Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 01:23 am GMT

PDB ID	:	4MEC
Title	:	Crystal structure of RAT Heme oxygenase-1 in complex with ZN(II)-Protoporphyrin IX
Authors	:	Sugishima, M.
Deposited on	:	2013-08-26
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

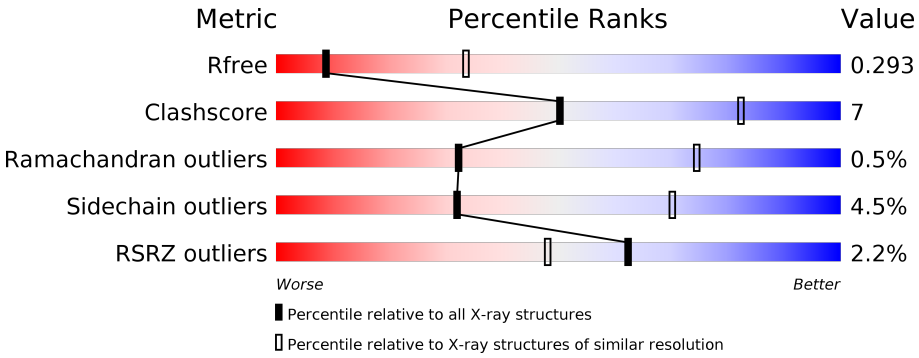
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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 <=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	232	73% 18% • 8%
1	B	232	75% 17% • 7%
1	C	232	% 72% 19% • 8%
1	D	232	2% 80% 12% • 7%
1	E	232	3% 76% 15% • 8%
1	F	232	2% 76% 8% • 15%

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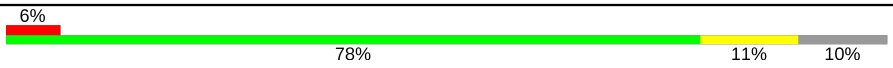
Mol	Chain	Length	Quality of chain
1	G	232	

2 Entry composition

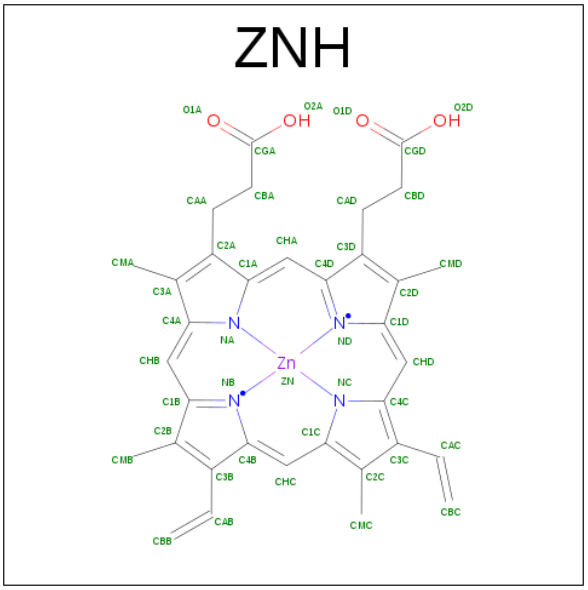
There are 2 unique types of molecules in this entry. The entry contains 11505 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Heme oxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1734	1110	296	322	6			
1	B	215	Total	C	N	O	S	0	0	0
			1730	1107	295	322	6			
1	C	213	Total	C	N	O	S	0	0	0
			1704	1092	286	320	6			
1	D	215	Total	C	N	O	S	0	0	0
			1680	1067	287	321	5			
1	E	213	Total	C	N	O	S	0	0	0
			1658	1065	276	311	6			
1	F	197	Total	C	N	O	S	0	0	0
			1339	833	242	260	4			
1	G	209	Total	C	N	O	S	0	0	0
			1475	930	260	281	4			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING ZN (three-letter code: ZNH) (formula: $C_{34}H_{32}N_4O_4Zn$).



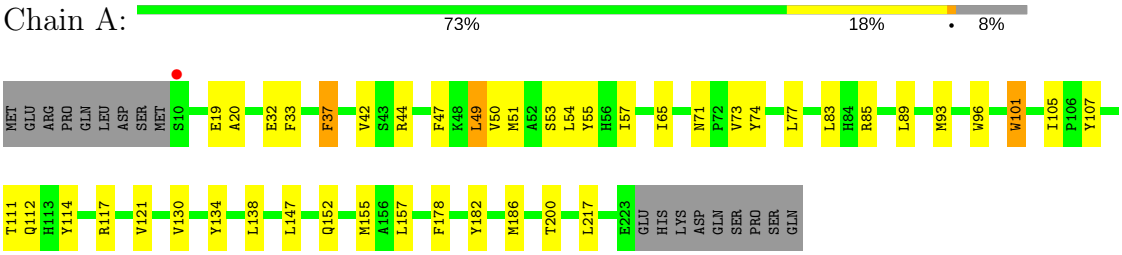
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O Zn 39 32 4 2 1	0	0
2	B	1	Total C N O Zn 39 32 4 2 1	0	0
2	C	1	Total C N Zn 35 30 4 1	0	0
2	D	1	Total C N Zn 35 30 4 1	0	0
2	E	1	Total C N Zn 35 30 4 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

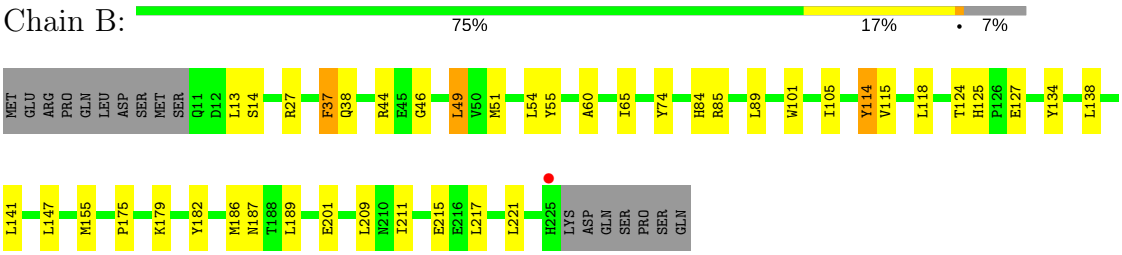
- Molecule 1: Heme oxygenase 1

Chain A:



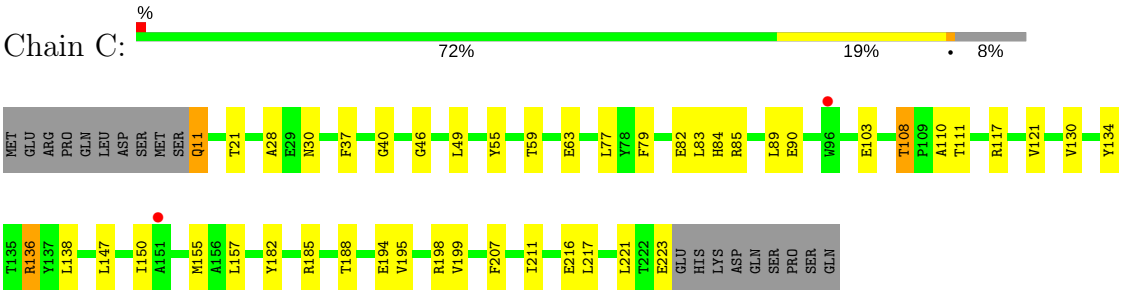
- Molecule 1: Heme oxygenase 1

Chain B:



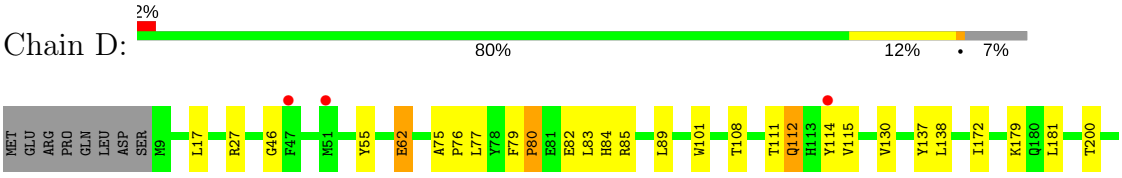
- Molecule 1: Heme oxygenase 1

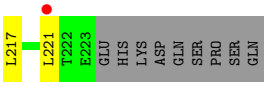
Chain C:



- Molecule 1: Heme oxygenase 1

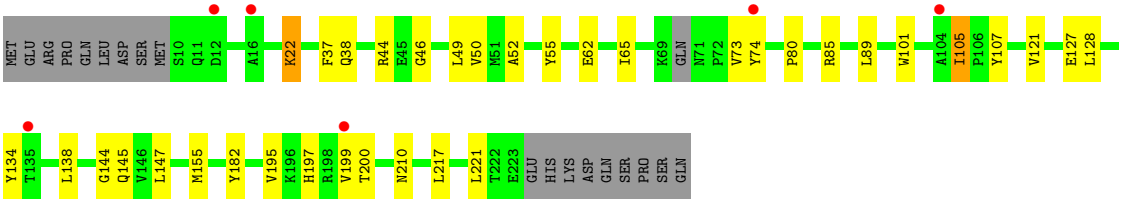
Chain D:





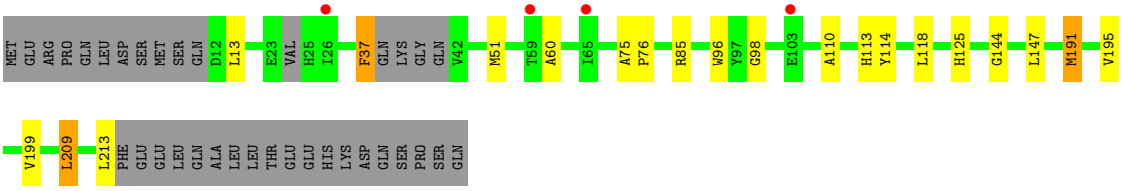
• Molecule 1: Heme oxygenase 1

Chain E:



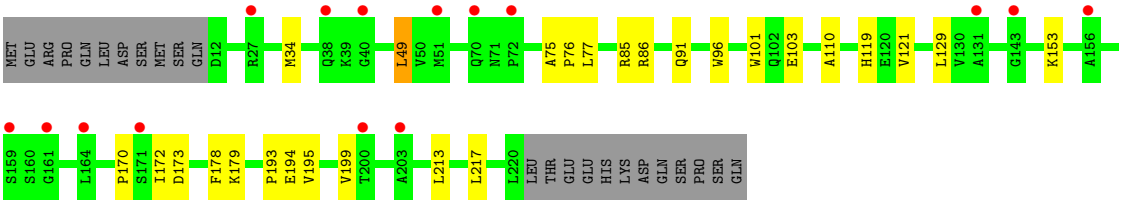
• Molecule 1: Heme oxygenase 1

Chain F:



• Molecule 1: Heme oxygenase 1

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	40.06Å 73.17Å 148.76Å 86.41° 87.62° 86.25°	Depositor
Resolution (Å)	38.94 – 3.20 38.94 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (38.94-3.20) 95.8 (38.94-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.249 , 0.299 0.245 , 0.293	Depositor DCC
R_{free} test set	1346 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	101.8	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 78.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11505	wwPDB-VP
Average B, all atoms (Å^2)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZNH

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	0.44	2/1778 (0.1%)	0.52	0/2408
1	B	0.44	0/1774	0.52	0/2406
1	C	0.43	0/1748	0.51	0/2374
1	D	0.43	1/1722 (0.1%)	0.47	0/2344
1	E	0.43	0/1701	0.48	0/2316
1	F	0.45	0/1369	0.48	0/1881
1	G	0.44	2/1511 (0.1%)	0.49	0/2073
All	All	0.44	5/11603 (0.0%)	0.50	0/15802

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	96	TRP	CD2-CE2	5.14	1.47	1.41
1	A	101	TRP	CD2-CE2	5.12	1.47	1.41
1	G	101	TRP	CD2-CE2	5.02	1.47	1.41
1	A	96	TRP	CD2-CE2	5.00	1.47	1.41
1	D	101	TRP	CD2-CE2	5.00	1.47	1.41

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	1734	0	1690	34	0
1	B	1730	0	1667	23	0
1	C	1704	0	1630	31	0
1	D	1680	0	1561	19	0
1	E	1658	0	1551	22	0
1	F	1339	0	1073	11	0
1	G	1475	0	1242	8	0
2	A	39	0	26	0	0
2	B	39	0	26	0	0
2	C	35	0	22	1	0
2	D	35	0	22	0	0
2	E	35	0	22	2	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
All	All	11505	0	10532	146	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 (146) 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:42:VAL:HG22	1:A:155:MET:HE3	1.61	0.80
1:F:110:ALA:HB1	1:F:213:LEU:HD11	1.68	0.75
1:C:55:TYR:HA	1:C:89:LEU:HD13	1.69	0.75
1:F:60:ALA:HB3	1:F:118:LEU:HD23	1.71	0.73
1:A:49:LEU:HD22	1:A:217:LEU:HD22	1.70	0.73
1:C:49:LEU:HD22	1:C:217:LEU:HD22	1.71	0.73
1:G:49:LEU:HD12	1:G:217:LEU:HD22	1.71	0.72
1:C:21:THR:HG21	1:C:207:PHE:CD1	2.28	0.69
1:B:124:THR:HG23	1:B:125:HIS:CD2	2.30	0.66
1:B:38:GLN:HE21	1:B:147:LEU:HD21	1.63	0.64
1:E:101:TRP:O	1:E:105:ILE:HD11	1.97	0.64
1:C:49:LEU:CD2	1:C:217:LEU:HD22	2.29	0.63
1:B:49:LEU:HD12	1:B:217:LEU:HD13	1.79	0.63
1:B:138:LEU:HD21	1:B:182:TYR:CD1	2.34	0.63
1:A:77:LEU:HD11	1:A:130:VAL:HG23	1.79	0.62
1:A:42:VAL:CG2	1:A:155:MET:HE3	2.30	0.62
1:B:51:MET:HE3	1:B:51:MET:HA	1.83	0.61
1:E:55:TYR:HA	1:E:89:LEU:HD13	1.82	0.61
1:A:77:LEU:CD1	1:A:130:VAL:HG23	2.30	0.61
1:F:98:GLY:HA2	1:G:193:PRO:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:TYR:HA	1:A:89:LEU:HD13	1.82	0.60
1:A:152:GLN:HA	1:A:157:LEU:HD23	1.83	0.60
1:B:65:ILE:HG23	1:B:74:TYR:CE2	2.37	0.59
1:A:53:SER:O	1:A:57:ILE:HD13	2.02	0.59
1:G:121:VAL:HG11	1:G:129:LEU:HD13	1.84	0.59
1:B:141:LEU:HD22	1:B:175:PRO:HB3	1.85	0.59
1:E:46:GLY:HA2	1:E:221:LEU:HD21	1.85	0.59
1:A:42:VAL:HG22	1:A:155:MET:CE	2.34	0.57
1:C:77:LEU:HD11	1:C:130:VAL:HG23	1.87	0.57
1:A:77:LEU:HD21	1:A:186:MET:HA	1.86	0.57
1:B:37:PHE:CD1	1:B:147:LEU:HD22	2.40	0.56
1:A:57:ILE:CD1	1:A:111:THR:HG23	2.36	0.56
1:C:77:LEU:CD1	1:C:130:VAL:HG23	2.35	0.56
1:C:11:GLN:HE21	1:C:11:GLN:C	2.09	0.56
1:C:134:TYR:HA	1:C:138:LEU:HD23	1.86	0.55
1:B:49:LEU:HD12	1:B:217:LEU:CD1	2.35	0.55
1:D:46:GLY:HA3	1:D:221:LEU:HD11	1.88	0.55
1:A:44:ARG:HA	1:A:155:MET:HE1	1.89	0.55
1:D:108:THR:HG21	1:D:217:LEU:HD21	1.89	0.55
1:E:44:ARG:HA	1:E:155:MET:HE3	1.89	0.55
1:E:52:ALA:HB1	1:E:105:ILE:CG2	2.37	0.54
1:D:77:LEU:HD11	1:D:130:VAL:HG23	1.90	0.54
1:G:195:VAL:O	1:G:199:VAL:HG23	2.08	0.54
1:A:33:PHE:CE2	1:A:50:VAL:HG11	2.43	0.53
1:C:195:VAL:O	1:C:199:VAL:HG23	2.09	0.53
1:A:37:PHE:CD1	1:A:147:LEU:HD22	2.44	0.52
1:E:38:GLN:HE22	2:E:300:ZNH:HMB1	1.75	0.52
1:D:80:PRO:HA	1:D:84:HIS:CD2	2.45	0.52
1:C:185:ARG:O	1:C:188:THR:HG22	2.10	0.52
1:E:37:PHE:CD1	1:E:147:LEU:HD22	2.45	0.52
1:B:60:ALA:HB2	1:B:115:VAL:HG13	1.91	0.51
1:E:46:GLY:O	1:E:50:VAL:HG23	2.10	0.51
1:B:55:TYR:HA	1:B:89:LEU:HD13	1.91	0.51
1:E:127:GLU:OE1	1:E:195:VAL:HG11	2.11	0.51
1:A:49:LEU:CD2	1:A:217:LEU:HD22	2.40	0.51
1:D:82:GLU:HB3	1:D:172:ILE:HD11	1.92	0.50
1:C:28:ALA:HB2	1:C:211:ILE:HD11	1.93	0.50
1:C:155:MET:HG3	1:C:157:LEU:HD23	1.93	0.50
1:C:37:PHE:CD1	1:C:147:LEU:HD22	2.46	0.50
1:A:65:ILE:HG23	1:A:74:TYR:CE2	2.47	0.50
1:B:13:LEU:HD23	1:B:186:MET:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:LEU:CD1	1:D:130:VAL:HG23	2.41	0.50
1:A:20:ALA:CB	1:A:200:THR:OG1	2.60	0.50
1:C:207:PHE:O	1:C:211:ILE:HG12	2.13	0.49
1:C:21:THR:HG21	1:C:207:PHE:CE1	2.47	0.49
1:C:110:ALA:HB3	1:C:216:GLU:OE1	2.11	0.49
1:F:60:ALA:CB	1:F:118:LEU:HD23	2.42	0.48
1:D:46:GLY:CA	1:D:221:LEU:HD21	2.43	0.48
1:E:195:VAL:O	1:E:199:VAL:HG23	2.14	0.48
1:F:113:HIS:ND1	1:F:209:LEU:HD11	2.28	0.48
1:A:117:ARG:O	1:A:121:VAL:HG23	2.14	0.48
1:D:138:LEU:HD22	1:D:179:LYS:HG3	1.95	0.48
1:A:42:VAL:O	1:A:155:MET:HE2	2.14	0.48
1:G:75:ALA:HB3	1:G:76:PRO:HD3	1.95	0.47
1:B:46:GLY:HA2	1:B:221:LEU:HD21	1.96	0.47
1:B:27:ARG:HD2	1:B:211:ILE:HD13	1.96	0.47
1:C:40:GLY:HA2	1:C:150:ILE:HD12	1.97	0.47
1:F:13:LEU:HD22	1:F:191:MET:HE3	1.96	0.47
1:C:108:THR:HG23	1:C:111:THR:OG1	2.15	0.46
1:A:47:PHE:HB2	1:A:155:MET:HE1	1.96	0.46
1:A:101:TRP:O	1:A:105:ILE:HG23	2.15	0.46
1:A:53:SER:O	1:A:57:ILE:CD1	2.63	0.46
1:C:136:ARG:HA	1:C:136:ARG:HE	1.81	0.46
1:B:186:MET:HA	1:B:189:LEU:HD13	1.98	0.46
1:C:110:ALA:CB	1:C:216:GLU:OE1	2.63	0.46
1:F:37:PHE:CE1	1:F:147:LEU:HD13	2.51	0.45
1:D:55:TYR:HA	1:D:89:LEU:HD13	1.98	0.45
1:E:73:VAL:HG11	1:E:127:GLU:HG2	1.98	0.45
1:F:96:TRP:HA	1:G:194:GLU:HB2	1.98	0.45
1:E:138:LEU:HD21	1:E:182:TYR:CE1	2.51	0.45
1:E:38:GLN:NE2	2:E:300:ZNH:HMB1	2.32	0.45
1:D:79:PHE:HB2	1:D:83:LEU:HD12	1.99	0.44
1:E:121:VAL:HG13	1:E:128:LEU:HB2	1.99	0.44
1:A:57:ILE:HD12	1:A:111:THR:HG23	1.99	0.44
1:F:114:TYR:HA	1:F:209:LEU:HD13	1.99	0.44
1:A:51:MET:CE	1:A:54:LEU:HD12	2.48	0.44
1:D:17:LEU:HD23	1:D:200:THR:HA	1.98	0.44
1:D:17:LEU:HD23	1:D:200:THR:HG22	1.99	0.44
1:C:28:ALA:HA	1:C:211:ILE:HD12	1.99	0.44
1:C:117:ARG:O	1:C:121:VAL:HG23	2.18	0.44
1:D:75:ALA:HB3	1:D:76:PRO:HD3	2.00	0.44
1:A:134:TYR:CD1	1:A:138:LEU:HD12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:TYR:CE2	1:A:112:GLN:HG2	2.53	0.43
1:C:28:ALA:HB1	2:C:300:ZNH:HMC2	1.99	0.43
1:B:114:TYR:CD1	1:B:209:LEU:HD13	2.53	0.43
1:E:49:LEU:HB3	1:E:217:LEU:HD22	2.01	0.43
1:E:134:TYR:HA	1:E:138:LEU:HD23	2.00	0.43
1:E:65:ILE:HG23	1:E:74:TYR:HE2	1.84	0.43
1:B:14:SER:HB3	1:B:187:ASN:HD21	1.83	0.43
1:A:47:PHE:HB2	1:A:155:MET:CE	2.48	0.43
1:B:65:ILE:HG23	1:B:74:TYR:HE2	1.82	0.43
1:A:51:MET:HE1	1:A:54:LEU:HD12	2.00	0.43
1:C:46:GLY:HA2	1:C:221:LEU:HD21	2.01	0.43
1:C:40:GLY:CA	1:C:150:ILE:HD12	2.49	0.43
1:C:79:PHE:HB3	1:C:82:GLU:HB2	1.99	0.42
1:F:195:VAL:O	1:F:199:VAL:HG23	2.19	0.42
1:G:110:ALA:HB3	1:G:213:LEU:HD12	2.01	0.42
1:D:79:PHE:HB3	1:D:82:GLU:HB2	2.02	0.42
1:A:51:MET:HB3	1:A:93:MET:HE1	2.02	0.42
1:A:77:LEU:HD21	1:A:186:MET:CA	2.50	0.42
1:D:111:THR:O	1:D:115:VAL:HG23	2.20	0.42
1:G:172:ILE:HG21	1:G:178:PHE:HB2	2.00	0.42
1:A:138:LEU:HD21	1:A:182:TYR:CD1	2.54	0.42
1:A:71:ASN:OD1	1:A:73:VAL:HG22	2.20	0.42
1:E:52:ALA:HB1	1:E:105:ILE:HG23	2.00	0.42
1:B:101:TRP:O	1:B:105:ILE:HG23	2.20	0.42
1:C:37:PHE:HD1	1:C:147:LEU:HD22	1.84	0.41
1:C:59:THR:O	1:C:63:GLU:HB2	2.20	0.41
1:E:22:LYS:HA	1:E:22:LYS:HE3	2.03	0.41
1:B:138:LEU:HD13	1:B:179:LYS:HG3	2.03	0.41
1:D:181:LEU:HD23	1:D:181:LEU:C	2.40	0.41
1:E:197:HIS:O	1:E:200:THR:HG22	2.21	0.41
1:B:44:ARG:NH2	1:B:155:MET:O	2.53	0.41
1:B:134:TYR:O	1:B:138:LEU:HB2	2.21	0.41
1:C:79:PHE:HB2	1:C:83:LEU:HD12	2.03	0.41
1:E:144:GLY:HA2	1:E:147:LEU:HD12	2.03	0.41
1:D:112:GLN:HB2	1:D:112:GLN:HE21	1.69	0.41
1:A:134:TYR:CE1	1:A:138:LEU:HD12	2.55	0.41
1:A:83:LEU:HD21	1:A:178:PHE:CE2	2.56	0.40
1:B:51:MET:HE3	1:B:54:LEU:HD12	2.02	0.40
1:C:37:PHE:CE1	1:C:147:LEU:HD13	2.55	0.40
1:D:62:GLU:OE2	1:D:137:TYR:OH	2.40	0.40
1:C:194:GLU:OE1	1:C:198:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:GLY:N	1:D:221:LEU:HD21	2.37	0.40
1:E:62:GLU:HA	1:E:65:ILE:HD12	2.04	0.40
1:F:75:ALA:HB3	1:F:76:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/232 (91%)	201 (95%)	11 (5%)	0	100	100
1	B	213/232 (92%)	208 (98%)	5 (2%)	0	100	100
1	C	211/232 (91%)	199 (94%)	12 (6%)	0	100	100
1	D	213/232 (92%)	206 (97%)	6 (3%)	1 (0%)	32	74
1	E	209/232 (90%)	194 (93%)	14 (7%)	1 (0%)	32	74
1	F	191/232 (82%)	173 (91%)	17 (9%)	1 (0%)	32	74
1	G	207/232 (89%)	185 (89%)	17 (8%)	5 (2%)	7	39
All	All	1456/1624 (90%)	1366 (94%)	82 (6%)	8 (0%)	32	74

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	77	LEU
1	G	153	LYS
1	G	170	PRO
1	F	144	GLY
1	G	103	GLU
1	E	80	PRO
1	G	179	LYS
1	D	80	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/201 (90%)	175 (97%)	6 (3%)	43	78
1	B	178/201 (89%)	169 (95%)	9 (5%)	28	66
1	C	175/201 (87%)	165 (94%)	10 (6%)	24	63
1	D	167/201 (83%)	162 (97%)	5 (3%)	46	79
1	E	165/201 (82%)	159 (96%)	6 (4%)	40	76
1	F	103/201 (51%)	97 (94%)	6 (6%)	23	62
1	G	121/201 (60%)	114 (94%)	7 (6%)	23	62
All	All	1090/1407 (78%)	1041 (96%)	49 (4%)	32	70

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	32	GLU
1	A	37	PHE
1	A	49	LEU
1	A	85	ARG
1	A	114	TYR
1	B	37	PHE
1	B	49	LEU
1	B	84	HIS
1	B	85	ARG
1	B	114	TYR
1	B	118	LEU
1	B	127	GLU
1	B	201	GLU
1	B	215	GLU
1	C	11	GLN
1	C	30	ASN
1	C	84	HIS
1	C	85	ARG
1	C	90	GLU

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Mol	Chain	Res	Type
1	C	103	GLU
1	C	108	THR
1	C	136	ARG
1	C	182	TYR
1	C	223	GLU
1	D	27	ARG
1	D	62	GLU
1	D	85	ARG
1	D	112	GLN
1	D	114	TYR
1	E	22	LYS
1	E	85	ARG
1	E	105	ILE
1	E	107	TYR
1	E	145	GLN
1	E	210	ASN
1	F	37	PHE
1	F	51	MET
1	F	85	ARG
1	F	125	HIS
1	F	191	MET
1	F	209	LEU
1	G	34	MET
1	G	49	LEU
1	G	85	ARG
1	G	86	ARG
1	G	91	GLN
1	G	119	HIS
1	G	173	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	B	36	ASN
1	B	38	GLN
1	B	68	ASN
1	B	125	HIS
1	B	210	ASN
1	C	11	GLN
1	C	36	ASN
1	C	132	HIS

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Mol	Chain	Res	Type
1	C	152	GLN
1	C	210	ASN
1	D	25	HIS
1	D	56	HIS
1	D	112	GLN
1	E	38	GLN
1	E	152	GLN
1	F	119	HIS
1	G	38	GLN
1	G	91	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are modelled with single atom - leaving 5 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	$\#\|Z\| > 2$
2	ZNH	A	300	1	29,46,50	4.44	22 (75%)	13,77,82	1.84	3 (23%)
2	ZNH	B	300	1	29,46,50	4.42	21 (72%)	13,77,82	1.81	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ZNH	C	300	1	29,42,50	4.78	22 (75%)	12,72,82	1.53	1 (8%)
2	ZNH	D	300	1	29,42,50	4.78	22 (75%)	12,72,82	1.65	2 (16%)
2	ZNH	E	300	1	29,42,50	4.78	22 (75%)	12,72,82	1.59	2 (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
2	ZNH	A	300	1	-	0/5/89/94	0/0/8/8
2	ZNH	B	300	1	-	0/5/89/94	0/0/8/8
2	ZNH	C	300	1	-	0/2/84/94	0/0/8/8
2	ZNH	D	300	1	-	0/2/84/94	0/0/8/8
2	ZNH	E	300	1	-	0/2/84/94	0/0/8/8

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	ZNH	CHC-C4B	-7.74	1.38	1.53
2	D	300	ZNH	CHC-C4B	-7.72	1.38	1.53
2	E	300	ZNH	CHC-C4B	-7.72	1.38	1.53
2	A	300	ZNH	CHB-C1B	-7.71	1.38	1.53
2	A	300	ZNH	CHD-C1D	-7.67	1.38	1.53
2	B	300	ZNH	CHC-C4B	-7.66	1.38	1.53
2	B	300	ZNH	CHB-C1B	-7.64	1.38	1.53
2	E	300	ZNH	CHB-C1B	-7.63	1.38	1.53
2	A	300	ZNH	CHA-C4D	-7.59	1.38	1.53
2	E	300	ZNH	CHA-C4D	-7.56	1.38	1.53
2	C	300	ZNH	CHC-C4B	-7.55	1.38	1.53
2	D	300	ZNH	CHD-C1D	-7.51	1.39	1.53
2	D	300	ZNH	CHA-C4D	-7.47	1.39	1.53
2	B	300	ZNH	CHD-C1D	-7.46	1.39	1.53
2	B	300	ZNH	CHA-C4D	-7.46	1.39	1.53
2	E	300	ZNH	CHD-C1D	-7.42	1.39	1.53
2	C	300	ZNH	CHB-C1B	-7.41	1.39	1.53
2	D	300	ZNH	CHB-C1B	-7.38	1.39	1.53
2	C	300	ZNH	CHD-C1D	-7.38	1.39	1.53
2	C	300	ZNH	CHA-C4D	-7.32	1.39	1.53
2	A	300	ZNH	CHD-C4C	-5.44	1.38	1.51
2	A	300	ZNH	CHA-C1A	-5.37	1.38	1.51
2	B	300	ZNH	CHB-C4A	-5.35	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	ZNH	CHB-C4A	-5.33	1.38	1.51
2	D	300	ZNH	CHC-C1C	-5.31	1.38	1.51
2	E	300	ZNH	CHB-C4A	-5.31	1.38	1.51
2	E	300	ZNH	CHA-C1A	-5.27	1.38	1.51
2	D	300	ZNH	CHA-C1A	-5.27	1.38	1.51
2	E	300	ZNH	CHD-C4C	-5.25	1.38	1.51
2	B	300	ZNH	CHC-C1C	-5.25	1.38	1.51
2	C	300	ZNH	CHB-C4A	-5.22	1.38	1.51
2	E	300	ZNH	CHC-C1C	-5.21	1.38	1.51
2	B	300	ZNH	CHD-C4C	-5.20	1.39	1.51
2	D	300	ZNH	CHD-C4C	-5.20	1.39	1.51
2	B	300	ZNH	CHA-C1A	-5.19	1.39	1.51
2	C	300	ZNH	CHA-C1A	-5.18	1.39	1.51
2	C	300	ZNH	CHC-C1C	-5.17	1.39	1.51
2	C	300	ZNH	CHD-C4C	-5.15	1.39	1.51
2	D	300	ZNH	CHB-C4A	-5.09	1.39	1.51
2	A	300	ZNH	CHC-C1C	-5.05	1.39	1.51
2	A	300	ZNH	C3C-C2C	-4.78	1.34	1.40
2	E	300	ZNH	C3C-C2C	-4.66	1.34	1.40
2	D	300	ZNH	C3C-C2C	-4.56	1.34	1.40
2	B	300	ZNH	C3C-C2C	-4.41	1.34	1.40
2	C	300	ZNH	C3C-C2C	-4.39	1.34	1.40
2	D	300	ZNH	C4B-C3B	-3.73	1.45	1.51
2	B	300	ZNH	C4B-C3B	-3.72	1.45	1.51
2	A	300	ZNH	C4B-C3B	-3.71	1.45	1.51
2	E	300	ZNH	C4B-C3B	-3.60	1.45	1.51
2	C	300	ZNH	C4B-C3B	-3.57	1.45	1.51
2	A	300	ZNH	C3A-C2A	-2.03	1.34	1.41
2	A	300	ZNH	CMD-C2D	2.45	1.54	1.50
2	E	300	ZNH	CMD-C2D	2.46	1.54	1.50
2	B	300	ZNH	CMD-C2D	2.62	1.54	1.50
2	C	300	ZNH	CMD-C2D	2.68	1.55	1.50
2	B	300	ZNH	CAD-C3D	2.70	1.54	1.51
2	B	300	ZNH	CMB-C2B	2.72	1.55	1.50
2	E	300	ZNH	CMB-C2B	2.72	1.55	1.50
2	D	300	ZNH	CMD-C2D	2.73	1.55	1.50
2	D	300	ZNH	CMB-C2B	2.74	1.55	1.50
2	E	300	ZNH	CAD-C3D	2.75	1.55	1.50
2	A	300	ZNH	CMB-C2B	2.75	1.55	1.50
2	C	300	ZNH	CAD-C3D	2.79	1.55	1.50
2	C	300	ZNH	CMB-C2B	2.85	1.55	1.50
2	D	300	ZNH	CAD-C3D	2.87	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	ZNH	CAD-C3D	2.97	1.55	1.51
2	A	300	ZNH	C1A-NA	3.33	1.38	1.34
2	A	300	ZNH	C4C-NC	3.37	1.38	1.34
2	D	300	ZNH	C3C-CAC	3.49	1.54	1.47
2	E	300	ZNH	C3C-CAC	3.49	1.54	1.47
2	C	300	ZNH	C3C-CAC	3.53	1.54	1.47
2	E	300	ZNH	C4C-NC	3.54	1.38	1.34
2	A	300	ZNH	C3C-CAC	3.58	1.55	1.47
2	C	300	ZNH	C4C-NC	3.60	1.38	1.34
2	B	300	ZNH	C4A-NA	3.60	1.38	1.34
2	D	300	ZNH	C1A-NA	3.61	1.38	1.34
2	B	300	ZNH	C1A-NA	3.63	1.38	1.34
2	A	300	ZNH	C1C-NC	3.65	1.38	1.34
2	B	300	ZNH	C3C-CAC	3.66	1.55	1.47
2	D	300	ZNH	C1C-NC	3.68	1.38	1.34
2	B	300	ZNH	C4C-NC	3.74	1.38	1.34
2	E	300	ZNH	C1A-NA	3.75	1.38	1.34
2	D	300	ZNH	C4C-NC	3.76	1.38	1.34
2	C	300	ZNH	C1A-NA	3.79	1.39	1.34
2	E	300	ZNH	C4A-NA	3.79	1.39	1.34
2	D	300	ZNH	C4A-NA	3.81	1.39	1.34
2	B	300	ZNH	C1C-NC	3.81	1.39	1.34
2	A	300	ZNH	C4A-NA	3.83	1.39	1.34
2	E	300	ZNH	C1C-NC	3.86	1.39	1.34
2	C	300	ZNH	C4A-NA	3.96	1.39	1.34
2	C	300	ZNH	C1C-NC	3.99	1.39	1.34
2	E	300	ZNH	C1C-C2C	5.23	1.45	1.38
2	D	300	ZNH	C1A-C2A	5.34	1.45	1.38
2	A	300	ZNH	C4A-C3A	5.36	1.45	1.38
2	B	300	ZNH	C4A-C3A	5.36	1.45	1.38
2	D	300	ZNH	C1C-C2C	5.37	1.45	1.38
2	A	300	ZNH	C1C-C2C	5.38	1.45	1.38
2	B	300	ZNH	C1C-C2C	5.41	1.45	1.38
2	A	300	ZNH	C1A-C2A	5.44	1.45	1.38
2	E	300	ZNH	C4A-C3A	5.52	1.45	1.38
2	C	300	ZNH	C1C-C2C	5.55	1.45	1.38
2	E	300	ZNH	C1A-C2A	5.59	1.45	1.38
2	C	300	ZNH	C4A-C3A	5.64	1.45	1.38
2	D	300	ZNH	C4A-C3A	5.66	1.46	1.38
2	B	300	ZNH	C1A-C2A	5.69	1.46	1.38
2	C	300	ZNH	C1A-C2A	5.69	1.46	1.38
2	E	300	ZNH	C3D-C2D	9.80	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	300	ZNH	C3D-C2D	9.90	1.54	1.33
2	C	300	ZNH	C3D-C2D	9.90	1.54	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	300	ZNH	CBD-CAD-C3D	-2.37	109.96	114.28
2	A	300	ZNH	CHD-C4C-C3C	-2.23	126.55	129.55
2	B	300	ZNH	CHD-C4C-C3C	-2.10	126.73	129.55
2	E	300	ZNH	CHD-C4C-C3C	-2.05	126.79	129.55
2	D	300	ZNH	C1A-C2A-C3A	2.03	108.28	105.81
2	B	300	ZNH	CAD-C3D-C4D	2.48	127.58	122.52
2	B	300	ZNH	C4C-C3C-C2C	2.76	108.25	104.13
2	A	300	ZNH	C4C-C3C-C2C	2.76	108.25	104.13
2	E	300	ZNH	C4C-C3C-C2C	2.80	108.32	104.13
2	A	300	ZNH	CAD-C3D-C4D	2.85	128.33	122.52
2	D	300	ZNH	C4C-C3C-C2C	2.95	108.55	104.13
2	C	300	ZNH	C4C-C3C-C2C	2.98	108.59	104.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	300	ZNH	1	0
2	E	300	ZNH	2	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, 95^{th} 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	214/232 (92%)	-0.15	1 (0%)	90	85	67, 93, 112, 132	0
1	B	215/232 (92%)	0.04	1 (0%)	90	85	79, 105, 136, 172	0
1	C	213/232 (91%)	-0.10	2 (0%)	84	75	86, 112, 157, 166	0
1	D	215/232 (92%)	0.08	4 (1%)	67	52	102, 139, 195, 247	0
1	E	213/232 (91%)	0.04	6 (2%)	53	39	117, 160, 202, 214	0
1	F	197/232 (84%)	0.13	4 (2%)	65	50	139, 174, 215, 237	0
1	G	209/232 (90%)	0.21	15 (7%)	16	10	117, 175, 218, 239	0
All	All	1476/1624 (90%)	0.03	33 (2%)	62	48	67, 138, 203, 247	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	104	ALA	5.2
1	B	225	HIS	4.9
1	G	156	ALA	3.7
1	G	203	ALA	3.4
1	G	40	GLY	3.3
1	E	74	TYR	3.0
1	E	135	THR	2.9
1	C	151	ALA	2.9
1	F	26	ILE	2.7
1	G	72	PRO	2.7
1	G	143	GLY	2.7
1	F	59	THR	2.6
1	G	38	GLN	2.6
1	D	221	LEU	2.4
1	D	51	MET	2.4
1	A	10	SER	2.3
1	G	200	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	159	SER	2.3
1	G	51	MET	2.3
1	E	12	ASP	2.2
1	C	96	TRP	2.2
1	F	103	GLU	2.2
1	E	16	ALA	2.2
1	E	199	VAL	2.2
1	D	47	PHE	2.1
1	G	27	ARG	2.1
1	G	131	ALA	2.0
1	G	164	LEU	2.0
1	G	70	GLN	2.0
1	G	171	SER	2.0
1	G	161	GLY	2.0
1	F	65	ILE	2.0
1	D	114	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, 95^{th} 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
2	ZNH	A	300	39/43	0.98	0.28	0.44	72,81,85,86	0
2	ZNH	E	300	35/43	0.94	0.27	0.36	147,160,175,180	0
2	ZNH	B	300	39/43	0.95	0.23	0.18	102,114,124,126	0
2	ZNH	D	300	35/43	0.93	0.27	0.02	128,144,158,163	0
2	ZNH	C	300	35/43	0.94	0.20	-0.75	116,130,141,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZNH	G	300	1/43	0.61	0.10	-	190,190,190,190	0
2	ZNH	F	300	1/43	0.91	0.20	-	185,185,185,185	0

6.5 Other polymers (i)

There are no such residues in this entry.