



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:00 AM GMT

PDB ID : 2OZ1
Title : The SoxAX Complex of Rhodovulum Sulfidophilum
Authors : Kihlken, M.A.; Berks, B.C.; Hemmings, A.M.
Deposited on : 2007-02-23
Resolution : 2.35 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

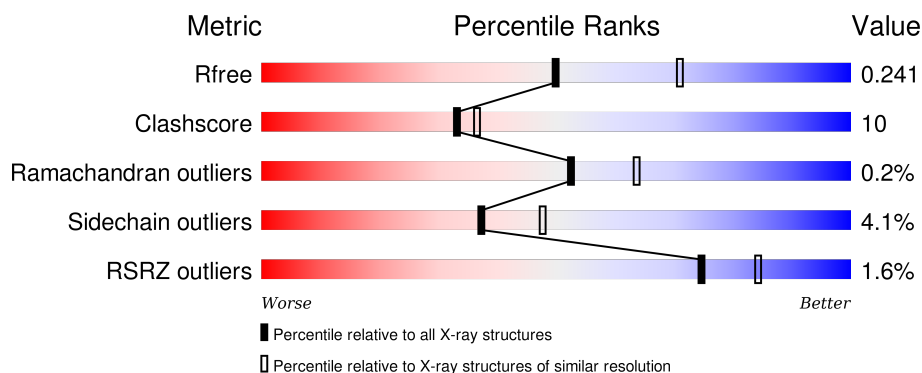
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	261	<div> <div></div> <div>87%11% •</div> </div>
1	C	261	<div> <div>%</div> <div>87%11% •</div> </div>
1	E	261	<div> <div></div> <div>87%11% •</div> </div>
1	G	261	<div> <div>%</div> <div>89%10% •</div> </div>
2	B	138	<div> <div>3%</div> <div>80%16% ••</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	138	<div><div></div><div>2%</div><div>81%</div><div>17%</div><div>••</div></div>
2	F	138	<div><div></div><div>3%</div><div>77%</div><div>22%</div><div>•</div></div>
2	H	138	<div><div></div><div>7%</div><div>82%</div><div>15%</div><div>•</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13668 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 Diheme cytochrome c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2031	1261	363	392	15			
1	C	261	Total	C	N	O	S	0	0	0
			2031	1261	363	392	15			
1	E	261	Total	C	N	O	S	0	0	0
			2031	1261	363	392	15			
1	G	261	Total	C	N	O	S	0	0	0
			2031	1261	363	392	15			

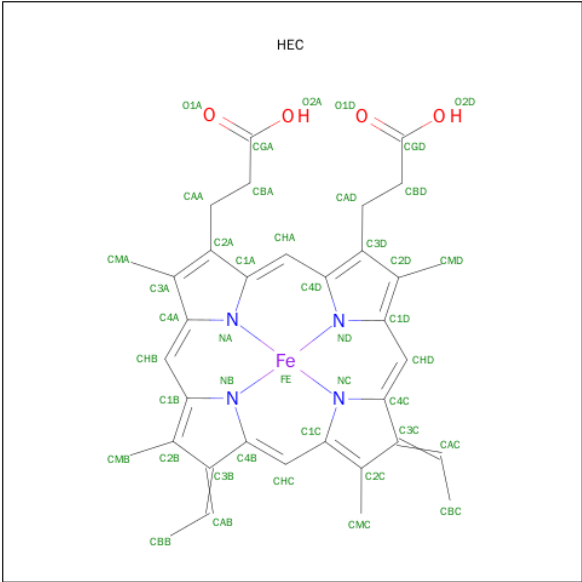
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	CSS	CYS	MODIFIED RESIDUE	UNP Q939U1
C	222	CSS	CYS	MODIFIED RESIDUE	UNP Q939U1
E	222	CSS	CYS	MODIFIED RESIDUE	UNP Q939U1
G	222	CSS	CYS	MODIFIED RESIDUE	UNP Q939U1

- Molecule 2 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	135	Total	C	N	O	S	0	0	0
			1005	631	175	191	8			
2	D	137	Total	C	N	O	S	0	0	0
			1022	640	177	197	8			
2	F	138	Total	C	N	O	S	0	0	0
			1031	645	179	199	8			
2	H	138	Total	C	N	O	S	0	0	0
			1031	645	179	199	8			

- Molecule 3 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

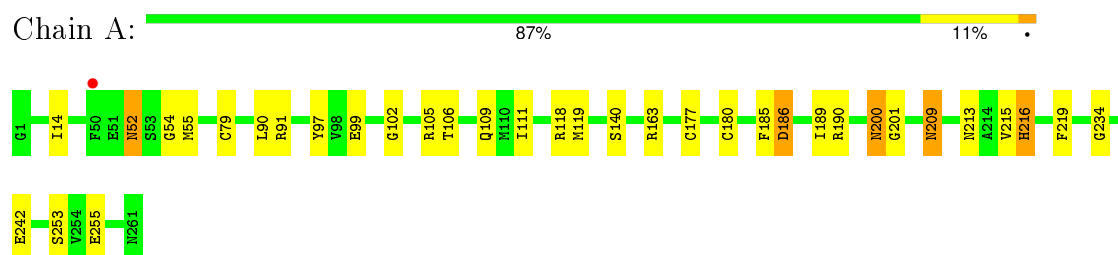
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total 162	O 162	0	0
4	B	71	Total 71	O 71	0	0
4	C	179	Total 179	O 179	0	0
4	D	67	Total 67	O 67	0	0
4	E	190	Total 190	O 190	0	0
4	F	66	Total 66	O 66	0	0
4	G	142	Total 142	O 142	0	0
4	H	62	Total 62	O 62	0	0

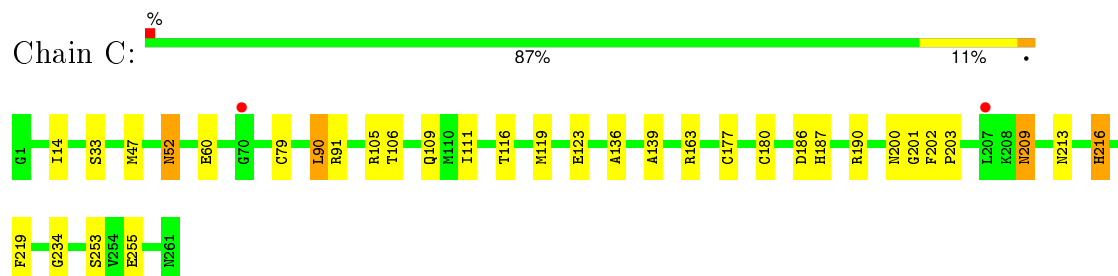
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

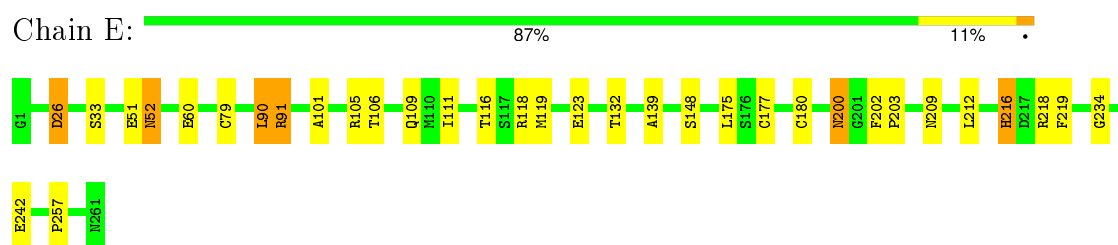
- Molecule 1: Diheme cytochrome c



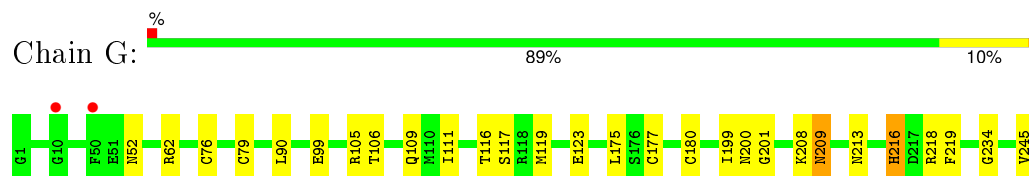
- Molecule 1: Diheme cytochrome c



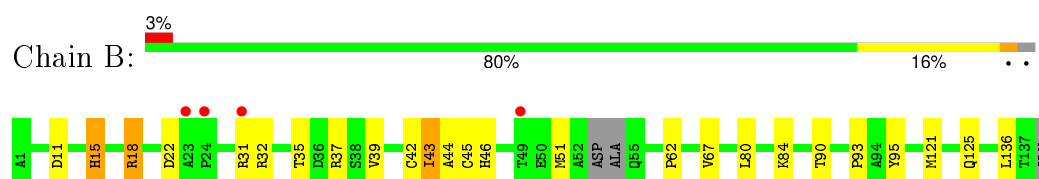
- Molecule 1: Diheme cytochrome c



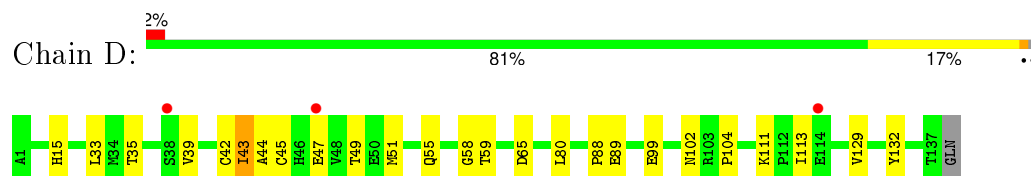
- Molecule 1: Diheme cytochrome c



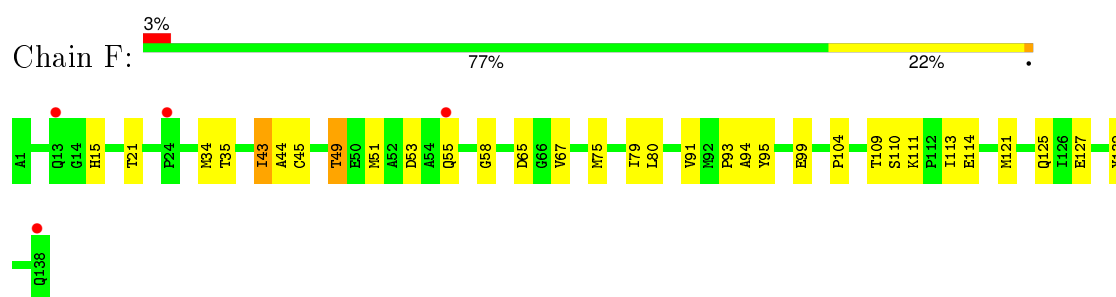
- Molecule 2: Cytochrome c



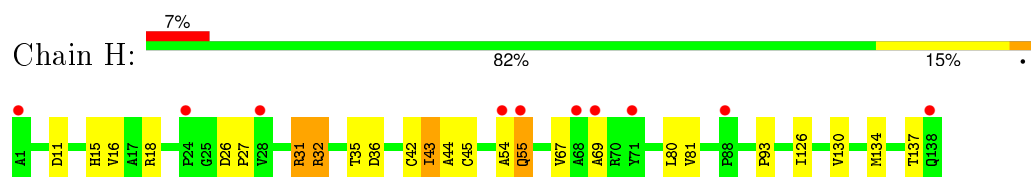
- Molecule 2: Cytochrome c



- Molecule 2: Cytochrome c



- Molecule 2: Cytochrome c



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.97Å 102.95Å 115.71Å 90.00° 110.22° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 42.62 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-2.35) 96.0 (42.62-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.242 0.187 , 0.241	Depositor DCC
R_{free} test set	3631 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.7	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 71773 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13668	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.23 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.8580e-03.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSS, HEC

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	0.53	0/2070	0.63	0/2805
1	C	0.51	0/2070	0.62	0/2805
1	E	0.52	0/2070	0.65	0/2805
1	G	0.49	0/2070	0.63	0/2805
2	B	0.49	0/1025	0.60	0/1395
2	D	0.48	0/1043	0.60	0/1421
2	F	0.49	0/1052	0.60	0/1433
2	H	0.51	0/1052	0.65	0/1433
All	All	0.50	0/12452	0.63	0/16902

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2031	0	1929	37	0
1	C	2031	0	1929	39	0
1	E	2031	0	1929	41	0
1	G	2031	0	1929	31	0
2	B	1005	0	996	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1022	0	1009	16	0
2	F	1031	0	1017	25	0
2	H	1031	0	1018	33	0
3	A	86	0	63	18	0
3	B	43	0	32	12	0
3	C	86	0	63	16	0
3	D	43	0	31	7	0
3	E	86	0	63	20	0
3	F	43	0	31	9	0
3	G	86	0	63	21	0
3	H	43	0	32	12	0
4	A	162	0	0	7	0
4	B	71	0	0	5	0
4	C	179	0	0	4	0
4	D	67	0	0	1	0
4	E	190	0	0	12	0
4	F	66	0	0	2	0
4	G	142	0	0	1	0
4	H	62	0	0	7	0
All	All	13668	0	12134	257	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 10.

All (257) 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:177:CYS:SG	3:A:953:HEC:HAB	1.45	1.56
1:C:177:CYS:SG	3:C:953:HEC:HAB	1.48	1.52
2:B:42:CYS:SG	3:B:951:HEC:HAB	1.54	1.46
1:G:76:CYS:SG	3:G:952:HEC:CAB	2.04	1.45
2:D:42:CYS:SG	3:D:951:HEC:CAB	2.05	1.41
2:H:42:CYS:SG	3:H:951:HEC:HAB	1.63	1.36
1:A:177:CYS:SG	3:A:953:HEC:CAB	2.09	1.36
1:E:177:CYS:SG	3:E:953:HEC:HAB	1.63	1.36
1:C:177:CYS:SG	3:C:953:HEC:CAB	2.13	1.35
2:B:42:CYS:SG	3:B:951:HEC:CAB	2.12	1.35
1:E:177:CYS:SG	3:E:953:HEC:CAB	2.14	1.35
2:B:67:VAL:HG12	4:B:1017:HOH:O	1.34	1.27
2:H:42:CYS:SG	3:H:951:HEC:CAB	2.20	1.27
1:A:180:CYS:SG	3:A:953:HEC:HAC	1.79	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:177:CYS:SG	3:G:953:HEC:CAB	2.36	1.14
1:A:180:CYS:SG	3:A:953:HEC:CAC	2.38	1.10
2:H:45:CYS:SG	3:H:951:HEC:CAC	2.41	1.09
1:E:180:CYS:SG	3:E:953:HEC:CAC	2.41	1.09
2:F:45:CYS:SG	3:F:951:HEC:CAC	2.41	1.08
1:C:180:CYS:SG	3:C:953:HEC:CAC	2.42	1.07
1:G:79:CYS:SG	3:G:952:HEC:CAC	2.43	1.06
2:F:45:CYS:SG	3:F:951:HEC:HAC	1.95	1.06
1:E:218:ARG:HG3	4:E:1143:HOH:O	1.51	1.06
1:A:79:CYS:SG	3:A:952:HEC:CAC	2.44	1.06
1:G:177:CYS:SG	3:G:953:HEC:HAB	1.95	1.04
1:G:180:CYS:SG	3:G:953:HEC:HAC	1.98	1.03
1:E:79:CYS:SG	3:E:952:HEC:CAC	2.47	1.03
2:D:45:CYS:SG	3:D:951:HEC:CAC	2.47	1.03
1:C:79:CYS:SG	3:C:952:HEC:CAC	2.47	1.01
2:H:54:ALA:HA	2:H:55:GLN:HB2	1.42	1.01
2:B:45:CYS:SG	3:B:951:HEC:CAC	2.49	1.01
1:G:180:CYS:SG	3:G:953:HEC:CAC	2.49	1.01
2:H:32:ARG:HG2	2:H:32:ARG:HH11	1.25	1.00
1:C:180:CYS:SG	3:C:953:HEC:HAC	2.04	0.97
2:H:42:CYS:HG	3:H:951:HEC:HAB	1.24	0.97
1:E:212:LEU:HD13	4:E:1141:HOH:O	1.65	0.97
1:E:216:HIS:HD2	1:E:234:GLY:H	1.13	0.96
1:A:180:CYS:HG	3:A:953:HEC:HAC	1.14	0.95
2:D:45:CYS:SG	3:D:951:HEC:HAC	2.08	0.92
1:C:216:HIS:HD2	1:C:234:GLY:H	1.08	0.92
2:H:45:CYS:SG	3:H:951:HEC:HAC	2.09	0.92
2:F:35:THR:HA	2:F:43:ILE:HD12	1.54	0.90
1:G:216:HIS:HD2	1:G:234:GLY:H	1.09	0.89
2:B:42:CYS:HG	3:B:951:HEC:HAB	0.98	0.88
1:A:216:HIS:HD2	1:A:234:GLY:H	1.16	0.87
1:C:216:HIS:CD2	1:C:234:GLY:H	1.94	0.86
2:B:45:CYS:SG	3:B:951:HEC:HAC	2.18	0.83
1:G:216:HIS:CD2	1:G:234:GLY:H	1.97	0.82
2:F:80:LEU:HD21	3:F:951:HEC:HMB2	1.59	0.82
1:E:218:ARG:HB3	4:E:1115:HOH:O	1.79	0.81
1:A:163:ARG:HD3	4:A:1110:HOH:O	1.79	0.81
1:A:111:ILE:HG12	3:A:952:HEC:HMB2	1.64	0.80
2:F:49:THR:HG23	2:F:65:ASP:OD2	1.82	0.80
2:H:80:LEU:HD21	3:H:951:HEC:HMB2	1.64	0.79
2:F:114:GLU:HB2	4:F:1011:HOH:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:LEU:HB3	4:E:1127:HOH:O	1.82	0.79
1:E:111:ILE:HG12	3:E:952:HEC:HMB2	1.65	0.78
1:G:209:ASN:HD21	1:G:213:ASN:HD21	1.32	0.78
1:E:216:HIS:CD2	1:E:234:GLY:H	2.03	0.74
1:C:106:THR:H	1:C:109:GLN:HE21	1.34	0.74
1:A:54:GLY:HA3	4:A:1102:HOH:O	1.87	0.74
2:B:32:ARG:HG3	1:E:60:GLU:OE2	1.88	0.73
1:A:209:ASN:HD21	1:A:213:ASN:HD21	1.36	0.73
3:E:952:HEC:HMC1	3:E:952:HEC:HBC3	1.71	0.71
2:H:54:ALA:CA	2:H:55:GLN:HB2	2.20	0.71
1:G:90:LEU:HD21	3:G:952:HEC:HBA2	1.73	0.71
2:F:35:THR:HG22	2:F:43:ILE:HG21	1.71	0.70
1:G:175:LEU:HD11	4:H:1012:HOH:O	1.90	0.70
1:E:91:ARG:HD2	1:E:139:ALA:HB2	1.73	0.70
1:E:132:THR:HG22	4:E:1141:HOH:O	1.92	0.70
2:H:32:ARG:HH11	2:H:32:ARG:CG	2.01	0.69
1:A:216:HIS:CD2	1:A:234:GLY:H	2.06	0.69
2:H:54:ALA:HA	2:H:55:GLN:CB	2.21	0.68
1:A:55:MET:HE1	4:A:1073:HOH:O	1.93	0.68
1:C:119:MET:HG3	3:C:952:HEC:HMC2	1.77	0.67
3:G:953:HEC:HMB1	3:G:953:HEC:HBB3	1.76	0.67
2:H:35:THR:HA	2:H:43:ILE:CG1	2.24	0.67
1:G:219:PHE:CD2	3:G:953:HEC:HMB2	2.29	0.67
1:E:106:THR:H	1:E:109:GLN:HE21	1.43	0.67
1:A:140:SER:HB2	4:A:1073:HOH:O	1.95	0.66
1:A:106:THR:H	1:A:109:GLN:HE21	1.44	0.65
3:C:952:HEC:HMC1	3:C:952:HEC:HBC3	1.78	0.64
2:F:104:PRO:HB2	2:F:113:ILE:HD12	1.79	0.64
2:D:80:LEU:HD21	3:D:951:HEC:HMB2	1.79	0.64
2:B:136:LEU:HB2	4:B:1017:HOH:O	1.95	0.64
2:B:42:CYS:HG	3:B:951:HEC:CAB	1.85	0.63
2:F:80:LEU:HD21	3:F:951:HEC:CMB	2.28	0.63
1:E:180:CYS:SG	3:E:953:HEC:HAC	2.37	0.63
1:G:199:ILE:HG12	1:G:245:VAL:HG12	1.80	0.63
2:D:33:LEU:HD22	2:D:39:VAL:HG11	1.81	0.63
1:E:33:SER:HB2	4:E:1112:HOH:O	1.97	0.63
2:B:80:LEU:HD21	3:B:951:HEC:HMB2	1.81	0.63
1:A:91:ARG:HD3	4:A:1072:HOH:O	1.99	0.62
1:G:208:LYS:HB3	4:G:1058:HOH:O	1.99	0.62
1:G:111:ILE:HG12	3:G:952:HEC:HMB2	1.82	0.62
3:G:952:HEC:HMC1	3:G:952:HEC:HBC3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:93:PRO:HG3	4:H:1012:HOH:O	1.99	0.61
1:C:90:LEU:HB3	4:C:1101:HOH:O	1.99	0.61
1:A:14:ILE:HG23	1:A:253:SER:HB2	1.83	0.61
1:E:219:PHE:CD2	3:E:953:HEC:HMB2	2.36	0.61
1:A:163:ARG:CD	4:A:1110:HOH:O	2.43	0.61
2:B:31:ARG:HD2	4:B:992:HOH:O	2.00	0.60
3:E:953:HEC:HBC2	4:E:1067:HOH:O	2.01	0.60
1:C:79:CYS:SG	3:C:952:HEC:C3C	2.90	0.60
1:C:116:THR:HG21	1:C:123:GLU:HG3	1.83	0.60
2:H:44:ALA:HB2	4:H:1011:HOH:O	2.02	0.60
2:F:75:MET:O	2:F:79:ILE:HG13	2.02	0.60
2:F:21:THR:HG22	2:F:127:GLU:HG3	1.84	0.59
2:B:35:THR:HA	2:B:43:ILE:CG1	2.32	0.59
1:A:90:LEU:HB3	4:A:1106:HOH:O	2.03	0.59
2:D:45:CYS:SG	3:D:951:HEC:C3C	2.91	0.58
1:C:60:GLU:OE2	2:H:32:ARG:HG2	2.03	0.58
1:C:116:THR:CG2	1:C:123:GLU:HG3	2.33	0.58
1:A:79:CYS:SG	3:A:952:HEC:C3C	2.92	0.58
1:C:119:MET:CG	3:C:952:HEC:HMC2	2.34	0.58
2:H:35:THR:HA	2:H:43:ILE:HG13	1.86	0.58
2:F:45:CYS:SG	3:F:951:HEC:C3C	2.91	0.57
1:E:91:ARG:HD2	1:E:139:ALA:CB	2.34	0.57
2:B:45:CYS:SG	3:B:951:HEC:C3C	2.93	0.57
1:A:79:CYS:SG	3:A:952:HEC:CB	2.93	0.56
2:H:45:CYS:SG	3:H:951:HEC:C3C	2.94	0.56
1:C:106:THR:H	1:C:109:GLN:NE2	2.02	0.56
1:E:257:PRO:HB2	4:E:1114:HOH:O	2.05	0.56
1:A:90:LEU:HD21	3:A:952:HEC:HBA2	1.88	0.56
3:A:952:HEC:HBC3	3:A:952:HEC:HMC1	1.88	0.56
1:C:209:ASN:HD21	1:C:213:ASN:HD21	1.53	0.55
1:G:116:THR:CG2	1:G:123:GLU:HG3	2.36	0.55
1:G:79:CYS:SG	3:G:952:HEC:C3C	2.95	0.55
2:H:35:THR:HA	2:H:43:ILE:HG12	1.86	0.55
1:C:180:CYS:SG	3:C:953:HEC:C3C	2.95	0.55
2:H:32:ARG:NH1	2:H:32:ARG:HG2	2.05	0.55
1:E:180:CYS:SG	3:E:953:HEC:C3C	2.95	0.54
3:H:951:HEC:HMC1	3:H:951:HEC:HBC3	1.89	0.54
2:D:80:LEU:HD21	3:D:951:HEC:CMB	2.37	0.54
1:G:201:GLY:HA2	1:G:255:GLU:HB3	1.88	0.54
1:A:219:PHE:CD2	3:A:953:HEC:HMB2	2.43	0.54
3:C:952:HEC:CB	3:C:952:HEC:HMC1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:PRO:HD3	3:B:951:HEC:HBC2	1.91	0.53
1:E:177:CYS:SG	3:E:953:HEC:C3B	2.96	0.53
2:H:16:VAL:HG21	2:H:81:VAL:HG21	1.90	0.53
2:B:51:MET:HE1	4:B:1022:HOH:O	2.08	0.52
2:H:67:VAL:HG21	3:H:951:HEC:HMA3	1.91	0.52
3:E:953:HEC:HMB1	3:E:953:HEC:HBB3	1.91	0.52
2:F:94:ALA:HA	4:F:957:HOH:O	2.10	0.52
2:H:130:VAL:O	2:H:134:MET:HG2	2.09	0.52
1:E:79:CYS:SG	3:E:952:HEC:HAC	2.44	0.52
2:B:80:LEU:HD21	3:B:951:HEC:CMB	2.39	0.52
1:E:105:ARG:HD3	4:E:987:HOH:O	2.09	0.52
1:E:218:ARG:CG	4:E:1143:HOH:O	2.31	0.52
2:B:121:MET:HE2	2:B:125:GLN:HB3	1.91	0.51
2:F:67:VAL:HG21	3:F:951:HEC:HMA3	1.91	0.51
1:C:187:HIS:HD2	2:D:59:THR:O	1.92	0.51
2:H:43:ILE:HG23	4:H:995:HOH:O	2.10	0.51
1:A:180:CYS:SG	3:A:953:HEC:C3C	2.99	0.51
1:G:79:CYS:SG	3:G:952:HEC:HAC	2.47	0.50
1:C:111:ILE:HG12	3:C:952:HEC:HMB2	1.94	0.50
1:A:177:CYS:SG	3:A:953:HEC:C3B	2.95	0.50
2:B:35:THR:HA	2:B:43:ILE:HG13	1.93	0.50
1:C:52:ASN:HD22	1:C:52:ASN:C	2.15	0.50
1:E:175:LEU:HD13	3:E:953:HEC:HBC3	1.94	0.50
1:C:47:MET:HE3	1:G:208:LYS:HG2	1.94	0.50
2:F:44:ALA:O	2:F:58:GLY:HA3	2.12	0.49
2:F:51:MET:HE2	2:F:132:TYR:CE2	2.46	0.49
3:E:952:HEC:HMC1	3:E:952:HEC:CBC	2.42	0.49
1:G:116:THR:HG21	1:G:123:GLU:HG3	1.94	0.49
1:E:52:ASN:HD22	1:E:52:ASN:C	2.14	0.49
1:G:79:CYS:SG	3:G:952:HEC:CBC	2.99	0.49
2:B:84:LYS:HE3	2:B:90:THR:O	2.11	0.49
2:D:111:LYS:HE3	4:D:992:HOH:O	2.12	0.49
1:G:106:THR:H	1:G:109:GLN:HE21	1.61	0.48
1:C:91:ARG:HD2	1:C:139:ALA:HB2	1.96	0.48
1:E:79:CYS:SG	3:E:952:HEC:C3C	3.01	0.48
1:A:106:THR:H	1:A:109:GLN:NE2	2.10	0.48
1:G:106:THR:H	1:G:109:GLN:NE2	2.11	0.48
2:F:93:PRO:HD3	3:F:951:HEC:HBC2	1.94	0.48
2:D:104:PRO:HB2	2:D:113:ILE:HD12	1.96	0.48
1:C:136:ALA:HB2	1:C:203:PRO:HG2	1.95	0.47
2:H:126:ILE:O	2:H:130:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:MET:HG2	3:A:952:HEC:HMC2	1.97	0.47
1:G:180:CYS:SG	3:G:953:HEC:C3C	3.03	0.47
2:F:121:MET:HE2	2:F:125:GLN:HB3	1.97	0.47
1:C:219:PHE:CD2	3:C:953:HEC:HMB2	2.50	0.46
2:D:49:THR:HG23	2:D:65:ASP:OD2	2.15	0.46
2:F:51:MET:HE2	2:F:132:TYR:CZ	2.51	0.46
2:H:36:ASP:N	4:H:992:HOH:O	2.49	0.46
1:G:177:CYS:SG	3:G:953:HEC:C3B	3.02	0.46
1:E:119:MET:CG	3:E:952:HEC:HMC2	2.45	0.46
2:D:51:MET:HE1	2:D:132:TYR:CE2	2.51	0.46
1:C:163:ARG:HD2	4:C:1016:HOH:O	2.15	0.46
1:E:119:MET:HG3	3:E:952:HEC:HMC2	1.97	0.46
1:A:119:MET:CG	3:A:952:HEC:HMC2	2.46	0.46
1:E:203:PRO:HB2	4:E:1141:HOH:O	2.14	0.46
2:F:51:MET:CE	2:F:132:TYR:CE2	2.99	0.46
1:C:90:LEU:HD23	4:C:1101:HOH:O	2.15	0.45
1:C:14:ILE:HG23	1:C:253:SER:HB2	1.99	0.45
1:G:209:ASN:ND2	1:G:213:ASN:HD21	2.07	0.45
1:G:119:MET:CG	3:G:952:HEC:HMC2	2.47	0.45
2:B:18:ARG:HH11	2:B:18:ARG:HG3	1.82	0.45
2:F:34:MET:HG3	2:F:51:MET:CE	2.46	0.45
2:H:32:ARG:NH1	2:H:32:ARG:CG	2.70	0.45
1:E:106:THR:H	1:E:109:GLN:NE2	2.11	0.45
1:C:201:GLY:HA2	1:C:255:GLU:HB3	1.99	0.45
3:G:952:HEC:CBC	3:G:952:HEC:HMC1	2.46	0.44
1:C:33:SER:HB2	4:C:1081:HOH:O	2.17	0.44
2:D:88:PRO:O	2:D:89:GLU:HB2	2.18	0.44
1:E:200:ASN:H	1:E:200:ASN:HD22	1.64	0.44
1:G:76:CYS:SG	3:G:952:HEC:C3B	2.99	0.44
1:A:200:ASN:H	1:A:200:ASN:HD22	1.66	0.44
2:B:42:CYS:SG	3:B:951:HEC:C3B	3.01	0.44
2:F:51:MET:C	2:F:53:ASP:H	2.20	0.44
1:E:118:ARG:HB3	3:E:952:HEC:HBC2	2.01	0.43
2:H:69:ALA:HB2	2:H:137:THR:O	2.17	0.43
1:C:209:ASN:C	1:C:209:ASN:HD22	2.20	0.43
1:C:60:GLU:OE2	2:H:32:ARG:CG	2.65	0.43
1:G:119:MET:HG3	3:G:952:HEC:HMC2	2.00	0.43
3:H:951:HEC:HBB3	3:H:951:HEC:HMB1	2.01	0.43
2:B:121:MET:CE	2:B:125:GLN:HB3	2.49	0.43
3:G:952:HEC:HMB1	3:G:952:HEC:HBB3	1.99	0.43
2:D:44:ALA:O	2:D:58:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ARG:HD3	1:E:51:GLU:HG2	1.99	0.43
1:A:118:ARG:HB3	3:A:952:HEC:HBC2	2.01	0.43
1:E:203:PRO:CB	4:E:1141:HOH:O	2.66	0.43
1:A:201:GLY:HA2	1:A:255:GLU:HB2	2.01	0.43
2:B:95:TYR:CE1	3:B:951:HEC:HBB2	2.54	0.42
1:C:79:CYS:SG	3:C:952:HEC:CBC	3.07	0.42
1:C:202:PHE:HA	1:C:203:PRO:C	2.39	0.42
1:E:202:PHE:HA	1:E:203:PRO:C	2.40	0.42
1:E:101:ALA:CB	1:E:105:ARG:HD2	2.50	0.42
2:F:95:TYR:OH	3:F:951:HEC:HMC2	2.20	0.42
2:D:35:THR:HA	2:D:43:ILE:HG13	2.02	0.42
2:H:93:PRO:HD3	3:H:951:HEC:HBC2	2.02	0.42
2:D:129:VAL:HG11	3:D:951:HEC:HMB1	2.01	0.42
1:C:14:ILE:HG21	1:C:255:GLU:HG3	2.02	0.41
2:H:26:ASP:HA	2:H:27:PRO:HD3	1.96	0.41
1:A:190:ARG:HD2	1:A:190:ARG:HA	1.80	0.41
1:G:216:HIS:HD2	1:G:234:GLY:N	1.93	0.41
1:E:116:THR:CG2	1:E:123:GLU:HG3	2.51	0.41
1:C:190:ARG:HA	1:C:190:ARG:HD2	1.95	0.41
1:E:216:HIS:CE1	1:E:242:GLU:OE2	2.74	0.41
3:A:952:HEC:CBC	3:A:952:HEC:HMC1	2.50	0.41
1:A:97:TYR:OH	1:A:102:GLY:HA2	2.21	0.41
1:C:216:HIS:HD2	1:C:234:GLY:N	1.93	0.41
1:A:52:ASN:C	1:A:52:ASN:HD22	2.24	0.41
1:E:180:CYS:SG	3:E:953:HEC:CBC	3.08	0.41
2:B:11:ASP:OD2	2:B:15:HIS:HB2	2.21	0.41
2:F:91:VAL:O	3:F:951:HEC:HBC2	2.21	0.40
2:B:37:ARG:NH2	4:B:976:HOH:O	2.45	0.40
1:A:185:PHE:O	1:A:186:ASP:HB2	2.21	0.40
2:F:109:THR:O	2:F:110:SER:HB2	2.21	0.40
2:B:46:HIS:HE1	2:B:62:PRO:HD2	1.85	0.40
2:H:42:CYS:SG	3:H:951:HEC:C3B	3.05	0.40
2:H:18:ARG:HD2	4:H:1004:HOH:O	2.20	0.40
1:C:79:CYS:SG	3:C:952:HEC:HAC	2.55	0.40
1:A:215:VAL:HG11	1:A:242:GLU:HG3	2.02	0.40
2:H:31:ARG:HD3	4:H:968:HOH:O	2.20	0.40
1:C:90:LEU:CD2	3:C:952:HEC:HMA3	2.51	0.40
1:A:189:ILE:HA	2:B:44:ALA:O	2.21	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	258/261 (99%)	250 (97%)	8 (3%)	0	100	100
1	C	258/261 (99%)	251 (97%)	7 (3%)	0	100	100
1	E	258/261 (99%)	249 (96%)	8 (3%)	1 (0%)	39	46
1	G	258/261 (99%)	252 (98%)	6 (2%)	0	100	100
2	B	131/138 (95%)	126 (96%)	4 (3%)	1 (1%)	24	26
2	D	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
2	F	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
2	H	136/138 (99%)	130 (96%)	5 (4%)	1 (1%)	26	29
All	All	1570/1596 (98%)	1519 (97%)	48 (3%)	3 (0%)	52	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	55	GLN
1	E	26	ASP
2	B	39	VAL

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	211/211 (100%)	204 (97%)	7 (3%)	45	58
1	C	211/211 (100%)	204 (97%)	7 (3%)	45	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	211/211 (100%)	203 (96%)	8 (4%)	40	52
1	G	211/211 (100%)	202 (96%)	9 (4%)	35	45
2	B	106/109 (97%)	102 (96%)	4 (4%)	40	52
2	D	108/109 (99%)	102 (94%)	6 (6%)	26	31
2	F	109/109 (100%)	103 (94%)	6 (6%)	27	32
2	H	109/109 (100%)	104 (95%)	5 (5%)	33	42
All	All	1276/1280 (100%)	1224 (96%)	52 (4%)	37	48

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	99	GLU
1	A	105	ARG
1	A	186	ASP
1	A	200	ASN
1	A	209	ASN
1	A	216	HIS
2	B	15	HIS
2	B	18	ARG
2	B	22	ASP
2	B	43	ILE
1	C	52	ASN
1	C	90	LEU
1	C	105	ARG
1	C	186	ASP
1	C	200	ASN
1	C	209	ASN
1	C	216	HIS
2	D	15	HIS
2	D	43	ILE
2	D	47	GLU
2	D	55	GLN
2	D	99	GLU
2	D	102	ASN
1	E	26	ASP
1	E	52	ASN
1	E	90	LEU
1	E	91	ARG
1	E	148	SER

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Mol	Chain	Res	Type
1	E	200	ASN
1	E	209	ASN
1	E	216	HIS
2	F	15	HIS
2	F	43	ILE
2	F	49	THR
2	F	55	GLN
2	F	99	GLU
2	F	111	LYS
1	G	52	ASN
1	G	62	ARG
1	G	99	GLU
1	G	105	ARG
1	G	117	SER
1	G	200	ASN
1	G	209	ASN
1	G	216	HIS
1	G	218	ARG
2	H	11	ASP
2	H	15	HIS
2	H	31	ARG
2	H	32	ARG
2	H	43	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	109	GLN
1	A	200	ASN
1	A	209	ASN
1	A	216	HIS
1	C	52	ASN
1	C	109	GLN
1	C	156	GLN
1	C	187	HIS
1	C	200	ASN
1	C	209	ASN
1	C	216	HIS
1	E	52	ASN
1	E	109	GLN
1	E	187	HIS

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Mol	Chain	Res	Type
1	E	200	ASN
1	E	209	ASN
1	E	216	HIS
2	F	55	GLN
1	G	52	ASN
1	G	109	GLN
1	G	200	ASN
1	G	209	ASN
1	G	216	HIS
2	H	13	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	CSS	A	222	1,3	4,6,7	0.74	0	3,6,8	1.19	0
1	CSS	C	222	1,3	4,6,7	0.74	0	3,6,8	1.63	1 (33%)
1	CSS	E	222	1,3	4,6,7	0.71	0	3,6,8	1.71	1 (33%)
1	CSS	G	222	1,3	4,6,7	0.73	0	3,6,8	1.44	1 (33%)

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
1	CSS	A	222	1,3	-	0/1/5/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSS	C	222	1,3	-	0/1/5/7	0/0/0/0
1	CSS	E	222	1,3	-	0/1/5/7	0/0/0/0
1	CSS	G	222	1,3	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	CSS	O-C-CA	-2.32	119.45	125.49
1	E	222	CSS	O-C-CA	-2.25	119.63	125.49
1	G	222	CSS	O-C-CA	-2.17	119.84	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	A	952	1	24,50,50	2.07	5 (20%)	19,82,82	3.30	9 (47%)
3	HEC	A	953	1	24,50,50	2.29	6 (25%)	19,82,82	2.59	6 (31%)
3	HEC	B	951	2	24,50,50	2.09	6 (25%)	19,82,82	2.82	9 (47%)
3	HEC	C	952	1	24,50,50	2.09	4 (16%)	19,82,82	2.82	10 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEC	C	953	1	24,50,50	2.18	4 (16%)	19,82,82	2.66	5 (26%)
3	HEC	D	951	2	24,50,50	2.15	4 (16%)	19,82,82	2.90	9 (47%)
3	HEC	E	952	1	24,50,50	2.18	5 (20%)	19,82,82	2.97	9 (47%)
3	HEC	E	953	1	24,50,50	2.22	4 (16%)	19,82,82	2.43	6 (31%)
3	HEC	F	951	2	24,50,50	2.21	4 (16%)	19,82,82	2.69	8 (42%)
3	HEC	G	952	1	24,50,50	2.30	3 (12%)	19,82,82	3.09	9 (47%)
3	HEC	G	953	1	24,50,50	2.29	6 (25%)	19,82,82	2.44	5 (26%)
3	HEC	H	951	2	24,50,50	2.22	3 (12%)	19,82,82	2.71	8 (42%)

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
3	HEC	A	952	1	-	0/6/54/54	0/0/8/8
3	HEC	A	953	1	-	0/6/54/54	0/0/8/8
3	HEC	B	951	2	-	0/6/54/54	0/0/8/8
3	HEC	C	952	1	-	0/6/54/54	0/0/8/8
3	HEC	C	953	1	-	0/6/54/54	0/0/8/8
3	HEC	D	951	2	-	0/6/54/54	0/0/8/8
3	HEC	E	952	1	-	0/6/54/54	0/0/8/8
3	HEC	E	953	1	-	0/6/54/54	0/0/8/8
3	HEC	F	951	2	-	0/6/54/54	0/0/8/8
3	HEC	G	952	1	-	0/6/54/54	0/0/8/8
3	HEC	G	953	1	-	0/6/54/54	0/0/8/8
3	HEC	H	951	2	-	0/6/54/54	0/0/8/8

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	953	HEC	C3B-C2B	-6.47	1.34	1.40
3	G	952	HEC	C3B-C2B	-6.25	1.34	1.40
3	G	953	HEC	C3B-C2B	-6.24	1.34	1.40
3	A	953	HEC	C3B-C2B	-6.14	1.34	1.40
3	H	951	HEC	C3B-C2B	-5.87	1.34	1.40
3	F	951	HEC	C3B-C2B	-5.47	1.35	1.40
3	E	952	HEC	C3B-C2B	-5.45	1.35	1.40
3	A	952	HEC	C3B-C2B	-5.21	1.35	1.40
3	B	951	HEC	C3B-C2B	-5.11	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	953	HEC	C3B-C2B	-5.09	1.35	1.40
3	C	952	HEC	C3B-C2B	-4.96	1.35	1.40
3	D	951	HEC	C3B-C2B	-4.95	1.35	1.40
3	H	951	HEC	C3C-C2C	-4.76	1.35	1.40
3	F	951	HEC	C3C-C2C	-4.60	1.35	1.40
3	C	953	HEC	C3C-C2C	-4.60	1.35	1.40
3	A	953	HEC	C3C-C2C	-4.58	1.36	1.40
3	G	952	HEC	C3C-C2C	-4.55	1.36	1.40
3	D	951	HEC	C3C-C2C	-4.31	1.36	1.40
3	C	952	HEC	C3C-C2C	-4.04	1.36	1.40
3	G	953	HEC	C3C-C2C	-3.96	1.36	1.40
3	B	951	HEC	C3C-C2C	-3.95	1.36	1.40
3	E	952	HEC	C3C-C2C	-3.92	1.36	1.40
3	A	952	HEC	C3C-C2C	-3.80	1.36	1.40
3	E	953	HEC	C3C-C2C	-3.57	1.37	1.40
3	B	951	HEC	CMA-C3A	2.00	1.56	1.51
3	E	952	HEC	CMA-C3A	2.02	1.56	1.51
3	G	953	HEC	C4A-NA	2.03	1.39	1.36
3	B	951	HEC	CMD-C2D	2.03	1.55	1.51
3	E	952	HEC	CAD-C3D	2.04	1.55	1.52
3	C	952	HEC	C4B-NB	2.05	1.39	1.36
3	A	952	HEC	CMD-C2D	2.09	1.56	1.51
3	A	952	HEC	CMB-C2B	2.10	1.56	1.51
3	C	953	HEC	CMC-C2C	2.15	1.56	1.51
3	B	951	HEC	C4B-NB	2.15	1.39	1.36
3	A	953	HEC	CAD-C3D	2.15	1.55	1.52
3	E	953	HEC	CMC-C2C	2.21	1.56	1.51
3	A	953	HEC	C4A-NA	2.24	1.39	1.36
3	G	953	HEC	CAD-C3D	2.24	1.55	1.52
3	F	951	HEC	C4A-NA	2.26	1.39	1.36
3	G	953	HEC	C1A-NA	2.26	1.39	1.36
3	A	953	HEC	CMC-C2C	2.28	1.56	1.51
3	D	951	HEC	CAD-C3D	2.32	1.56	1.52
3	A	952	HEC	C3D-C2D	5.31	1.53	1.37
3	A	953	HEC	C3D-C2D	5.50	1.54	1.37
3	E	953	HEC	C3D-C2D	5.50	1.54	1.37
3	G	952	HEC	C3D-C2D	5.51	1.54	1.37
3	C	952	HEC	C3D-C2D	5.52	1.54	1.37
3	C	953	HEC	C3D-C2D	5.60	1.54	1.37
3	H	951	HEC	C3D-C2D	5.65	1.54	1.37
3	B	951	HEC	C3D-C2D	5.74	1.54	1.37
3	G	953	HEC	C3D-C2D	5.75	1.54	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	952	HEC	C3D-C2D	5.79	1.54	1.37
3	F	951	HEC	C3D-C2D	5.80	1.54	1.37
3	D	951	HEC	C3D-C2D	5.98	1.55	1.37

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	952	HEC	CBB-CAB-C3B	-8.42	108.64	127.35
3	G	952	HEC	CBB-CAB-C3B	-7.81	109.99	127.35
3	A	953	HEC	CBB-CAB-C3B	-7.35	111.01	127.35
3	C	953	HEC	CBB-CAB-C3B	-7.28	111.17	127.35
3	E	953	HEC	CBB-CAB-C3B	-7.22	111.31	127.35
3	A	952	HEC	CBA-CAA-C2A	-7.05	99.90	112.53
3	A	952	HEC	CBB-CAB-C3B	-7.01	111.77	127.35
3	D	951	HEC	CBB-CAB-C3B	-6.99	111.83	127.35
3	F	951	HEC	CBB-CAB-C3B	-6.93	111.95	127.35
3	C	952	HEC	CBB-CAB-C3B	-6.91	111.98	127.35
3	G	953	HEC	CBB-CAB-C3B	-6.56	112.77	127.35
3	H	951	HEC	CBB-CAB-C3B	-6.51	112.89	127.35
3	B	951	HEC	CBB-CAB-C3B	-6.26	113.44	127.35
3	B	951	HEC	CBA-CAA-C2A	-6.19	101.44	112.53
3	C	953	HEC	CBC-CAC-C3C	-6.17	113.64	127.35
3	A	952	HEC	CBD-CAD-C3D	-5.83	102.08	112.53
3	G	952	HEC	CBA-CAA-C2A	-5.66	102.39	112.53
3	A	953	HEC	CBC-CAC-C3C	-5.62	114.87	127.35
3	G	953	HEC	CBC-CAC-C3C	-5.44	115.27	127.35
3	H	951	HEC	CBC-CAC-C3C	-5.08	116.06	127.35
3	E	952	HEC	CBC-CAC-C3C	-4.91	116.44	127.35
3	D	951	HEC	CBC-CAC-C3C	-4.86	116.54	127.35
3	G	952	HEC	CBD-CAD-C3D	-4.86	103.83	112.53
3	F	951	HEC	CBA-CAA-C2A	-4.69	104.12	112.53
3	C	952	HEC	CBD-CAD-C3D	-4.63	104.24	112.53
3	C	952	HEC	CBC-CAC-C3C	-4.44	117.48	127.35
3	E	953	HEC	CBC-CAC-C3C	-4.37	117.63	127.35
3	H	951	HEC	CBA-CAA-C2A	-4.37	104.69	112.53
3	D	951	HEC	CBA-CAA-C2A	-4.32	104.78	112.53
3	A	952	HEC	CBC-CAC-C3C	-4.26	117.88	127.35
3	B	951	HEC	CBC-CAC-C3C	-4.16	118.11	127.35
3	H	951	HEC	CAA-C2A-C1A	-4.12	122.54	127.01
3	F	951	HEC	CBC-CAC-C3C	-3.94	118.60	127.35
3	E	952	HEC	CBD-CAD-C3D	-3.92	105.50	112.53
3	D	951	HEC	CMB-C2B-C1B	-3.90	121.91	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	952	HEC	CBC-CAC-C3C	-3.77	118.97	127.35
3	G	952	HEC	CAA-C2A-C1A	-3.72	122.97	127.01
3	A	952	HEC	CMC-C2C-C1C	-3.53	122.53	128.36
3	C	952	HEC	CBA-CAA-C2A	-3.43	106.38	112.53
3	E	953	HEC	CMC-C2C-C1C	-3.34	122.85	128.36
3	D	951	HEC	CMC-C2C-C1C	-3.28	122.93	128.36
3	F	951	HEC	CAD-CBD-CGD	-3.25	106.79	112.75
3	B	951	HEC	CAD-CBD-CGD	-3.21	106.86	112.75
3	F	951	HEC	CMC-C2C-C1C	-3.19	123.08	128.36
3	A	952	HEC	CAA-C2A-C1A	-3.14	123.60	127.01
3	H	951	HEC	CMB-C2B-C1B	-3.11	123.22	128.36
3	B	951	HEC	CMB-C2B-C1B	-3.07	123.29	128.36
3	D	951	HEC	CAD-CBD-CGD	-3.04	107.17	112.75
3	C	953	HEC	CMC-C2C-C1C	-2.91	123.56	128.36
3	B	951	HEC	CAA-C2A-C1A	-2.91	123.85	127.01
3	E	952	HEC	CBA-CAA-C2A	-2.80	107.52	112.53
3	G	953	HEC	CMC-C2C-C1C	-2.78	123.76	128.36
3	E	952	HEC	C3B-C4B-NB	-2.78	105.70	110.94
3	C	953	HEC	CBA-CAA-C2A	-2.77	107.57	112.53
3	C	952	HEC	CMB-C2B-C1B	-2.69	123.92	128.36
3	A	953	HEC	CMC-C2C-C1C	-2.67	123.95	128.36
3	C	952	HEC	CAA-C2A-C1A	-2.67	124.11	127.01
3	A	953	HEC	CAA-C2A-C1A	-2.65	124.13	127.01
3	C	952	HEC	CMC-C2C-C1C	-2.64	123.99	128.36
3	E	952	HEC	CAA-C2A-C1A	-2.63	124.15	127.01
3	F	951	HEC	CAA-C2A-C1A	-2.63	124.16	127.01
3	E	952	HEC	CMC-C2C-C1C	-2.63	124.02	128.36
3	B	951	HEC	CMC-C2C-C1C	-2.62	124.03	128.36
3	D	951	HEC	C3B-C4B-NB	-2.60	106.03	110.94
3	G	952	HEC	C3B-C4B-NB	-2.58	106.08	110.94
3	D	951	HEC	CAA-C2A-C1A	-2.54	124.25	127.01
3	C	953	HEC	CMB-C2B-C1B	-2.53	124.17	128.36
3	G	953	HEC	CMB-C2B-C1B	-2.49	124.25	128.36
3	F	951	HEC	CMB-C2B-C1B	-2.47	124.28	128.36
3	E	953	HEC	CMB-C2B-C1B	-2.42	124.36	128.36
3	G	952	HEC	CMC-C2C-C1C	-2.39	124.41	128.36
3	D	951	HEC	CAD-C3D-C4D	-2.39	124.41	127.01
3	C	952	HEC	C3B-C4B-NB	-2.37	106.48	110.94
3	E	953	HEC	CBD-CAD-C3D	-2.32	108.37	112.53
3	E	953	HEC	CBA-CAA-C2A	-2.24	108.52	112.53
3	A	952	HEC	C3B-C4B-NB	-2.22	106.75	110.94
3	G	953	HEC	CBA-CAA-C2A	-2.20	108.59	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	951	HEC	CMC-C2C-C1C	-2.20	124.73	128.36
3	H	951	HEC	CAD-CBD-CGD	-2.08	108.93	112.75
3	B	951	HEC	C3B-C4B-NB	-2.06	107.05	110.94
3	H	951	HEC	C3B-C4B-NB	-2.06	107.05	110.94
3	A	953	HEC	C3B-C4B-NB	-2.06	107.05	110.94
3	F	951	HEC	C3B-C4B-NB	-2.02	107.13	110.94
3	G	952	HEC	CAA-CBA-CGA	2.16	116.71	112.75
3	C	952	HEC	C4B-C3B-C2B	2.18	108.71	106.35
3	A	952	HEC	C4B-C3B-C2B	2.19	108.72	106.35
3	E	952	HEC	CAA-CBA-CGA	2.23	116.83	112.75
3	B	951	HEC	CAA-CBA-CGA	2.30	116.95	112.75
3	A	953	HEC	C4B-C3B-C2B	2.33	108.87	106.35
3	E	952	HEC	C4B-C3B-C2B	2.60	109.16	106.35
3	A	952	HEC	CAA-CBA-CGA	2.76	117.80	112.75
3	C	952	HEC	CAA-CBA-CGA	2.84	117.95	112.75
3	G	952	HEC	C4B-C3B-C2B	2.86	109.44	106.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 115 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	952	HEC	10	0
3	A	953	HEC	8	0
3	B	951	HEC	12	0
3	C	952	HEC	10	0
3	C	953	HEC	6	0
3	D	951	HEC	7	0
3	E	952	HEC	9	0
3	E	953	HEC	11	0
3	F	951	HEC	9	0
3	G	952	HEC	13	0
3	G	953	HEC	8	0
3	H	951	HEC	12	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	260/261 (99%)	0.07	1 (0%) 93 97	4, 12, 22, 27	0
1	C	260/261 (99%)	0.15	2 (0%) 87 93	5, 11, 19, 27	0
1	E	260/261 (99%)	0.10	0 100 100	5, 11, 21, 25	0
1	G	260/261 (99%)	0.19	2 (0%) 87 93	5, 14, 24, 29	0
2	B	135/138 (97%)	0.41	4 (2%) 54 66	8, 18, 32, 35	0
2	D	137/138 (99%)	0.20	3 (2%) 65 77	10, 17, 27, 33	0
2	F	138/138 (100%)	0.16	4 (2%) 55 67	8, 15, 27, 29	0
2	H	138/138 (100%)	0.66	10 (7%) 18 28	8, 20, 34, 38	0
All	All	1588/1596 (99%)	0.21	26 (1%) 74 84	4, 14, 26, 38	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	54	ALA	4.6
1	A	50	PHE	3.5
2	F	24	PRO	3.4
2	B	23	ALA	3.2
2	B	24	PRO	3.1
2	H	1	ALA	3.1
2	B	49	THR	3.1
1	G	10	GLY	3.1
2	F	55	GLN	2.8
2	D	114	GLU	2.7
1	G	50	PHE	2.6
2	H	88	PRO	2.5
2	H	71	TYR	2.5
2	H	138	GLN	2.5
2	F	138	GLN	2.4
2	H	69	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	38	SER	2.4
2	H	28	VAL	2.3
2	B	31	ARG	2.3
1	C	70	GLY	2.2
2	H	24	PRO	2.2
2	H	68	ALA	2.2
2	F	13	GLN	2.2
2	D	47	GLU	2.1
2	H	55	GLN	2.1
1	C	207	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSS	G	222	7/8	0.98	0.11	-	7,8,8,10	0
1	CSS	A	222	7/8	0.98	0.13	-	5,7,7,9	0
1	CSS	C	222	7/8	0.97	0.11	-	8,10,12,15	0
1	CSS	E	222	7/8	0.98	0.11	-	6,6,8,8	0

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
3	HEC	F	951	43/43	0.95	0.14	0.77	7,9,12,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	HEC	D	951	43/43	0.93	0.15	0.69	8,11,16,17	0
3	HEC	A	953	43/43	0.96	0.15	0.69	3,6,8,11	0
3	HEC	E	953	43/43	0.97	0.15	0.66	2,5,7,7	0
3	HEC	H	951	43/43	0.94	0.18	0.65	10,13,18,19	0
3	HEC	C	953	43/43	0.96	0.16	0.44	4,6,9,12	0
3	HEC	E	952	43/43	0.94	0.17	0.31	11,14,17,20	0
3	HEC	C	952	43/43	0.94	0.17	0.25	11,14,17,18	0
3	HEC	G	952	43/43	0.97	0.14	0.18	6,11,18,19	0
3	HEC	G	953	43/43	0.96	0.14	0.10	6,9,11,14	0
3	HEC	B	951	43/43	0.96	0.15	-0.01	9,10,12,15	0
3	HEC	A	952	43/43	0.97	0.14	-0.04	4,8,12,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.