



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:12 PM GMT

PDB ID : 4WZB
Title : Crystal Structure of MgAMPPCP-bound Av2-Av1 complex
Authors : Tezcan, F.A.; Kaiser, J.T.; Mustafi, D.; Walton, M.Y.; Howard, J.B.; Rees, D.C.
Deposited on : 2014-11-19
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

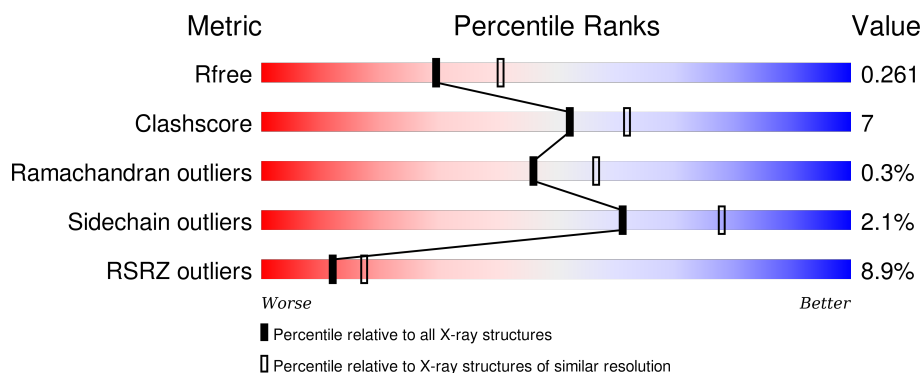
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	477	<div> <div>9%</div> <div>83%</div> <div>16%</div> </div>
1	C	477	<div> <div>6%</div> <div>84%</div> <div>16%</div> </div>
2	B	522	<div> <div>3%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
2	D	522	<div> <div>4%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
3	E	272	<div> <div>25%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	272	<div><div></div><div>15%</div><div>74%</div><div>21%</div><div></div><div></div></div>
3	G	272	<div><div></div><div>11%</div><div>86%</div><div>13%</div><div></div><div></div></div>
3	H	272	<div><div></div><div>11%</div><div>79%</div><div>17%</div><div></div><div></div></div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 25156 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 molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3790	2410	647	708	25			
1	C	476	Total	C	N	O	S	0	0	0
			3782	2405	646	707	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	GLN	GLU	variant	UNP P07328
C	440	GLN	GLU	variant	UNP P07328

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

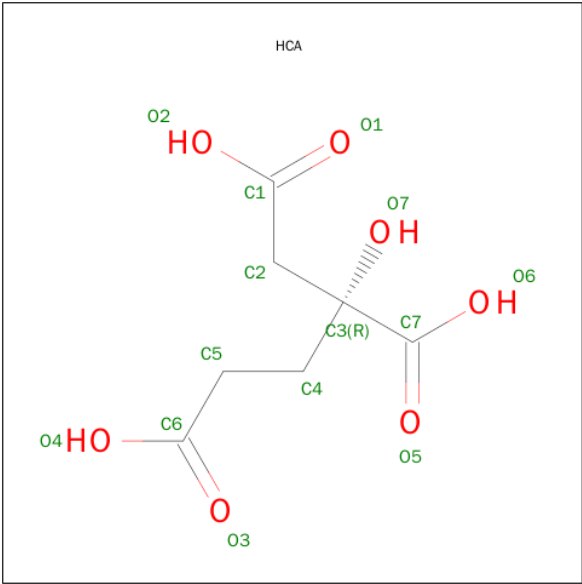
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	1	0	0
			4174	2666	705	775	28			

- Molecule 3 is a protein called Nitrogenase iron protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	270	Total	C	N	O	S	151	0	0
			2042	1274	349	399	20			
3	F	263	Total	C	N	O	S	94	0	0
			1983	1236	342	386	19			
3	G	272	Total	C	N	O	S	91	0	0
			2057	1285	351	401	20			
3	H	262	Total	C	N	O	S	31	0	0
			1974	1231	341	383	19			

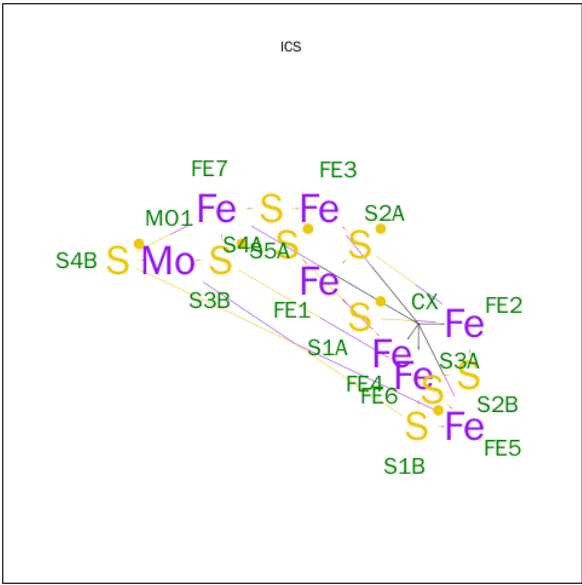
- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (for-

mula: C₇H₁₀O₇).



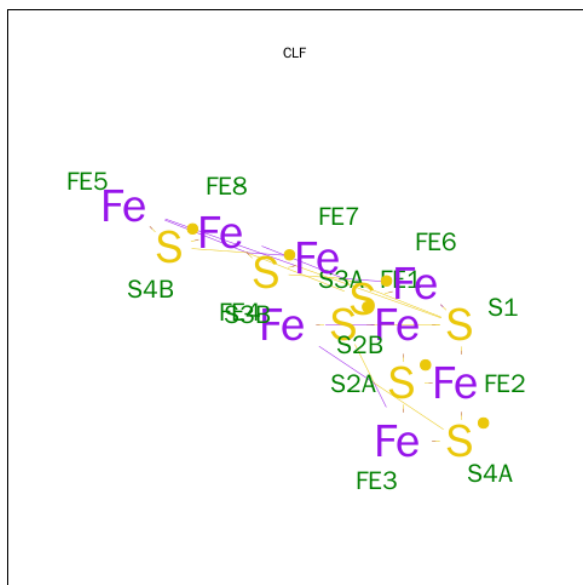
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	7	7		
4	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is iron-sulfur-molybdenum cluster with interstitial carbon (three-letter code: ICS) (formula: CFe₇MoS₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Fe	Mo	S	
			18	1	7	1	9	
5	C	1	Total	C	Fe	Mo	S	
			18	1	7	1	9	

- Molecule 6 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe₈S₇).



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

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Fe		
			1	1		
7	D	1	Total	Fe		
			1	1		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

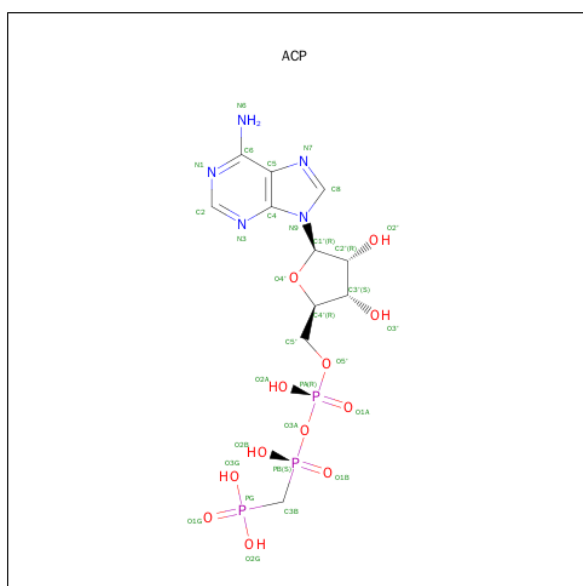
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total	Mg		
			1	1		

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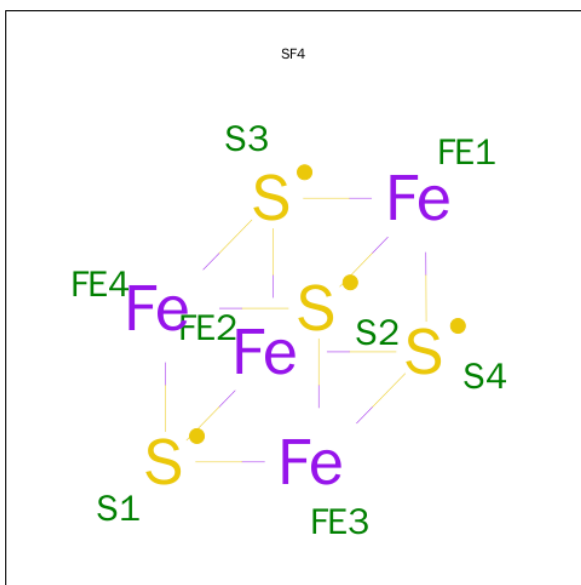
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		
8	E	1	Total	Mg	0	0
			1	1		

- Molecule 9 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
9	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
9	G	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
9	H	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	Fe	S	0	0
			8	4	4		
10	G	1	Total	Fe	S	0	0
			8	4	4		

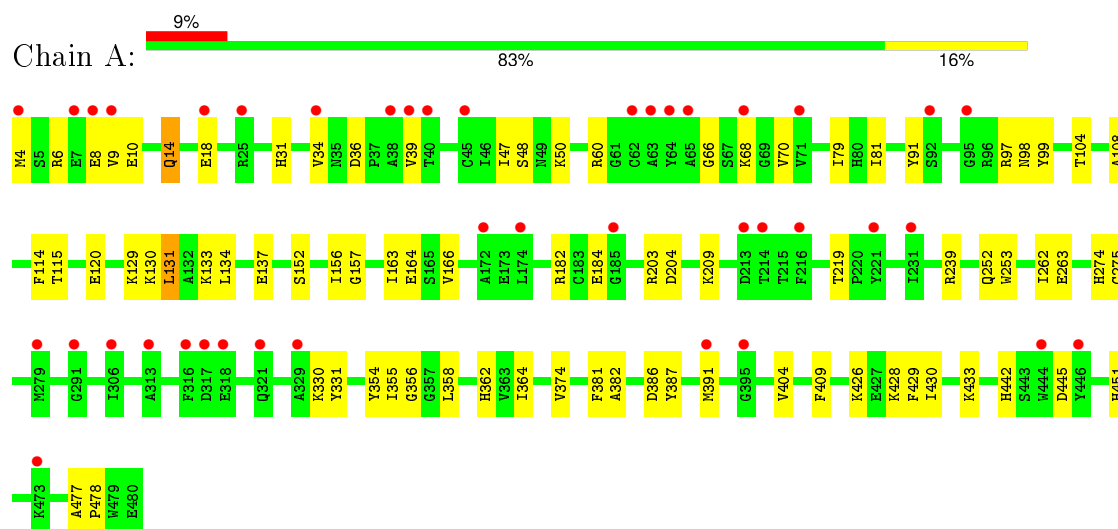
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	131	Total	O	0	0
			131	131		
11	B	243	Total	O	0	0
			243	243		
11	C	172	Total	O	0	0
			172	172		
11	D	213	Total	O	0	0
			213	213		
11	E	23	Total	O	0	0
			23	23		
11	F	42	Total	O	0	0
			42	42		
11	G	54	Total	O	0	0
			54	54		
11	H	62	Total	O	0	0
			62	62		

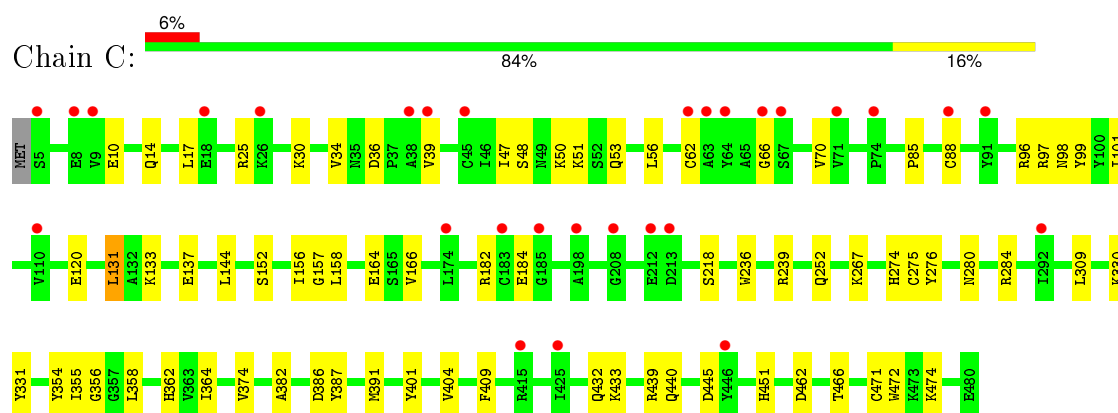
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

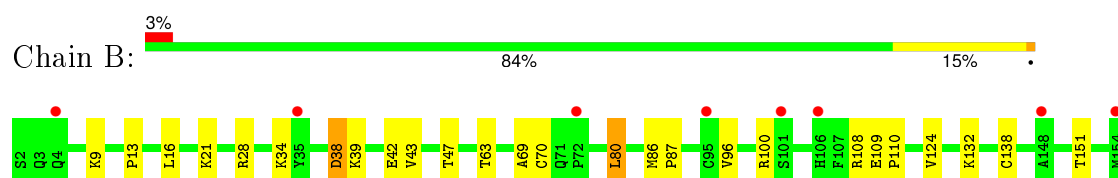
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

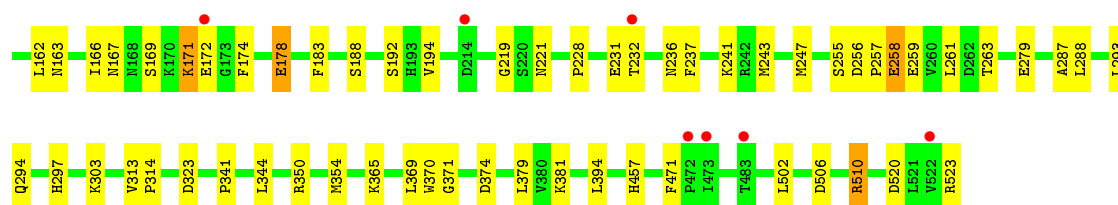


- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

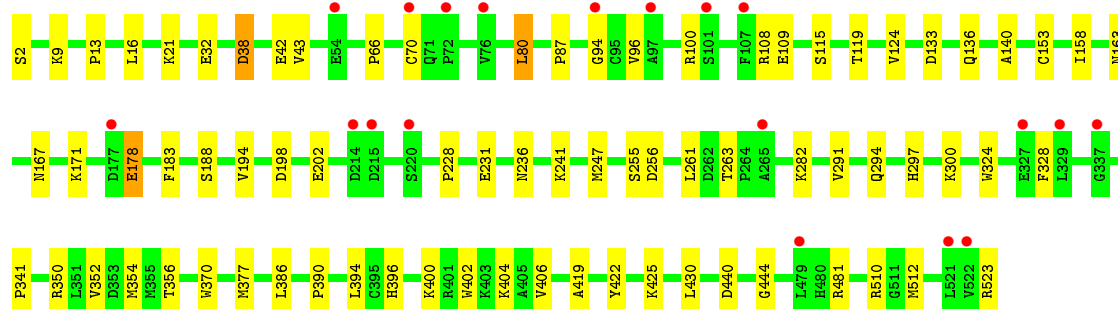
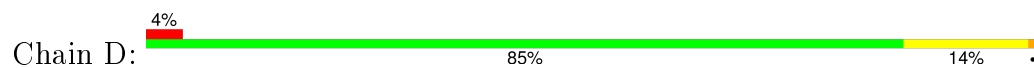


- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

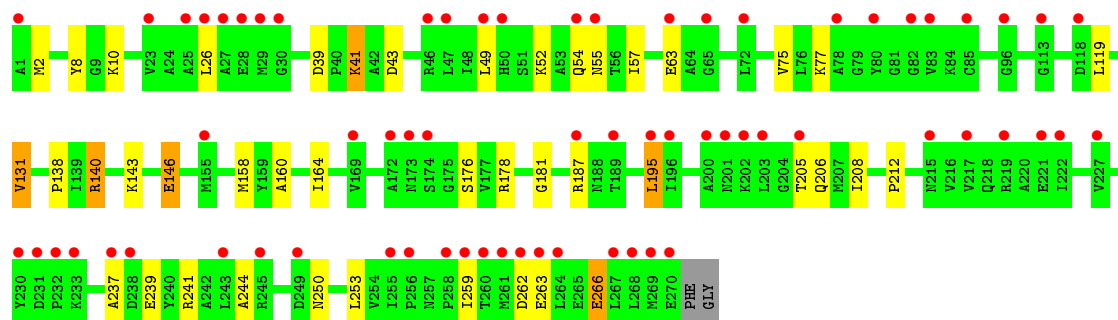
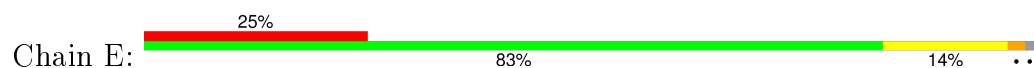




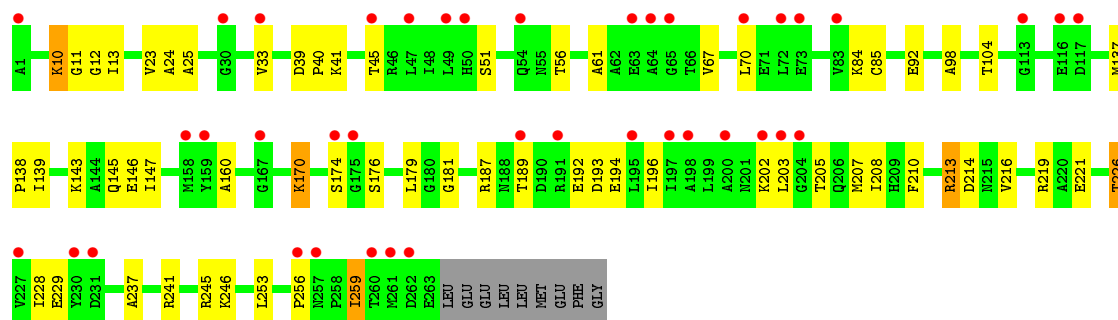
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain



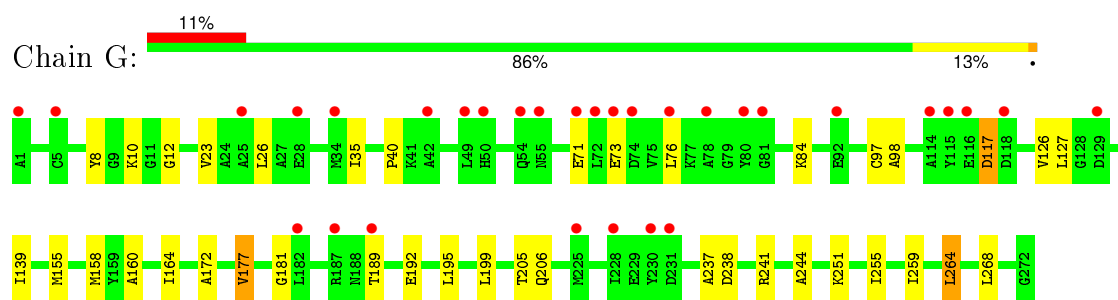
• Molecule 3: Nitrogenase iron protein 1



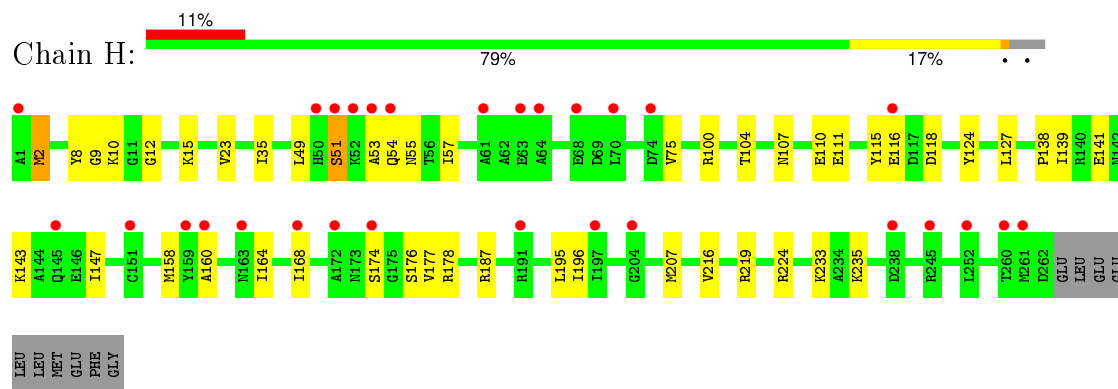
• Molecule 3: Nitrogenase iron protein 1



• Molecule 3: Nitrogenase iron protein 1



• Molecule 3: Nitrogenase iron protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.53Å 120.89Å 264.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 2.30 49.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.2 (49.38-2.30) 88.7 (49.38-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.255 0.215 , 0.261	Depositor DCC
R_{free} test set	9916 reflections (7.58%)	DCC
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 159724 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25156	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.52% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, HCA, SF4, ACP, FE2, ICS, CLF

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	0/3878	0.66	0/5229
1	C	0.59	1/3870 (0.0%)	0.70	0/5219
2	B	0.61	0/4280	0.69	2/5786 (0.0%)
2	D	0.63	0/4280	0.68	0/5786
3	E	0.39	0/2065	0.64	0/2782
3	F	0.44	0/2006	0.65	0/2703
3	G	0.48	0/2081	0.66	0/2803
3	H	0.51	0/1997	0.73	0/2691
All	All	0.56	1/24457 (0.0%)	0.68	2/32999 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	88	CYS	CB-SG	-6.80	1.70	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	510	ARG	NE-CZ-NH2	-5.77	117.42	120.30
2	B	506	ASP	CB-CG-OD1	5.54	123.28	118.30

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	3790	0	3731	52	0
1	C	3782	0	3722	53	0
2	B	4174	0	4088	53	0
2	D	4174	0	4088	54	0
3	E	2042	0	2059	27	0
3	F	1983	0	1999	46	0
3	G	2057	0	2071	22	0
3	H	1974	0	1993	28	0
4	A	14	0	6	2	0
4	C	14	0	6	1	0
5	A	18	0	0	0	0
5	C	18	0	0	1	0
6	A	15	0	0	0	0
6	C	15	0	0	1	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
9	E	31	0	14	0	0
9	F	31	0	14	3	0
9	G	31	0	14	1	0
9	H	31	0	14	1	0
10	E	8	0	0	0	0
10	G	8	0	0	0	0
11	A	131	0	0	7	0
11	B	243	0	0	7	0
11	C	172	0	0	8	0
11	D	213	0	0	14	0
11	E	23	0	0	3	0
11	F	42	0	0	4	0
11	G	54	0	0	1	0
11	H	62	0	0	3	0
All	All	25156	0	23819	318	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 7.

All (318) 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:H:178:ARG:NH1	11:H:1312:HOH:O	2.01	0.93
3:E:206:GLN:HE21	3:E:208:ILE:HD13	1.39	0.86
3:G:259:ILE:HD11	3:G:264:LEU:HD13	1.59	0.84
2:D:136:GLN:NE2	11:D:1618:HOH:O	2.11	0.84
1:A:157:GLY:HA3	1:A:184:GLU:HG2	1.66	0.78
1:C:51:LYS:O	11:C:1581:HOH:O	2.03	0.77
2:D:481:ARG:O	11:D:1604:HOH:O	2.03	0.76
2:D:2:SER:N	11:D:1663:HOH:O	2.18	0.75
2:B:510:ARG:NH2	11:B:1627:HOH:O	2.21	0.74
1:C:267:LYS:O	11:C:1570:HOH:O	2.07	0.72
2:D:32:GLU:OE1	11:D:1619:HOH:O	2.07	0.72
2:D:422:TYR:HB3	2:D:425:LYS:HG3	1.70	0.71
1:C:239:ARG:HH11	1:C:252:GLN:HE21	1.38	0.71
2:D:440:ASP:OD1	11:D:1697:HOH:O	2.07	0.70
3:F:61:ALA:HA	3:F:70:LEU:HD11	1.73	0.69
1:A:239:ARG:HD2	1:A:252:GLN:NE2	2.08	0.69
3:F:67:VAL:HA	3:F:70:LEU:HD13	1.74	0.69
3:F:12:GLY:HA2	9:F:1292:ACP:H3B1	1.74	0.68
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.74	0.68
3:H:233:LYS:NZ	11:H:1301:HOH:O	2.27	0.68
3:G:84:LYS:NZ	3:G:117:ASP:OD2	2.27	0.68
3:F:139:ILE:HG21	3:F:147:ILE:HD11	1.75	0.68
3:E:2:MET:HE2	3:E:119:LEU:HB2	1.77	0.67
1:C:239:ARG:HD2	1:C:252:GLN:NE2	2.10	0.67
3:F:10:LYS:HD2	3:F:160:ALA:HB2	1.77	0.66
3:G:139:ILE:HB	3:G:177:VAL:HG11	1.77	0.66
2:D:231:GLU:CD	2:D:236:ASN:HD22	1.96	0.66
2:B:520:ASP:OD2	1:C:97:ARG:HD2	1.96	0.66
2:D:386:LEU:O	11:D:1540:HOH:O	2.14	0.66
3:E:49:LEU:O	11:E:1320:HOH:O	2.14	0.65
1:A:91:TYR:O	11:A:1571:HOH:O	2.13	0.65
1:A:97:ARG:NH1	1:A:99:TYR:OH	2.30	0.65
1:C:382:ALA:HB1	1:C:386:ASP:HB2	1.79	0.64
2:D:167:ASN:HB2	3:H:174:SER:HB2	1.79	0.64
3:E:43:ASP:OD1	11:E:1322:HOH:O	2.16	0.62
3:F:39:ASP:O	11:F:1316:HOH:O	2.16	0.62
2:B:171:LYS:HD3	2:B:172:GLU:HG3	1.81	0.61
3:G:12:GLY:HA2	9:G:1290:ACP:H3B1	1.81	0.61
2:B:9:LYS:HB3	2:B:13:PRO:HD2	1.82	0.61
2:B:39:LYS:NZ	2:B:42:GLU:OE2	2.30	0.60
3:H:51:SER:HA	3:H:224:ARG:HD3	1.83	0.60
3:G:71:GLU:HB3	3:G:73:GLU:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:181:GLY:HA2	3:E:205:THR:CG2	2.32	0.60
3:E:181:GLY:HA2	3:E:205:THR:HG23	1.83	0.60
1:A:47:ILE:HD12	1:A:48:SER:H	1.67	0.60
3:F:40:PRO:HG3	3:F:98:ALA:HB1	1.84	0.59
1:A:433:LYS:NZ	2:B:263:THR:O	2.36	0.59
1:A:381:PHE:HA	11:A:1552:HOH:O	2.02	0.59
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.84	0.59
1:A:129:LYS:NZ	11:A:1501:HOH:O	2.34	0.59
1:A:81:ILE:HD12	1:A:134:LEU:HD21	1.85	0.59
3:E:131:VAL:HG13	3:F:98:ALA:HB3	1.84	0.58
2:D:133:ASP:OD2	11:D:1699:HOH:O	2.17	0.58
2:D:247:MET:HG2	2:D:341:PRO:HD3	1.86	0.58
1:A:36:ASP:HB3	1:A:39:VAL:HG23	1.86	0.58
3:F:214:ASP:OD1	3:F:216:VAL:HG23	2.04	0.57
3:F:226:THR:HB	3:F:229:GLU:H	1.69	0.57
3:F:221:GLU:OE2	9:F:1292:ACP:O3'	2.18	0.57
1:C:164:GLU:OE2	1:C:182:ARG:HD3	2.04	0.57
3:H:51:SER:HA	3:H:224:ARG:HH11	1.69	0.57
2:B:28:ARG:HD2	2:B:34:LYS:HD3	1.87	0.57
3:H:49:LEU:HD13	3:H:53:ALA:HB2	1.87	0.57
2:D:282:LYS:NZ	11:D:1684:HOH:O	2.38	0.57
3:F:241:ARG:O	3:F:245:ARG:HG3	2.05	0.56
2:B:231:GLU:CD	2:B:236:ASN:HD22	2.09	0.56
3:E:39:ASP:OD1	3:E:41:LYS:HG2	2.04	0.56
1:A:387:TYR:O	1:A:391:MET:HG3	2.05	0.56
2:B:70:CYS:HB2	2:B:188:SER:HB2	1.87	0.56
2:D:394:LEU:HD13	2:D:430:LEU:HB2	1.87	0.56
2:D:153:CYS:HB3	2:D:188:SER:OG	2.04	0.56
1:C:157:GLY:HA3	1:C:184:GLU:HG2	1.88	0.56
3:E:250:ASN:O	11:E:1313:HOH:O	2.17	0.56
1:C:440:GLN:NE2	11:C:1614:HOH:O	2.24	0.56
2:B:323:ASP:OD1	1:C:474:LYS:NZ	2.29	0.56
2:D:80:LEU:HD13	2:D:87:PRO:HG2	1.88	0.56
2:D:510:ARG:NH1	11:D:1550:HOH:O	2.39	0.55
4:C:1494:HCA:O2	4:C:1494:HCA:O7	2.24	0.55
1:A:14:GLN:O	1:A:18:GLU:HG3	2.06	0.55
2:D:178:GLU:H	2:D:178:GLU:CD	2.08	0.55
1:C:276:TYR:OH	1:C:284:ARG:NH2	2.40	0.55
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.87	0.55
1:C:120:GLU:OE2	3:H:104:THR:OG1	2.25	0.55
1:A:354:TYR:HB2	1:A:409:PHE:HE2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ALA:HB1	1:A:386:ASP:HB2	1.88	0.54
1:A:164:GLU:OE2	1:A:182:ARG:HD3	2.07	0.54
3:H:139:ILE:O	3:H:177:VAL:HG21	2.08	0.54
3:F:207:MET:HE1	3:F:210:PHE:HB2	1.90	0.54
3:F:61:ALA:CA	3:F:70:LEU:HD11	2.38	0.54
3:G:76:LEU:HD11	3:G:84:LYS:HB3	1.89	0.54
1:A:354:TYR:HB2	1:A:409:PHE:CE2	2.43	0.54
1:C:355:ILE:HG22	1:C:356:GLY:H	1.72	0.53
2:B:132:LYS:HD3	2:B:174:PHE:CE2	2.44	0.53
3:E:54:GLN:HG2	3:E:77:LYS:HD2	1.91	0.53
1:C:439:ARG:HB3	11:C:1639:HOH:O	2.08	0.53
1:C:97:ARG:NH1	1:C:99:TYR:OH	2.42	0.53
3:F:146:GLU:HG2	3:F:253:LEU:HD21	1.91	0.53
3:E:146:GLU:HB3	3:E:253:LEU:HD21	1.89	0.53
2:B:228:PRO:O	2:B:294:GLN:HG3	2.09	0.53
1:C:131:LEU:HD13	1:C:166:VAL:HG11	1.91	0.53
2:D:202:GLU:HG3	2:D:300:LYS:HG2	1.91	0.52
3:F:10:LYS:HE3	3:F:11:GLY:H	1.73	0.52
3:F:23:VAL:HG22	3:F:33:VAL:HG11	1.92	0.52
2:B:247:MET:HG2	2:B:341:PRO:HD3	1.91	0.52
3:G:237:ALA:O	3:G:241:ARG:HG3	2.09	0.52
3:H:141:GLU:HG2	11:H:1338:HOH:O	2.09	0.52
1:A:133:LYS:O	1:A:137:GLU:HG3	2.09	0.51
1:A:355:ILE:HG22	1:A:356:GLY:H	1.76	0.51
1:C:274:HIS:CE1	1:C:451:HIS:CE1	2.99	0.51
3:H:110:GLU:OE1	3:H:143:LYS:NZ	2.36	0.51
2:B:241:LYS:NZ	2:B:256:ASP:OD2	2.42	0.51
3:G:251:LYS:O	11:G:1301:HOH:O	2.19	0.51
1:A:163:ILE:HD11	1:A:182:ARG:HD2	1.93	0.51
3:H:8:TYR:HB3	3:H:164:ILE:HD13	1.92	0.51
4:A:1494:HCA:O7	4:A:1494:HCA:O2	2.28	0.51
1:C:387:TYR:O	1:C:391:MET:HG3	2.11	0.51
1:A:430:ILE:HG13	2:B:110:PRO:HB3	1.92	0.51
2:D:119:THR:HB	11:D:1514:HOH:O	2.10	0.51
3:E:26:LEU:HD12	3:E:244:ALA:HB1	1.93	0.51
3:F:92:GLU:O	11:F:1313:HOH:O	2.19	0.50
2:B:237:PHE:CE1	2:B:257:PRO:HD2	2.46	0.50
2:D:38:ASP:OD1	2:D:38:ASP:N	2.40	0.50
2:B:86:MET:HG2	2:B:138:CYS:SG	2.52	0.50
3:G:158:MET:HE2	3:G:199:LEU:HD22	1.92	0.50
2:D:228:PRO:O	2:D:294:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:GLU:OE1	11:D:1644:HOH:O	2.20	0.50
2:D:9:LYS:HB3	2:D:13:PRO:HD2	1.94	0.50
1:A:330:LYS:HE2	1:A:331:TYR:CZ	2.47	0.50
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.47	0.50
3:F:39:ASP:OD1	3:F:41:LYS:HG2	2.11	0.50
2:B:523:ARG:OXT	2:D:108:ARG:NH2	2.30	0.50
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.47	0.49
3:E:10:LYS:HD3	3:E:160:ALA:HB2	1.93	0.49
3:E:187:ARG:NH1	3:F:187:ARG:HE	2.09	0.49
3:H:10:LYS:HD3	3:H:160:ALA:HB2	1.94	0.49
1:A:4:MET:HG3	1:A:8:GLU:OE2	2.11	0.49
2:B:108:ARG:NH2	2:D:523:ARG:OXT	2.23	0.49
3:F:213:ARG:N	11:F:1342:HOH:O	2.45	0.49
2:B:38:ASP:N	2:B:38:ASP:OD1	2.45	0.49
3:F:137:MET:HB3	3:F:138:PRO:HD3	1.93	0.49
1:C:274:HIS:ND1	11:C:1629:HOH:O	2.28	0.49
1:A:442:HIS:HB3	4:A:1494:HCA:O5	2.12	0.49
2:B:350:ARG:O	2:B:354:MET:HG3	2.12	0.49
1:C:330:LYS:HE2	1:C:331:TYR:CZ	2.47	0.49
2:B:80:LEU:HD13	2:B:87:PRO:CG	2.43	0.49
3:G:155:MET:HG2	3:G:268:LEU:HD13	1.95	0.49
1:C:85:PRO:HB2	6:C:1498:CLF:S2B	2.53	0.48
3:F:237:ALA:O	3:F:241:ARG:HG3	2.13	0.48
11:A:1594:HOH:O	3:E:140:ARG:HD3	2.12	0.48
3:F:45:THR:HG21	3:F:85:CYS:HB3	1.95	0.48
1:C:36:ASP:HB3	1:C:39:VAL:HG23	1.95	0.48
1:A:209:LYS:NZ	1:A:263:GLU:OE2	2.31	0.48
1:A:9:VAL:HG12	1:A:34:VAL:HG22	1.94	0.48
2:D:241:LYS:NZ	2:D:256:ASP:OD2	2.45	0.48
3:F:145:GLN:HE22	3:F:176:SER:HB3	1.76	0.48
1:A:253:TRP:CZ2	1:A:262:ILE:HG23	2.48	0.48
3:E:187:ARG:HH22	3:F:187:ARG:HG3	1.79	0.48
3:E:158:MET:HE1	3:E:195:LEU:HD22	1.94	0.48
3:F:202:LYS:HB3	3:F:259:ILE:HD12	1.96	0.48
1:C:133:LYS:O	1:C:137:GLU:HG3	2.14	0.48
2:D:96:VAL:O	2:D:100:ARG:HG3	2.14	0.48
2:B:247:MET:HG2	2:B:341:PRO:CD	2.44	0.48
3:F:193:ASP:OD1	3:F:194:GLU:N	2.48	0.47
2:B:369:LEU:HD13	2:B:379:LEU:HD23	1.95	0.47
3:G:205:THR:OG1	3:G:206:GLN:N	2.48	0.47
3:F:25:ALA:HB2	3:F:228:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ARG:HD2	1:A:252:GLN:HE21	1.78	0.47
3:F:147:ILE:O	3:F:179:LEU:HD12	2.14	0.47
1:C:432:GLN:HG2	1:C:472:TRP:HH2	1.80	0.47
2:B:80:LEU:HD13	2:B:87:PRO:HG2	1.95	0.47
3:H:124:TYR:CG	3:H:138:PRO:HB3	2.50	0.47
3:F:139:ILE:CG2	3:F:147:ILE:HD11	2.45	0.47
1:A:404:VAL:HG11	1:A:409:PHE:HD2	1.79	0.47
1:A:428:LYS:HD3	1:A:429:PHE:CE1	2.50	0.47
2:D:390:PRO:O	2:D:419:ALA:HB2	2.15	0.47
2:D:70:CYS:HB2	2:D:188:SER:HB2	1.97	0.47
2:D:80:LEU:HD13	2:D:87:PRO:CG	2.43	0.47
3:F:143:LYS:HA	3:F:143:LYS:HD3	1.65	0.47
1:C:433:LYS:NZ	2:D:263:THR:O	2.48	0.47
1:A:157:GLY:HA3	1:A:184:GLU:CG	2.43	0.46
3:H:158:MET:SD	3:H:195:LEU:HD11	2.55	0.46
2:D:140:ALA:HA	11:D:1651:HOH:O	2.15	0.46
3:F:189:THR:HB	3:F:192:GLU:HB2	1.96	0.46
3:H:12:GLY:HA2	9:H:1292:ACP:H3B1	1.96	0.46
2:D:400:LYS:O	2:D:404:LYS:HG3	2.16	0.46
1:A:274:HIS:CE1	1:A:451:HIS:CE1	3.03	0.46
2:B:163:ASN:HB2	2:B:183:PHE:CZ	2.50	0.46
3:H:51:SER:HA	3:H:224:ARG:CD	2.45	0.46
1:A:120:GLU:OE2	3:F:104:THR:OG1	2.34	0.46
1:C:239:ARG:HD2	1:C:252:GLN:HE21	1.78	0.46
1:A:131:LEU:HD13	1:A:166:VAL:HG11	1.97	0.46
2:D:291:VAL:HG11	2:D:328:PHE:HE1	1.81	0.46
2:D:370:TRP:CE2	2:D:444:GLY:HA3	2.51	0.46
3:G:189:THR:O	3:G:192:GLU:HB2	2.15	0.46
3:G:23:VAL:HG11	3:G:35:ILE:HD11	1.97	0.46
3:F:181:GLY:HA2	3:F:205:THR:OG1	2.16	0.46
2:D:163:ASN:HB2	2:D:183:PHE:CZ	2.51	0.45
2:B:258:GLU:HG3	2:B:259:GLU:N	2.32	0.45
1:C:50:LYS:HD3	1:C:50:LYS:HA	1.73	0.45
1:A:364:ILE:HG23	1:A:374:VAL:HG21	1.99	0.45
3:G:10:LYS:HD3	3:G:160:ALA:HB2	1.99	0.45
1:C:218:SER:HB2	11:C:1570:HOH:O	2.16	0.45
2:D:158:ILE:HG22	3:G:97:CYS:HB2	1.99	0.45
1:C:152:SER:HB3	1:C:156:ILE:HB	1.99	0.44
1:A:60:ARG:NH2	11:A:1564:HOH:O	2.51	0.44
2:B:381:LYS:HD2	11:B:1679:HOH:O	2.17	0.44
2:B:96:VAL:O	2:B:100:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:181:GLY:HA2	3:G:205:THR:OG1	2.18	0.44
1:C:466:THR:O	1:C:472:TRP:NE1	2.50	0.44
3:F:67:VAL:HA	3:F:70:LEU:CD1	2.44	0.44
2:B:166:ILE:O	2:B:169:SER:HB2	2.18	0.44
3:G:40:PRO:HG3	3:G:98:ALA:HB1	1.99	0.44
1:C:17:LEU:O	1:C:25:ARG:HG3	2.18	0.44
3:E:263:GLU:O	3:E:266:GLU:HB3	2.18	0.44
3:E:178:ARG:HD3	3:E:178:ARG:HA	1.86	0.44
2:B:232:THR:HG21	2:B:471:PHE:CD1	2.53	0.44
1:A:203:ARG:HD2	1:A:204:ASP:OD1	2.18	0.44
3:H:107:ASN:O	3:H:111:GLU:HG2	2.18	0.44
2:B:28:ARG:HD3	11:B:1632:HOH:O	2.18	0.44
2:B:279:GLU:HG2	11:B:1641:HOH:O	2.18	0.44
3:G:8:TYR:HB3	3:G:164:ILE:HD13	2.00	0.44
1:A:66:GLY:O	1:A:70:VAL:HB	2.17	0.43
3:F:208:ILE:O	3:F:246:LYS:HD3	2.18	0.43
3:E:176:SER:O	3:E:178:ARG:HG2	2.18	0.43
3:E:8:TYR:HB3	3:E:164:ILE:HD13	1.99	0.43
2:D:324:TRP:HH2	2:D:377:MET:HE2	1.83	0.43
1:C:47:ILE:HD12	1:C:48:SER:H	1.84	0.43
1:A:115:THR:HG23	2:B:63:THR:HB	2.00	0.43
1:A:275:CYS:CA	1:A:358:LEU:HD22	2.43	0.43
2:B:43:VAL:O	2:B:47:THR:HG23	2.19	0.43
3:H:57:ILE:HA	3:H:75:VAL:HG11	2.00	0.43
2:D:370:TRP:CZ2	2:D:444:GLY:HA3	2.53	0.43
3:G:126:VAL:HG12	3:G:127:LEU:N	2.34	0.43
2:D:350:ARG:O	2:D:354:MET:HG3	2.18	0.43
2:D:247:MET:HG2	2:D:341:PRO:CD	2.47	0.43
3:F:24:ALA:CB	3:F:226:THR:HG21	2.48	0.43
2:B:457:HIS:ND1	2:D:512:MET:HB3	2.33	0.43
2:B:374:ASP:OD1	11:B:1521:HOH:O	2.21	0.43
3:H:196:ILE:HB	3:H:207:MET:HE2	2.00	0.43
2:B:502:LEU:HD23	2:B:502:LEU:HA	1.80	0.43
1:C:276:TYR:O	1:C:280:ASN:HB3	2.18	0.43
3:G:26:LEU:HD12	3:G:244:ALA:HB1	2.00	0.43
1:C:62:CYS:HB3	2:D:94:GLY:HA3	2.00	0.43
1:A:50:LYS:HD3	1:A:50:LYS:HA	1.83	0.43
2:B:167:ASN:HB2	3:F:174:SER:HB2	2.00	0.43
3:F:203:LEU:O	3:F:256:PRO:HA	2.19	0.43
1:C:471:CYS:HB3	11:C:1529:HOH:O	2.17	0.43
2:D:510:ARG:HD3	11:D:1538:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:VAL:HB	2:B:297:HIS:CG	2.54	0.42
3:E:237:ALA:O	3:E:241:ARG:HG3	2.19	0.42
2:D:9:LYS:HE3	11:D:1531:HOH:O	2.18	0.42
2:D:194:VAL:HB	2:D:297:HIS:CG	2.54	0.42
3:H:53:ALA:O	3:H:55:ASN:N	2.53	0.42
1:C:10:GLU:HG3	1:C:34:VAL:HG21	2.01	0.42
2:B:303:LYS:HG3	11:B:1676:HOH:O	2.18	0.42
2:B:313:VAL:HA	2:B:314:PRO:HD3	1.90	0.42
3:F:216:VAL:HG22	3:F:219:ARG:NH2	2.34	0.42
2:D:198:ASP:HB2	2:D:297:HIS:O	2.20	0.42
1:A:104:THR:HA	1:A:108:ALA:O	2.20	0.42
2:D:109:GLU:HG3	2:D:261:LEU:O	2.20	0.42
2:B:370:TRP:HA	2:B:394:LEU:O	2.19	0.42
2:B:371:GLY:HA2	11:B:1709:HOH:O	2.19	0.42
1:C:356:GLY:HA3	5:C:1496:ICS:S1B	2.60	0.42
2:D:96:VAL:HG21	2:D:115:SER:HB2	2.01	0.42
3:H:100:ARG:HA	3:H:100:ARG:HD2	1.90	0.42
1:A:130:LYS:NZ	11:A:1509:HOH:O	2.41	0.42
3:G:8:TYR:CE2	3:G:126:VAL:HG11	2.54	0.42
1:A:68:LYS:C	1:A:68:LYS:HD3	2.40	0.42
1:C:53:GLN:HB2	1:C:56:LEU:HD12	2.00	0.42
1:C:56:LEU:HD23	1:C:56:LEU:HA	1.85	0.42
3:E:205:THR:HG22	3:E:206:GLN:O	2.20	0.42
2:B:221:ASN:OD1	2:B:287:ALA:HA	2.20	0.42
1:A:426:LYS:HG3	11:A:1510:HOH:O	2.20	0.42
2:D:66:PRO:HB3	2:D:396:HIS:HE1	1.84	0.42
3:H:176:SER:O	3:H:178:ARG:HG2	2.19	0.42
2:D:231:GLU:OE2	2:D:236:ASN:ND2	2.40	0.42
3:H:143:LYS:HA	3:H:143:LYS:HD3	1.85	0.42
1:C:101:ILE:HG12	1:C:236:TRP:CZ2	2.55	0.42
3:H:23:VAL:HG11	3:H:35:ILE:HD11	2.01	0.42
2:B:69:ALA:O	2:B:192:SER:HB2	2.20	0.42
1:C:364:ILE:HG12	1:C:374:VAL:HG21	2.02	0.41
3:H:9:GLY:N	3:H:15:LYS:HD3	2.35	0.41
3:F:12:GLY:CA	9:F:1292:ACP:H3B1	2.47	0.41
2:D:402:TRP:CZ2	2:D:406:VAL:HG21	2.55	0.41
1:C:280:ASN:O	1:C:284:ARG:HG3	2.21	0.41
1:C:96:ARG:HH11	1:C:96:ARG:HD3	1.66	0.41
3:E:205:THR:CG2	3:E:206:GLN:N	2.84	0.41
1:A:239:ARG:HH11	1:A:252:GLN:HE21	1.68	0.41
2:B:109:GLU:HG3	2:B:261:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:57:ILE:HA	3:E:75:VAL:HG11	2.02	0.41
3:E:212:PRO:HD2	3:E:239:GLU:HG3	2.03	0.41
1:C:309:LEU:HD23	1:C:309:LEU:HA	1.83	0.41
2:B:365:LYS:HD3	2:B:365:LYS:HA	1.89	0.41
1:C:144:LEU:HD21	2:D:43:VAL:HG21	2.02	0.41
1:A:477:ALA:HA	1:A:478:PRO:HD3	1.92	0.41
3:H:216:VAL:HG22	3:H:219:ARG:NH2	2.35	0.41
2:B:243:MET:HG2	2:B:344:LEU:HD21	2.03	0.41
3:F:196:ILE:HA	3:F:196:ILE:HD13	1.89	0.41
1:C:66:GLY:O	1:C:70:VAL:HB	2.20	0.41
3:G:172:ALA:HB1	3:G:255:ILE:HG12	2.03	0.41
1:A:31:HIS:ND1	1:A:47:ILE:O	2.54	0.41
1:C:354:TYR:HB2	1:C:409:PHE:CE2	2.56	0.41
1:A:6:ARG:O	1:A:10:GLU:HG3	2.21	0.41
3:F:56:THR:OG1	11:F:1308:HOH:O	2.16	0.41
1:C:96:ARG:HG3	11:C:1543:HOH:O	2.20	0.41
3:H:147:ILE:HG21	3:H:168:ILE:HD11	2.03	0.41
3:H:2:MET:CE	3:H:115:TYR:HB3	2.50	0.41
1:A:79:ILE:HG23	1:A:114:PHE:CD1	2.55	0.40
1:C:158:LEU:HA	1:C:158:LEU:HD23	1.92	0.40
2:D:352:VAL:O	2:D:356:THR:HG23	2.21	0.40
1:C:30:LYS:HB3	1:C:47:ILE:HG22	2.03	0.40
1:A:152:SER:HB3	1:A:156:ILE:HB	2.04	0.40
3:F:170:LYS:HE2	3:F:170:LYS:HB3	1.64	0.40
2:B:178:GLU:H	2:B:178:GLU:CD	2.23	0.40
1:C:439:ARG:CZ	1:C:462:ASP:HB3	2.52	0.40
2:B:228:PRO:HA	2:B:293:LEU:HD12	2.04	0.40
3:E:138:PRO:O	3:E:143:LYS:HB3	2.22	0.40
2:B:219:GLY:HA2	2:B:288:LEU:HA	2.02	0.40
3:F:145:GLN:OE1	3:F:176:SER:HB2	2.22	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	475/477 (100%)	456 (96%)	19 (4%)	0	100	100
1	C	474/477 (99%)	453 (96%)	21 (4%)	0	100	100
2	B	520/522 (100%)	507 (98%)	12 (2%)	1 (0%)	52	64
2	D	520/522 (100%)	507 (98%)	12 (2%)	1 (0%)	52	64
3	E	268/272 (98%)	255 (95%)	10 (4%)	3 (1%)	17	18
3	F	261/272 (96%)	254 (97%)	6 (2%)	1 (0%)	39	48
3	G	270/272 (99%)	262 (97%)	8 (3%)	0	100	100
3	H	260/272 (96%)	250 (96%)	8 (3%)	2 (1%)	24	27
All	All	3048/3086 (99%)	2944 (97%)	96 (3%)	8 (0%)	46	57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	52	LYS
3	E	262	ASP
3	H	54	GLN
3	E	55	ASN
3	H	51	SER
2	B	255	SER
2	D	255	SER
3	F	51	SER

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	407/407 (100%)	401 (98%)	6 (2%)	72	85
1	C	406/407 (100%)	400 (98%)	6 (2%)	72	85
2	B	454/454 (100%)	446 (98%)	8 (2%)	66	82
2	D	454/454 (100%)	447 (98%)	7 (2%)	72	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	217/218 (100%)	209 (96%)	8 (4%)	41	55
3	F	210/218 (96%)	203 (97%)	7 (3%)	45	61
3	G	218/218 (100%)	213 (98%)	5 (2%)	58	75
3	H	209/218 (96%)	203 (97%)	6 (3%)	50	66
All	All	2575/2594 (99%)	2522 (98%)	53 (2%)	61	78

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	98	ASN
1	A	131	LEU
1	A	219	THR
1	A	362	HIS
1	A	445	ASP
2	B	16	LEU
2	B	21	LYS
2	B	38	ASP
2	B	80	LEU
2	B	124	VAL
2	B	171	LYS
2	B	178	GLU
2	B	258	GLU
1	C	14	GLN
1	C	98	ASN
1	C	131	LEU
1	C	362	HIS
1	C	401	TYR
1	C	445	ASP
2	D	16	LEU
2	D	21	LYS
2	D	38	ASP
2	D	80	LEU
2	D	124	VAL
2	D	171	LYS
2	D	178	GLU
3	E	41	LYS
3	E	63	GLU
3	E	131	VAL
3	E	140	ARG
3	E	146	GLU

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Mol	Chain	Res	Type
3	E	195	LEU
3	E	259	ILE
3	E	266	GLU
3	F	10	LYS
3	F	13	ILE
3	F	84	LYS
3	F	170	LYS
3	F	213	ARG
3	F	226	THR
3	F	259	ILE
3	G	117	ASP
3	G	177	VAL
3	G	195	LEU
3	G	238	ASP
3	G	264	LEU
3	H	2	MET
3	H	116	GLU
3	H	118	ASP
3	H	127	LEU
3	H	187	ARG
3	H	235	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	GLN
1	A	274	HIS
1	A	440	GLN
2	B	418	ASN
1	C	252	GLN
1	C	321	GLN
2	D	18	GLN
3	E	201	ASN
3	E	206	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 6 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$
4	HCA	A	1494	-	4,13,13	0.80	0	3,18,18	2.32	1 (33%)
5	ICS	A	1496	1	6,30,30	1.95	2 (33%)	0,78,78	0.00	-
6	CLF	A	1498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
4	HCA	C	1494	-	4,13,13	0.74	0	3,18,18	2.40	1 (33%)
5	ICS	C	1496	1	6,30,30	1.64	1 (16%)	0,78,78	0.00	-
6	CLF	C	1498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
10	SF4	E	1290	3	0,12,12	0.00	-	0,24,24	0.00	-
9	ACP	E	1292	8	25,33,33	1.86	7 (28%)	31,52,52	1.94	7 (22%)
9	ACP	F	1292	8	25,33,33	1.70	5 (20%)	31,52,52	2.02	6 (19%)
9	ACP	G	1290	8	25,33,33	1.95	7 (28%)	31,52,52	1.99	8 (25%)
10	SF4	G	1292	3	0,12,12	0.00	-	0,24,24	0.00	-
9	ACP	H	1292	8	25,33,33	1.79	5 (20%)	31,52,52	2.01	6 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HCA	A	1494	-	-	0/7/17/17	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ICS	A	1496	1	-	0/0/204/204	0/0/13/13
6	CLF	A	1498	1,2	-	0/0/132/132	0/12/10/10
4	HCA	C	1494	-	-	0/7/17/17	0/0/0/0
5	ICS	C	1496	1	-	0/0/204/204	0/0/13/13
6	CLF	C	1498	1,2	-	0/0/132/132	0/12/10/10
10	SF4	E	1290	3	-	0/0/48/48	0/6/5/5
9	ACP	E	1292	8	-	0/15/38/38	0/3/3/3
9	ACP	F	1292	8	-	0/15/38/38	0/3/3/3
9	ACP	G	1290	8	-	0/15/38/38	0/3/3/3
10	SF4	G	1292	3	-	0/0/48/48	0/6/5/5
9	ACP	H	1292	8	-	0/15/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1496	ICS	S2B-FE6	-3.60	2.16	2.24
9	E	1292	ACP	PB-O2B	-3.13	1.48	1.56
9	H	1292	ACP	PG-O3G	-2.91	1.47	1.54
9	G	1290	ACP	PB-O2B	-2.81	1.49	1.56
5	C	1496	ICS	S2B-FE6	-2.77	2.18	2.24
9	E	1292	ACP	PG-O2G	-2.74	1.48	1.54
9	G	1290	ACP	PG-O2G	-2.57	1.48	1.54
9	F	1292	ACP	PG-O3G	-2.49	1.48	1.54
5	A	1496	ICS	S5A-FE7	-2.18	2.19	2.24
9	E	1292	ACP	PB-O3A	2.03	1.60	1.58
9	F	1292	ACP	O4'-C1'	2.21	1.44	1.41
9	E	1292	ACP	PG-O3G	2.53	1.61	1.54
9	H	1292	ACP	PG-O2G	2.68	1.61	1.54
9	G	1290	ACP	PG-O3G	2.82	1.61	1.54
9	H	1292	ACP	C5-C4	2.94	1.47	1.40
9	E	1292	ACP	C5-C4	3.00	1.47	1.40
9	F	1292	ACP	C5-C4	3.09	1.47	1.40
9	F	1292	ACP	PG-O2G	3.24	1.62	1.54
9	G	1290	ACP	C5-C4	3.26	1.47	1.40
9	G	1290	ACP	PB-O3A	3.45	1.62	1.58
9	G	1290	ACP	PB-O1B	3.82	1.61	1.51
9	E	1292	ACP	PB-O1B	3.83	1.61	1.51
9	H	1292	ACP	PG-O1G	4.53	1.60	1.50
9	H	1292	ACP	PB-O3A	4.59	1.63	1.58
9	E	1292	ACP	PG-O1G	4.93	1.61	1.50
9	G	1290	ACP	PG-O1G	5.03	1.61	1.50
9	F	1292	ACP	PG-O1G	5.13	1.61	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	1292	ACP	N3-C2-N1	-7.39	123.23	128.89
9	F	1292	ACP	N3-C2-N1	-7.01	123.53	128.89
9	E	1292	ACP	N3-C2-N1	-6.78	123.70	128.89
9	G	1290	ACP	N3-C2-N1	-6.43	123.97	128.89
9	H	1292	ACP	C2'-C1'-N9	-4.86	106.87	114.29
9	G	1290	ACP	C2'-C1'-N9	-4.64	107.20	114.29
9	F	1292	ACP	PA-O3A-PB	-3.93	121.70	132.73
9	E	1292	ACP	PA-O3A-PB	-3.86	121.89	132.73
9	E	1292	ACP	C2'-C1'-N9	-3.84	108.42	114.29
4	A	1494	HCA	C3-C2-C1	-3.72	109.01	114.96
4	C	1494	HCA	C3-C2-C1	-3.71	109.03	114.96
9	F	1292	ACP	C2'-C1'-N9	-3.58	108.83	114.29
9	G	1290	ACP	PA-O3A-PB	-3.54	122.79	132.73
9	H	1292	ACP	C4-C5-N7	-2.89	106.82	109.48
9	F	1292	ACP	C4-C5-N7	-2.83	106.88	109.48
9	G	1290	ACP	C4-C5-N7	-2.69	107.00	109.48
9	H	1292	ACP	PA-O3A-PB	-2.11	126.80	132.73
9	G	1290	ACP	O3'-C3'-C2'	-2.05	105.15	111.83
9	E	1292	ACP	C4-C5-N7	-2.05	107.59	109.48
9	F	1292	ACP	C2-N1-C6	2.01	122.36	118.77
9	H	1292	ACP	O4'-C1'-N9	2.03	112.34	108.10
9	G	1290	ACP	C2-N1-C6	2.07	122.47	118.77
9	E	1292	ACP	C2-N1-C6	2.08	122.48	118.77
9	E	1292	ACP	O4'-C1'-N9	2.14	112.59	108.10
9	H	1292	ACP	O3G-PG-C3B	2.28	111.92	106.40
9	G	1290	ACP	O4'-C1'-N9	2.36	113.04	108.10
9	E	1292	ACP	O2G-PG-C3B	2.42	112.28	106.40
9	F	1292	ACP	O4'-C1'-N9	2.82	114.01	108.10
9	G	1290	ACP	O2G-PG-C3B	3.04	113.78	106.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1494	HCA	2	0
4	C	1494	HCA	1	0
5	C	1496	ICS	1	0
6	C	1498	CLF	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	1292	ACP	3	0
9	G	1290	ACP	1	0
9	H	1292	ACP	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	477/477 (100%)	0.77	41 (8%)	13 18	18, 31, 52, 70	0
1	C	476/477 (99%)	0.60	29 (6%)	25 33	15, 26, 43, 57	0
2	B	522/522 (100%)	0.47	15 (2%)	55 64	16, 24, 34, 46	0
2	D	522/522 (100%)	0.47	19 (3%)	46 55	15, 23, 33, 48	1 (0%)
3	E	267/272 (98%)	1.33	67 (25%)	1 1	26, 53, 69, 87	26 (9%)
3	F	260/272 (95%)	1.06	40 (15%)	3 4	23, 48, 69, 98	16 (6%)
3	G	270/272 (99%)	0.83	31 (11%)	6 10	20, 37, 52, 65	15 (5%)
3	H	262/272 (96%)	0.85	29 (11%)	7 11	18, 37, 58, 78	7 (2%)
All	All	3056/3086 (99%)	0.73	271 (8%)	12 17	15, 30, 58, 98	65 (2%)

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	1	ALA	8.3
3	H	53	ALA	7.0
3	H	1	ALA	6.2
3	H	51	SER	6.0
3	F	198	ALA	5.9
3	E	232	PRO	5.9
3	F	261	MET	5.9
3	F	1	ALA	5.5
1	A	40	THR	5.4
3	E	49	LEU	5.3
3	F	203	LEU	5.3
2	B	148	ALA	5.2
3	F	167	GLY	5.0
3	E	118	ASP	5.0
1	A	38	ALA	4.9
3	F	260	THR	4.8

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Mol	Chain	Res	Type	RSRZ
3	H	116	GLU	4.8
3	H	50	HIS	4.7
3	F	200	ALA	4.6
3	F	30	GLY	4.5
3	E	54	GLN	4.5
1	C	39	VAL	4.5
3	H	168	ILE	4.4
3	E	169	VAL	4.4
3	E	238	ASP	4.4
3	F	33	VAL	4.3
3	E	173	ASN	4.2
1	A	214	THR	4.2
1	C	5	SER	4.1
3	H	63	GLU	3.9
3	E	27	ALA	3.9
2	D	177	ASP	3.9
3	E	261	MET	3.9
3	F	54	GLN	3.9
3	F	174	SER	3.7
3	E	231	ASP	3.7
3	H	52	LYS	3.7
1	A	4	MET	3.7
3	E	85	CYS	3.7
3	E	205	THR	3.7
3	E	233	LYS	3.6
1	A	291	GLY	3.6
1	A	34	VAL	3.6
1	A	317	ASP	3.6
3	E	230	TYR	3.6
2	D	337	GLY	3.5
1	A	9	VAL	3.5
3	G	118	ASP	3.5
3	F	195	LEU	3.5
3	F	159	TYR	3.5
3	G	187	ARG	3.4
3	E	72	LEU	3.4
3	E	268	LEU	3.4
3	E	172	ALA	3.4
3	E	259	ILE	3.4
3	E	227	VAL	3.4
3	E	201	ASN	3.4
3	G	71	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	316	PHE	3.3
1	A	45	CYS	3.3
1	A	231	ILE	3.3
1	C	425	ILE	3.3
1	C	63	ALA	3.2
3	E	174	SER	3.2
3	H	70	LEU	3.2
1	C	45	CYS	3.2
2	D	214	ASP	3.2
1	A	213	ASP	3.2
3	F	257	ASN	3.2
1	A	216	PHE	3.2
3	E	267	LEU	3.2
3	F	64	ALA	3.2
3	G	1	ALA	3.2
3	E	50	HIS	3.2
3	G	50	HIS	3.1
3	G	73	GLU	3.1
3	F	191	ARG	3.1
3	G	92	GLU	3.1
1	A	172	ALA	3.1
3	F	231	ASP	3.1
1	A	8	GLU	3.1
3	E	30	GLY	3.1
3	E	82	GLY	3.0
1	A	221	TYR	3.0
3	G	115	TYR	3.0
3	E	80	TYR	3.0
3	H	245	ARG	3.0
3	F	158	MET	3.0
3	G	80	TYR	3.0
1	A	95	GLY	3.0
3	E	255	ILE	3.0
1	C	62	CYS	2.9
2	D	94	GLY	2.9
2	D	522	VAL	2.9
1	A	329	ALA	2.9
3	E	200	ALA	2.9
3	E	263	GLU	2.9
3	E	249	ASP	2.9
3	E	47	LEU	2.9
3	F	49	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	G	25	ALA	2.9
3	E	217	VAL	2.9
3	E	256	PRO	2.9
1	C	18	GLU	2.8
2	B	35	TYR	2.8
2	D	70	CYS	2.8
3	E	258	PRO	2.8
3	E	55	ASN	2.8
1	A	64	TYR	2.8
3	F	70	LEU	2.8
1	A	395	GLY	2.8
3	F	204	GLY	2.8
3	G	129	ASP	2.8
2	B	101	SER	2.8
2	D	521	LEU	2.8
3	G	225	MET	2.8
3	E	219	ARG	2.7
1	C	110	VAL	2.7
3	E	237	ALA	2.7
3	E	83	VAL	2.7
3	H	172	ALA	2.7
2	D	215	ASP	2.7
2	B	522	VAL	2.7
3	G	74	ASP	2.7
3	E	269	MET	2.7
1	A	65	ALA	2.7
1	C	198	ALA	2.7
1	A	39	VAL	2.7
3	F	202	LYS	2.6
3	G	42	ALA	2.6
3	E	155	MET	2.6
3	F	117	ASP	2.6
1	C	8	GLU	2.6
3	E	23	VAL	2.6
3	G	54	GLN	2.6
1	C	91	TYR	2.6
2	D	72	PRO	2.6
3	E	189	THR	2.6
3	E	29	MET	2.6
3	H	145	GLN	2.5
3	F	73	GLU	2.5
3	G	49	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	H	197	ILE	2.5
2	B	4	GLN	2.5
3	H	61	ALA	2.5
3	H	204	GLY	2.5
3	H	160	ALA	2.5
1	A	306	ILE	2.5
3	G	228	ILE	2.5
1	A	7	GLU	2.5
1	A	318	GLU	2.5
3	G	28	GLU	2.5
3	G	116	GLU	2.5
1	C	415	ARG	2.5
3	E	270	GLU	2.5
3	F	45	THR	2.5
1	A	71	VAL	2.5
3	H	238	ASP	2.5
1	A	63	ALA	2.4
1	A	321	GLN	2.4
1	A	446	TYR	2.4
3	G	114	ALA	2.4
2	B	95	CYS	2.4
1	A	313	ALA	2.4
3	E	245	ARG	2.4
3	E	25	ALA	2.4
2	B	214	ASP	2.4
3	E	215	ASN	2.4
1	A	18	GLU	2.4
3	F	116	GLU	2.4
2	B	472	PRO	2.4
1	A	391	MET	2.4
3	E	96	GLY	2.4
3	G	81	GLY	2.4
2	D	54	GLU	2.4
3	H	151	CYS	2.4
3	H	54	GLN	2.4
1	A	92	SER	2.3
3	G	5	CYS	2.3
3	H	163	ASN	2.3
2	D	220	SER	2.3
2	D	265	ALA	2.3
3	E	260	THR	2.3
3	F	47	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	212	GLU	2.3
3	F	256	PRO	2.3
3	E	28	GLU	2.3
3	E	264	LEU	2.3
3	F	72	LEU	2.3
2	D	97	ALA	2.3
3	E	63	GLU	2.3
3	E	243	LEU	2.3
3	E	262	ASP	2.3
3	G	72	LEU	2.3
3	G	76	LEU	2.3
2	D	327	GLU	2.3
1	C	446	TYR	2.3
3	H	159	TYR	2.3
2	D	101	SER	2.3
1	A	473	LYS	2.3
3	E	202	LYS	2.3
3	E	26	LEU	2.3
1	C	9	VAL	2.2
3	F	83	VAL	2.2
1	C	67	SER	2.2
3	F	175	GLY	2.2
2	B	473	ILE	2.2
3	H	64	ALA	2.2
3	H	68	GLU	2.2
1	A	62	CYS	2.2
1	C	88	CYS	2.2
1	C	183	CYS	2.2
2	D	329	LEU	2.2
2	B	72	PRO	2.2
3	E	113	GLY	2.2
3	F	113	GLY	2.2
2	B	232	THR	2.2
1	A	444	TRP	2.2
3	E	196	ILE	2.2
3	F	65	GLY	2.2
3	H	191	ARG	2.2
3	E	221	GLU	2.2
3	E	46	ARG	2.2
3	F	50	HIS	2.2
3	H	174	SER	2.2
3	E	78	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	65	GLY	2.2
2	B	106	HIS	2.2
3	F	189	THR	2.2
1	A	68	LYS	2.1
3	F	197	ILE	2.1
3	G	231	ASP	2.1
2	D	76	VAL	2.1
3	G	78	ALA	2.1
3	F	63	GLU	2.1
3	G	55	ASN	2.1
2	B	154	MET	2.1
2	D	479	LEU	2.1
3	H	252	LEU	2.1
1	C	213	ASP	2.1
3	E	187	ARG	2.1
3	H	260	THR	2.1
2	B	172	GLU	2.1
3	H	74	ASP	2.1
3	G	182	LEU	2.1
3	G	189	THR	2.1
1	C	292	ILE	2.1
1	A	279	MET	2.1
1	C	64	TYR	2.1
1	C	174	LEU	2.1
3	E	203	LEU	2.1
3	G	34	MET	2.1
1	A	185	GLY	2.1
1	C	185	GLY	2.1
1	C	208	GLY	2.1
1	C	71	VAL	2.1
1	C	26	LYS	2.1
1	C	66	GLY	2.1
3	F	230	TYR	2.1
2	B	483	THR	2.0
2	D	107	PHE	2.0
3	E	195	LEU	2.0
3	H	261	MET	2.0
3	F	262	ASP	2.0
1	A	25	ARG	2.0
1	C	74	PRO	2.0
3	E	222	ILE	2.0
3	F	227	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	174	LEU	2.0
1	C	38	ALA	2.0
3	G	230	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	HCA	A	1494	14/14	0.93	0.25	0.12	19,21,23,24	0
4	HCA	C	1494	14/14	0.96	0.22	-0.46	15,17,20,23	0
9	ACP	F	1292	31/31	0.89	0.16	-0.70	34,47,53,54	0
9	ACP	H	1292	31/31	0.94	0.14	-0.79	22,30,35,35	0
9	ACP	E	1292	31/31	0.93	0.14	-0.97	37,47,51,52	0
6	CLF	A	1498	15/15	0.86	0.17	-0.99	17,20,106,128	0
9	ACP	G	1290	31/31	0.91	0.15	-1.11	29,40,44,47	0
5	ICS	A	1496	18/18	0.97	0.14	-1.42	20,24,26,29	0
6	CLF	C	1498	15/15	0.97	0.15	-1.66	12,15,18,19	0
5	ICS	C	1496	18/18	0.97	0.12	-1.88	15,19,24,26	0
10	SF4	E	1290	8/8	0.98	0.10	-2.14	21,23,26,27	0
8	MG	F	1291	1/1	0.93	0.12	-2.34	41,41,41,41	0
7	FE2	B	1492	1/1	0.92	0.10	-2.86	22,22,22,22	1
8	MG	H	1291	1/1	0.91	0.11	-2.89	25,25,25,25	0
8	MG	G	1291	1/1	0.93	0.08	-2.93	34,34,34,34	0
10	SF4	G	1292	8/8	0.97	0.12	-3.19	16,20,22,22	0
7	FE2	D	1492	1/1	0.95	0.04	-4.05	27,27,27,27	1
8	MG	E	1291	1/1	0.87	0.10	-	40,40,40,40	0

6.5 Other polymers

There are no such residues in this entry.