
1	D	430/431 (100%)	420 (98%)	10 (2%)	44	14
2	B	389/388 (100%)	383 (98%)	6 (2%)	57	27
2	E	389/388 (100%)	383 (98%)	6 (2%)	57	27
3	C	110/110 (100%)	108 (98%)	2 (2%)	51	21
3	F	110/110 (100%)	108 (98%)	2 (2%)	51	21
All	All	1863/1858 (100%)	1822 (98%)	41 (2%)	45	15

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	44	ILE
1	A	73	VAL
1	A	108	VAL
1	A	182	LYS
1	A	233[A]	SER
1	A	233[B]	SER
1	A	244	LEU
1	A	354	LYS
1	A	359	TYR
1	A	374	ARG
1	A	454	LEU
1	A	461	LYS
1	A	508	ARG
1	A	516	LYS
2	B	159	VAL
2	B	219	VAL
2	B	255	LYS
2	B	303	LEU
2	B	428	THR
2	B	458	VAL
3	C	24	ARG
3	C	87	ASP
1	D	20	VAL
1	D	44	ILE
1	D	244	LEU
1	D	354	LYS
1	D	359	TYR
1	D	374	ARG
1	D	453	GLN
1	D	454	LEU
1	D	467	TRP
1	D	508	ARG
2	E	145	VAL
2	E	167	GLU
2	E	219	VAL
2	E	263	ILE
2	E	358	LYS
2	E	428	THR
3	F	18	VAL
3	F	24	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	89	ASN
1	A	117	GLN
1	A	128	GLN
1	A	136	GLN
1	A	148	ASN
1	A	203	HIS
1	A	345	HIS
1	A	426	HIS
1	A	494	GLN
2	B	15	ASN
2	B	43	GLN
2	B	254	GLN
2	B	278	GLN
2	B	385	ASN
2	B	407	ASN
2	B	454	ASN
3	C	96	ASN
1	D	18	HIS
1	D	89	ASN
1	D	136	GLN
1	D	148	ASN
1	D	426	HIS
1	D	453	GLN
2	E	21	GLN
2	E	200	ASN
2	E	407	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic and 2 are modelled with single atom - leaving 6 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
6	CLF	A	603	2,1	0,24,24	-	-	-		
5	HCA	A	602	4	13,13,13	1.14	0	15,18,18	1.41	2 (13%)
6	CLF	E	501	2,1	0,24,24	-	-	-		
4	S5Q	A	601	1,5,7	6,30,30	1.45	1 (16%)	-		
5	HCA	D	602	4	13,13,13	0.99	0	15,18,18	1.40	2 (13%)
4	S5Q	D	601	1,5,7	6,30,30	1.18	1 (16%)	-		

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	HCA	D	602	4	-	2/17/17/17	-
5	HCA	A	602	4	-	4/17/17/17	-
6	CLF	E	501	2,1	-	-	0/12/10/10
6	CLF	A	603	2,1	-	-	0/12/10/10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	S5Q	S2B-FE6	-2.94	2.18	2.24
4	D	601	S5Q	S2B-FE6	-2.46	2.19	2.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HCA	O7-C3-C4	3.27	114.12	108.88
5	D	602	HCA	O7-C3-C4	2.95	113.61	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HCA	O5-C7-C3	-2.67	116.91	122.09
5	D	602	HCA	O5-C7-C3	-2.27	117.69	122.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	602	HCA	C4-C5-C6-O4
5	A	602	HCA	C4-C5-C6-O4
5	D	602	HCA	C4-C5-C6-O3
5	A	602	HCA	C4-C5-C6-O3
5	A	602	HCA	O1-C1-C2-C3
5	A	602	HCA	O2-C1-C2-C3

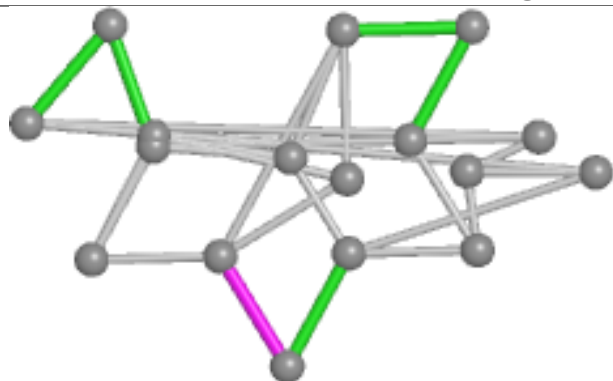
There are no ring outliers.

4 monomers are involved in 5 short contacts:

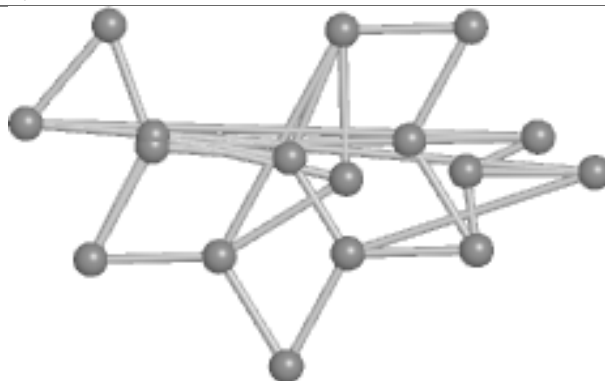
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	HCA	1	0
6	E	501	CLF	1	0
4	A	601	S5Q	1	0
4	D	601	S5Q	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

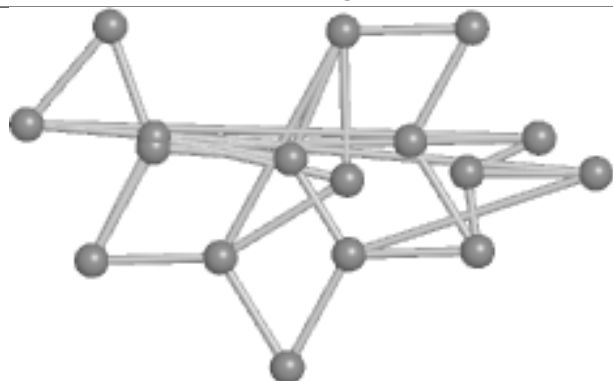
Ligand S5Q A 601



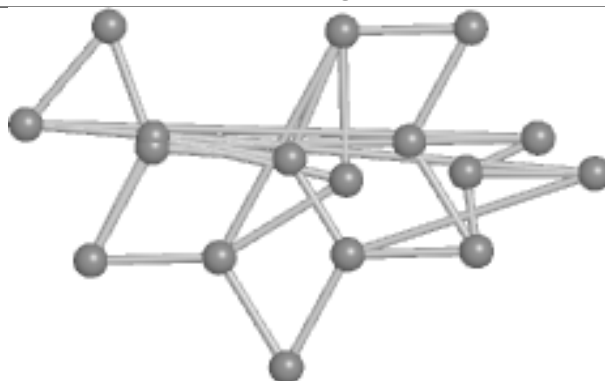
Bond lengths



Bond angles

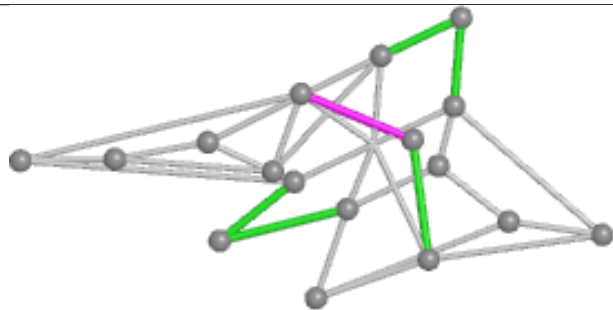


Torsions

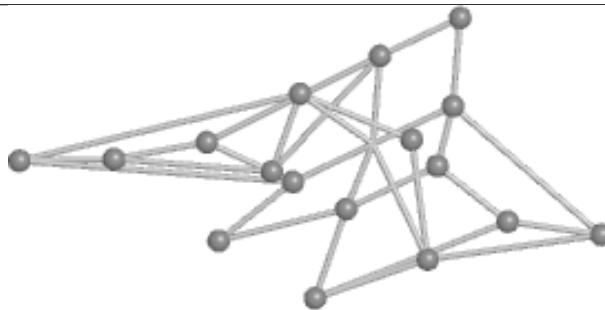


Rings

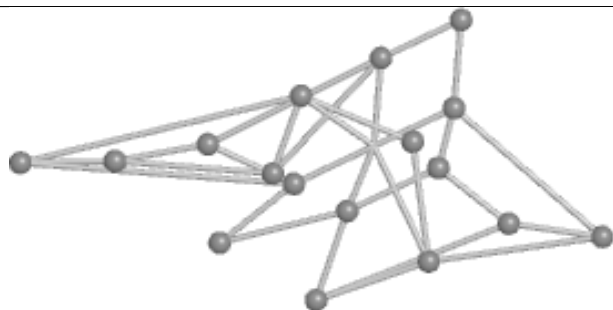
Ligand S5Q D 601



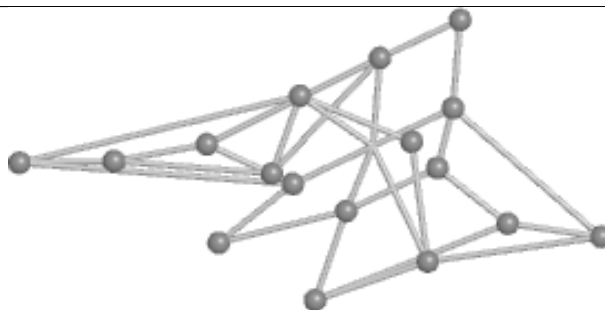
Bond lengths



Bond angles



Torsions



Rings

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	515/515 (100%)	0.13	11 (2%) 63 73	9, 25, 49, 92	4 (0%)
1	D	513/515 (99%)	0.36	16 (3%) 51 61	12, 30, 57, 95	1 (0%)
2	B	461/461 (100%)	-0.17	0 100 100	9, 21, 39, 53	1 (0%)
2	E	461/461 (100%)	0.02	6 (1%) 75 81	8, 24, 44, 59	1 (0%)
3	C	119/119 (100%)	0.95	13 (10%) 10 14	24, 41, 58, 68	0
3	F	119/119 (100%)	1.40	27 (22%) 2 3	31, 51, 72, 86	0
All	All	2188/2190 (99%)	0.21	73 (3%) 49 58	8, 27, 55, 95	7 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	467	TRP	11.7
1	D	467	TRP	9.6
1	A	465	PRO	5.4
1	D	464	ALA	5.2
1	D	465	PRO	4.9
1	A	512	ALA	4.3
3	C	14	VAL	4.2
1	D	468	GLY	4.1
1	D	109	PHE	4.0
3	F	94	TRP	3.7
1	D	512	ALA	3.6
1	D	513	PHE	3.3
1	A	464	ALA	3.3
1	D	108	VAL	3.2
3	F	14	VAL	3.2
1	D	199	ILE	3.2
3	F	110	LEU	3.2
3	F	18	VAL	3.1
1	A	511	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	95	ILE	3.1
3	C	103	ILE	3.1
3	F	63	CYS	3.0
3	F	95	ILE	2.9
3	C	67	VAL	2.9
3	F	82	VAL	2.9
3	F	103	ILE	2.8
3	C	106	LEU	2.8
3	F	67	VAL	2.7
3	C	25	ILE	2.7
3	F	25	ILE	2.7
3	F	106	LEU	2.7
1	A	469	ASN	2.7
1	D	469	ASN	2.7
1	D	302	ASP	2.7
3	F	105	SER	2.7
1	A	516	LYS	2.6
3	C	62	LEU	2.5
1	A	108	VAL	2.5
3	F	88	TYR	2.5
3	C	101	GLU	2.4
1	D	299	GLY	2.4
3	F	20	PRO	2.4
1	A	199	ILE	2.4
3	F	28	LEU	2.4
3	F	62	LEU	2.4
1	D	482	LEU	2.3
2	E	230	ILE	2.3
3	F	23	ALA	2.3
3	C	63	CYS	2.3
1	D	463	ASN	2.3
3	F	29	THR	2.3
1	A	468	GLY	2.3
2	E	257	PHE	2.2
3	F	16	ALA	2.2
1	D	200	THR	2.2
3	C	92	TYR	2.2
3	F	61	LEU	2.1
3	F	66	PRO	2.1
3	F	101	GLU	2.1
2	E	130	PRO	2.1
3	F	17	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	84	LEU	2.1
3	F	85	ALA	2.1
1	A	109	PHE	2.1
1	D	300	ILE	2.1
2	E	252	TYR	2.1
3	C	93	PRO	2.1
3	C	18	VAL	2.0
2	E	165	LYS	2.0
3	F	91	HIS	2.0
2	E	127	GLU	2.0
3	C	16	ALA	2.0
3	F	117	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	HCA	A	602	14/14	0.94	0.06	12,14,17,17	0
5	HCA	D	602	14/14	0.96	0.05	15,18,20,20	0
4	S5Q	A	601	18/18	0.99	0.02	13,15,16,17	1
4	S5Q	D	601	18/18	0.99	0.03	16,18,20,21	1
6	CLF	A	603	15/15	0.99	0.02	13,15,17,19	0
6	CLF	E	501	15/15	0.99	0.03	17,18,20,21	0
8	H2S	A	605	1/1	0.99	0.02	14,14,14,14	1
8	H2S	D	604	1/1	0.99	0.05	18,18,18,18	1
9	MG	B	501	1/1	0.99	0.01	16,16,16,16	0
9	MG	B	502	1/1	0.99	0.05	15,15,15,15	0
7	O	A	604	1/1	1.00	0.02	16,16,16,16	1

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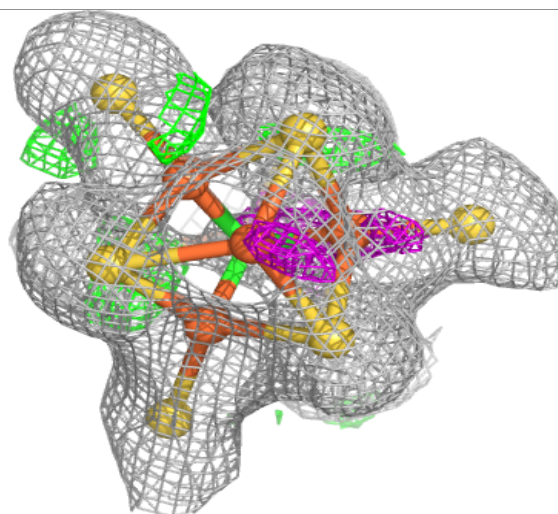
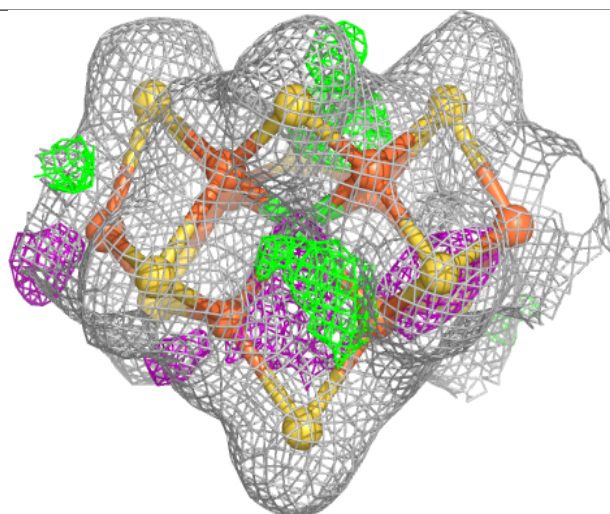
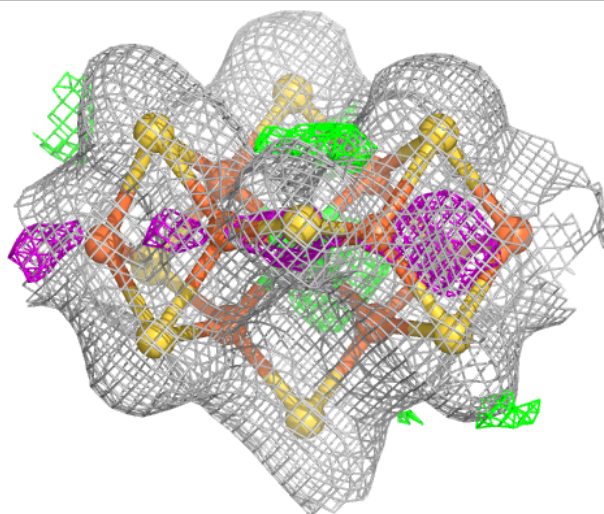
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	O	D	603	1/1	1.00	0.02	10,10,10,10	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

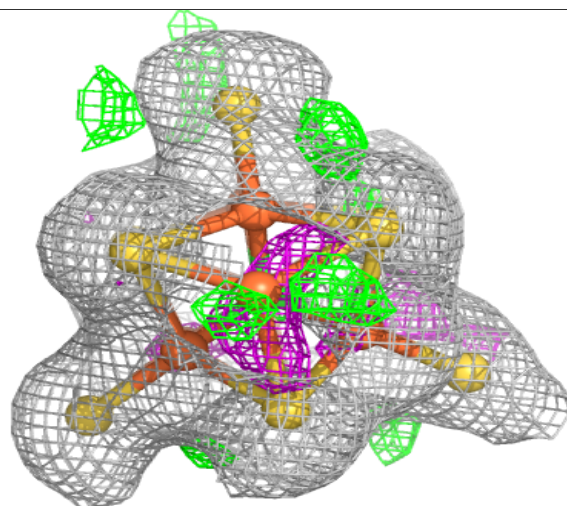
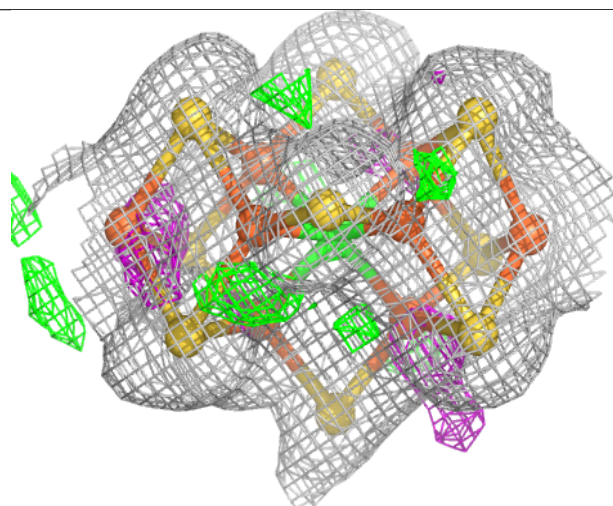
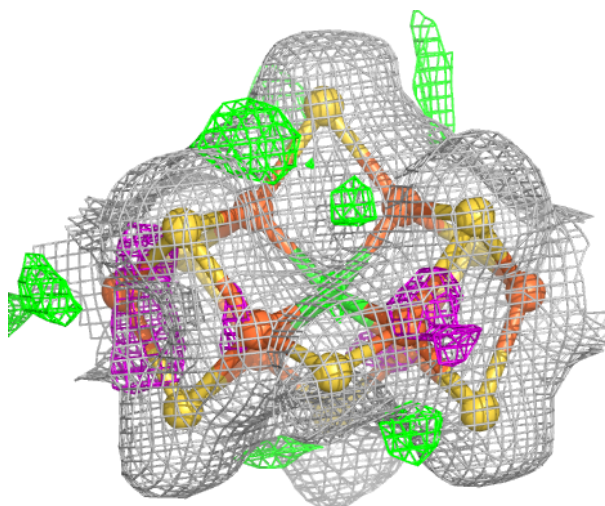
Electron density around S5Q A 601:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around S5Q D 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.