Full wwPDB X-ray Structure Validation Report (i)

Feb 12, 2024 – 05:43 AM EST

PDB ID	:	3H90
Title	:	Structural basis for the autoregulation of the zinc transporter YiiP
Authors	:	Lu, M.
Deposited on	:	2009-04-29
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

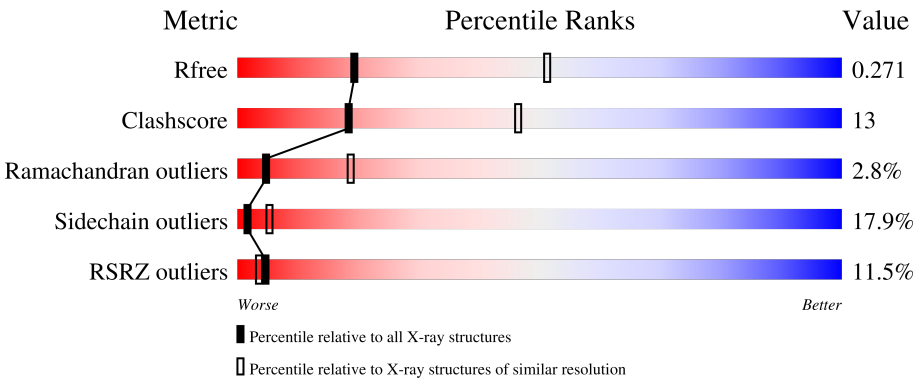
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	283	10% 59% 33% 8%
1	B	283	11% 63% 33% 5%
1	C	283	13% 60% 32% 8%
1	D	283	12% 61% 35% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9001 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 Ferrous-iron efflux pump fieF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	283	2178	1402	372	393	11	0	0	0
1	B	283	2178	1402	372	393	11	0	0	0
1	C	283	2178	1402	372	393	11	0	0	0
1	D	283	2178	1402	372	393	11	0	0	0

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	4	4	4	0	0
3	B	4	4	4	0	0
3	C	4	4	4	0	0
3	D	4	4	4	0	0

- Molecule 4 is water.

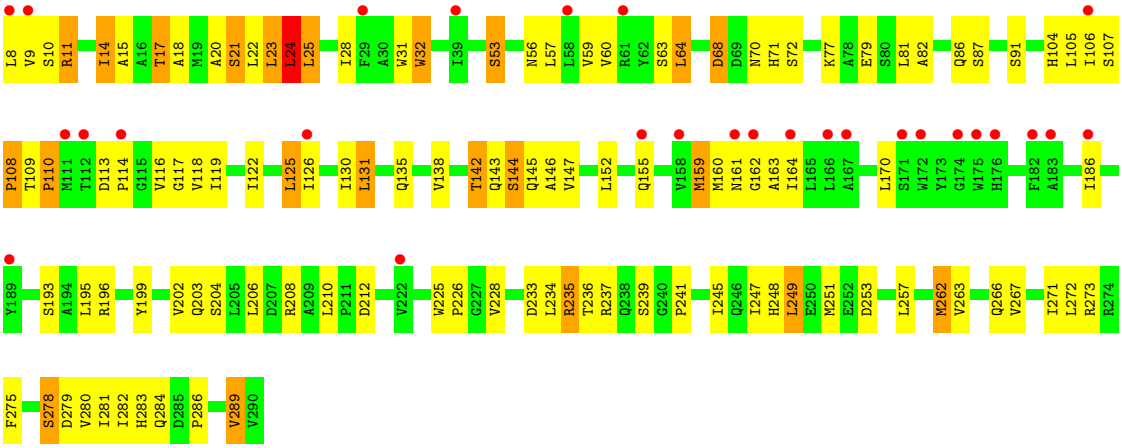
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	58	58	58	0	0
			Total	O		
4	B	77	77	77	0	0
			Total	O		
4	C	67	67	67	0	0
			Total	O		
4	D	63	63	63	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

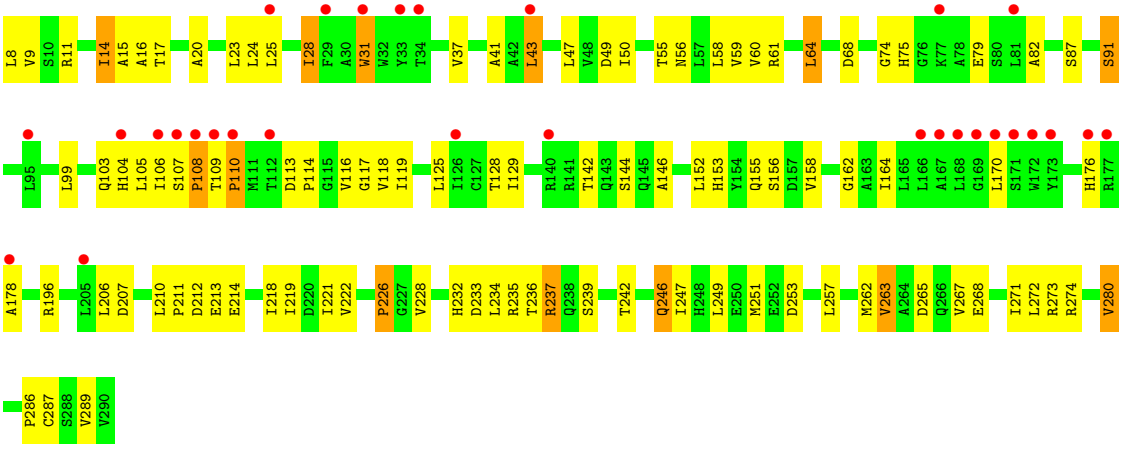
• Molecule 1: Ferrous-iron efflux pump fieF

Chain A:



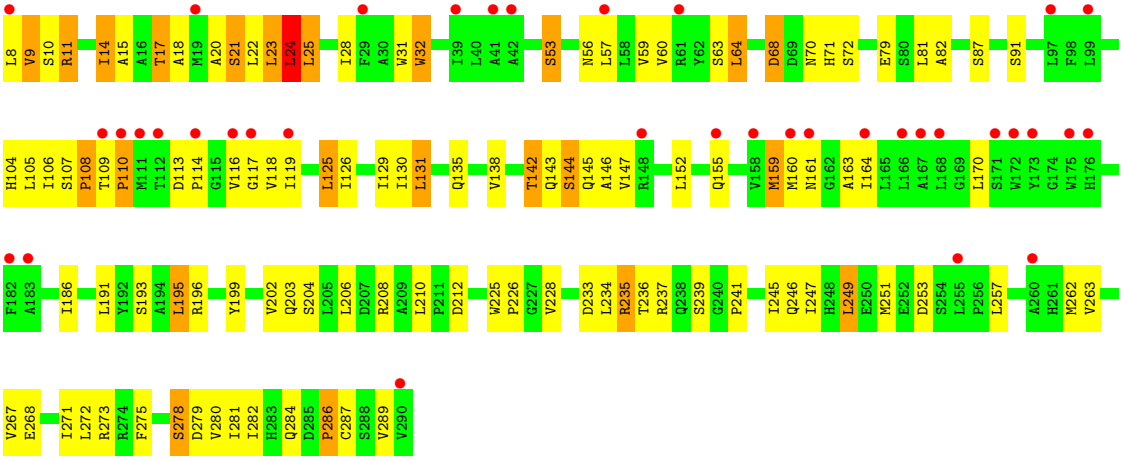
• Molecule 1: Ferrous-iron efflux pump fieF

Chain B:



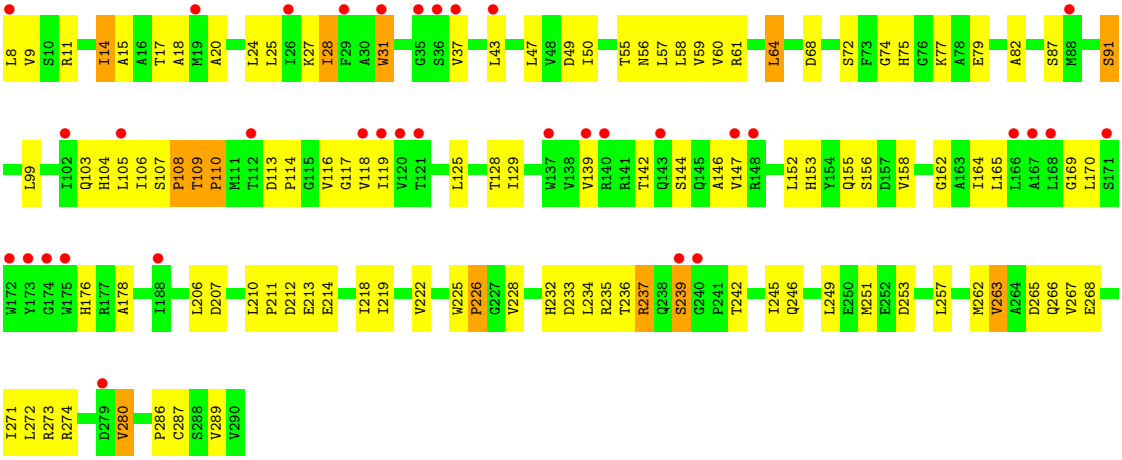
• Molecule 1: Ferrous-iron efflux pump fieF

Chain C:



- Molecule 1: Ferrous-iron efflux pump fieF

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.66Å 130.70Å 115.76Å 90.00° 93.28° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 48.91 – 2.89	Depositor EDS
% Data completeness (in resolution range)	93.8 (20.00-2.90) 79.4 (48.91-2.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.261 , 0.277 0.257 , 0.271	Depositor DCC
R_{free} test set	3315 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	78.7	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9001	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.45	0/2224	0.70	1/3032 (0.0%)
1	B	0.43	0/2224	0.69	0/3032
1	C	0.45	0/2224	0.70	1/3032 (0.0%)
1	D	0.44	0/2224	0.68	0/3032
All	All	0.44	0/8896	0.69	2/12128 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	24	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	24	LEU	CA-CB-CG	5.78	128.59	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	74	GLY	Peptide
1	D	74	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2178	0	2214	65	0
1	B	2178	0	2213	55	0
1	C	2178	0	2214	59	0
1	D	2178	0	2214	57	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	58	0	0	5	0
4	B	77	0	0	3	0
4	C	67	0	0	1	0
4	D	63	0	0	1	0
All	All	9001	0	8855	233	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 13.

All (233) 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:11:ARG:HH11	1:A:14:ILE:HG21	1.41	0.85
1:C:79:GLU:HG2	1:C:146:ALA:HB2	1.60	0.83
1:C:11:ARG:HH11	1:C:14:ILE:HG21	1.41	0.82
1:D:68:ASP:HB2	1:D:75:HIS:CE1	2.18	0.79
1:A:79:GLU:HG2	1:A:146:ALA:HB2	1.65	0.78
1:B:162:GLY:HA3	4:B:304:HOH:O	1.82	0.78
1:D:268:GLU:HG3	1:D:280:VAL:HG22	1.65	0.78
1:C:152:LEU:HA	1:C:155:GLN:HE21	1.47	0.78
1:C:267:VAL:O	1:C:271:ILE:HD12	1.84	0.77
1:C:126:ILE:O	1:C:130:ILE:HG12	1.84	0.76
1:A:21:SER:OG	1:A:53:SER:HB2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:SER:OG	1:C:53:SER:HB2	1.86	0.75
1:B:268:GLU:HG3	1:B:280:VAL:HG22	1.67	0.75
1:A:126:ILE:O	1:A:130:ILE:HG12	1.86	0.75
1:B:68:ASP:HB2	1:B:75:HIS:CE1	2.23	0.74
1:C:233:ASP:O	1:C:247:ILE:HA	1.87	0.74
1:A:233:ASP:O	1:A:247:ILE:HA	1.87	0.74
1:A:152:LEU:HA	1:A:155:GLN:HE21	1.51	0.73
1:A:267:VAL:O	1:A:271:ILE:HD12	1.87	0.73
1:B:14:ILE:HG13	1:B:15:ALA:N	2.04	0.72
1:D:268:GLU:HG3	1:D:280:VAL:CG2	2.22	0.70
1:B:246:GLN:NE2	4:B:297:HOH:O	2.24	0.69
1:D:14:ILE:HG13	1:D:15:ALA:N	2.07	0.68
1:C:14:ILE:HG13	1:C:15:ALA:N	2.09	0.67
1:D:68:ASP:HB2	1:D:75:HIS:HE1	1.55	0.67
1:B:268:GLU:HG3	1:B:280:VAL:CG2	2.24	0.67
1:B:87:SER:O	1:B:91:SER:HB2	1.96	0.66
1:C:79:GLU:HG2	1:C:146:ALA:CB	2.26	0.65
1:C:22:LEU:O	1:C:25:LEU:HB2	1.97	0.64
1:C:144:SER:OG	1:C:147:VAL:HG13	1.97	0.64
1:A:249:LEU:HD22	1:A:282:ILE:HG21	1.79	0.64
1:B:68:ASP:HB2	1:B:75:HIS:HE1	1.61	0.64
1:A:22:LEU:O	1:A:25:LEU:HB2	1.98	0.64
1:D:162:GLY:HA3	4:D:304:HOH:O	1.97	0.64
1:A:14:ILE:HG13	1:A:15:ALA:N	2.14	0.61
1:D:107:SER:HB2	1:D:108:PRO:HD3	1.83	0.61
1:A:79:GLU:HG2	1:A:146:ALA:CB	2.31	0.60
1:D:87:SER:O	1:D:91:SER:HB2	2.01	0.60
1:A:87:SER:O	1:A:91:SER:HB2	2.01	0.60
1:B:107:SER:HB2	1:B:108:PRO:HD3	1.84	0.59
1:A:162:GLY:HA3	4:A:312:HOH:O	2.01	0.59
1:C:18:ALA:HB1	1:C:57:LEU:HB2	1.84	0.59
1:B:233:ASP:OD2	1:B:235:ARG:HD3	2.04	0.58
1:C:225:TRP:CD1	1:C:226:PRO:HD2	2.38	0.58
1:A:107:SER:HB2	1:A:108:PRO:HD3	1.85	0.58
1:D:233:ASP:OD2	1:D:235:ARG:HD3	2.04	0.58
1:A:144:SER:OG	1:A:147:VAL:HG13	2.04	0.57
1:B:110:PRO:HG3	1:B:178:ALA:HB2	1.87	0.57
1:A:18:ALA:HB1	1:A:57:LEU:HB2	1.86	0.57
1:A:20:ALA:O	1:A:23:LEU:HB3	2.04	0.57
1:D:262:MET:HA	1:D:262:MET:CE	2.34	0.57
1:C:56:ASN:O	1:C:60:VAL:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ILE:O	1:D:222:VAL:HG23	2.04	0.57
1:A:56:ASN:O	1:A:60:VAL:HG13	2.05	0.57
1:D:125:LEU:O	1:D:129:ILE:HG12	2.05	0.56
1:A:225:TRP:CD1	1:A:226:PRO:HD2	2.40	0.56
1:D:110:PRO:HG3	1:D:178:ALA:HB2	1.87	0.56
1:A:235:ARG:NH2	1:C:279:ASP:OD2	2.39	0.56
1:C:60:VAL:O	1:C:64:LEU:HD22	2.06	0.56
1:C:107:SER:HB2	1:C:108:PRO:HD3	1.86	0.56
1:C:87:SER:O	1:C:91:SER:HB2	2.05	0.55
1:C:20:ALA:O	1:C:23:LEU:HB3	2.05	0.55
1:A:60:VAL:O	1:A:64:LEU:HD22	2.06	0.55
1:C:203:GLN:CG	1:C:208:ARG:HE	2.20	0.55
1:B:125:LEU:O	1:B:129:ILE:HG12	2.07	0.54
1:C:233:ASP:OD2	1:C:235:ARG:HD2	2.07	0.54
1:D:47:LEU:O	1:D:50:ILE:HG22	2.06	0.54
1:A:233:ASP:OD2	1:A:235:ARG:HD2	2.07	0.54
1:A:159:MET:HB3	1:A:186:ILE:HD13	1.90	0.54
1:A:11:ARG:NH1	1:A:14:ILE:HG21	2.19	0.54
1:B:113:ASP:N	1:B:114:PRO:CD	2.71	0.53
1:C:249:LEU:HB3	1:C:251:MET:CE	2.38	0.53
1:D:113:ASP:N	1:D:114:PRO:CD	2.71	0.53
1:D:56:ASN:O	1:D:60:VAL:HG13	2.08	0.53
1:B:47:LEU:O	1:B:50:ILE:HG22	2.09	0.53
1:B:25:LEU:O	1:B:28:ILE:HG22	2.09	0.53
1:B:113:ASP:H	1:B:114:PRO:CD	2.22	0.53
1:C:113:ASP:N	1:C:114:PRO:CD	2.72	0.53
1:A:24:LEU:HD22	1:A:24:LEU:O	2.08	0.53
1:A:113:ASP:N	1:A:114:PRO:CD	2.72	0.53
1:B:262:MET:HA	1:B:262:MET:CE	2.39	0.53
1:C:68:ASP:HB2	1:C:71:HIS:HB2	1.91	0.53
1:A:59:VAL:HG11	1:A:82:ALA:HB2	1.90	0.52
1:A:32:TRP:CE3	1:A:32:TRP:HA	2.44	0.52
1:A:122:ILE:HG22	4:A:312:HOH:O	2.09	0.52
1:D:207:ASP:HB3	1:D:237:ARG:HD2	1.92	0.52
1:A:125:LEU:CD1	1:A:160:MET:HB3	2.40	0.52
1:B:17:THR:HA	1:B:20:ALA:HB3	1.91	0.52
1:B:210:LEU:HG	1:B:236:THR:HB	1.92	0.52
1:C:24:LEU:HD22	1:C:24:LEU:O	2.09	0.52
1:D:113:ASP:H	1:D:114:PRO:CD	2.22	0.52
1:C:161:ASN:C	1:C:163:ALA:H	2.13	0.51
1:B:211:PRO:HG2	1:B:214:GLU:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:TRP:HA	1:C:32:TRP:CE3	2.46	0.51
1:A:203:GLN:CG	1:A:208:ARG:HE	2.23	0.51
1:C:59:VAL:HG11	1:C:82:ALA:HB2	1.91	0.51
1:C:249:LEU:HD22	1:C:282:ILE:HG21	1.91	0.51
1:D:25:LEU:O	1:D:28:ILE:HG22	2.11	0.51
1:A:199:TYR:O	1:A:203:GLN:HB2	2.11	0.51
1:A:279:ASP:OD2	1:C:235:ARG:NH2	2.44	0.51
1:D:210:LEU:HG	1:D:236:THR:HB	1.93	0.51
1:A:159:MET:HG2	1:A:186:ILE:HG12	1.93	0.51
1:B:56:ASN:O	1:B:60:VAL:HG13	2.10	0.51
1:C:159:MET:HB3	1:C:186:ILE:HD13	1.93	0.50
1:A:262:MET:O	1:A:266:GLN:HG3	2.11	0.50
1:D:211:PRO:HG2	1:D:214:GLU:HG3	1.93	0.50
1:B:25:LEU:HD13	1:B:50:ILE:HD11	1.93	0.50
1:B:263:VAL:O	1:B:267:VAL:HG23	2.11	0.50
1:C:159:MET:HG2	1:C:186:ILE:HG12	1.94	0.50
1:D:267:VAL:O	1:D:271:ILE:HD12	2.12	0.50
1:C:164:ILE:HG13	1:C:164:ILE:O	2.12	0.50
1:C:275:PHE:O	1:C:278:SER:HB2	2.11	0.50
1:A:249:LEU:HB3	1:A:251:MET:CE	2.42	0.49
1:B:218:ILE:O	1:B:222:VAL:HG23	2.13	0.49
1:B:24:LEU:HD23	1:B:49:ASP:HB2	1.95	0.49
1:C:125:LEU:CD1	1:C:160:MET:HB3	2.43	0.49
1:D:25:LEU:HD13	1:D:50:ILE:HD11	1.94	0.49
1:A:161:ASN:C	1:A:163:ALA:H	2.16	0.48
1:C:11:ARG:NH1	1:C:14:ILE:HG21	2.21	0.48
1:A:164:ILE:HG13	1:A:164:ILE:O	2.14	0.48
1:B:232:HIS:CD2	1:B:233:ASP:H	2.32	0.48
1:C:21:SER:O	1:C:24:LEU:HD12	2.14	0.48
1:B:164:ILE:HG13	1:B:164:ILE:O	2.14	0.48
1:D:17:THR:HA	1:D:20:ALA:HB3	1.95	0.47
1:A:68:ASP:HB2	1:A:71:HIS:HB2	1.97	0.47
1:A:142:THR:O	1:A:144:SER:N	2.46	0.47
1:D:104:HIS:C	1:D:106:ILE:H	2.18	0.47
1:C:131:LEU:HD22	1:C:135:GLN:HG3	1.97	0.47
1:D:24:LEU:HD23	1:D:49:ASP:HB2	1.96	0.47
1:D:249:LEU:HD23	1:D:251:MET:CE	2.45	0.47
1:A:275:PHE:O	1:A:278:SER:HB2	2.15	0.47
1:B:267:VAL:O	1:B:271:ILE:HD12	2.14	0.47
1:C:108:PRO:HG3	4:C:352:HOH:O	2.15	0.46
1:D:60:VAL:O	1:D:64:LEU:HD22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:VAL:O	1:B:64:LEU:HD22	2.14	0.46
1:A:68:ASP:HB3	1:A:71:HIS:H	1.81	0.46
1:B:104:HIS:HA	1:B:108:PRO:HD2	1.97	0.46
1:B:235:ARG:HG2	1:D:72:SER:HB2	1.97	0.46
1:D:152:LEU:HA	1:D:155:GLN:HE21	1.81	0.46
1:B:16:ALA:CB	4:B:310:HOH:O	2.64	0.46
1:B:106:ILE:HD12	1:B:176:HIS:HB2	1.98	0.46
1:D:104:HIS:HA	1:D:108:PRO:HD2	1.97	0.46
1:B:104:HIS:C	1:B:106:ILE:H	2.19	0.46
1:C:9:VAL:HG12	1:C:10:SER:H	1.80	0.46
1:B:249:LEU:HD23	1:B:251:MET:HE2	1.98	0.46
1:A:116:VAL:O	1:A:118:VAL:N	2.49	0.46
1:C:104:HIS:C	1:C:106:ILE:H	2.19	0.46
1:A:9:VAL:HG12	1:A:10:SER:H	1.81	0.45
1:A:210:LEU:HG	1:A:236:THR:HB	1.98	0.45
1:B:113:ASP:H	1:B:114:PRO:HD3	1.80	0.45
1:D:106:ILE:HD12	1:D:176:HIS:HB2	1.97	0.45
1:B:104:HIS:C	1:B:106:ILE:N	2.70	0.45
1:C:116:VAL:O	1:C:118:VAL:N	2.49	0.45
1:C:152:LEU:HA	1:C:155:GLN:NE2	2.24	0.45
1:A:60:VAL:O	1:A:63:SER:HB3	2.16	0.45
1:A:104:HIS:C	1:A:106:ILE:H	2.20	0.45
1:C:68:ASP:HB3	1:C:71:HIS:H	1.82	0.45
1:C:199:TYR:O	1:C:203:GLN:HB2	2.16	0.45
1:D:18:ALA:HB1	1:D:57:LEU:HB2	1.98	0.45
1:D:262:MET:HA	1:D:262:MET:HE2	1.99	0.45
1:D:24:LEU:HD11	1:D:27:LYS:HD3	1.98	0.45
1:D:128:THR:HG22	1:D:158:VAL:HG23	1.97	0.45
1:A:106:ILE:HG23	1:A:110:PRO:HD3	1.98	0.44
1:B:249:LEU:HD23	1:B:251:MET:CE	2.47	0.44
1:D:113:ASP:H	1:D:114:PRO:HD3	1.82	0.44
1:D:28:ILE:O	1:D:31:TRP:CE3	2.71	0.44
1:D:170:LEU:HD12	1:D:170:LEU:H	1.82	0.44
1:A:144:SER:HB3	1:A:147:VAL:HG22	1.98	0.44
1:B:59:VAL:HG11	1:B:82:ALA:HB2	1.99	0.44
1:C:106:ILE:HG23	1:C:110:PRO:HD3	1.99	0.44
1:D:104:HIS:C	1:D:106:ILE:N	2.70	0.44
1:D:153:HIS:O	1:D:156:SER:HB3	2.17	0.44
1:D:164:ILE:O	1:D:164:ILE:HG13	2.16	0.44
1:D:77:LYS:HG2	1:D:239:SER:HB2	1.99	0.44
1:A:14:ILE:HA	1:A:17:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:HA	1:B:155:GLN:HE21	1.82	0.44
1:B:210:LEU:HB3	1:B:211:PRO:HD2	2.00	0.44
1:A:289:VAL:HG12	4:A:315:HOH:O	2.18	0.44
1:D:245:ILE:O	1:D:280:VAL:HA	2.18	0.44
1:B:128:THR:HG22	1:B:158:VAL:HG23	2.00	0.44
1:B:170:LEU:HD12	1:B:170:LEU:H	1.82	0.44
1:B:207:ASP:HB3	1:B:237:ARG:HD2	2.00	0.44
1:C:203:GLN:HG3	1:C:208:ARG:HE	1.83	0.44
1:D:249:LEU:HD23	1:D:251:MET:HE3	1.99	0.44
1:A:21:SER:O	1:A:24:LEU:HD12	2.18	0.43
1:A:233:ASP:OD2	1:A:235:ARG:CD	2.66	0.43
1:B:153:HIS:O	1:B:156:SER:HB3	2.18	0.43
1:A:161:ASN:HB3	1:A:164:ILE:HG23	2.00	0.43
1:A:281:ILE:HA	4:A:346:HOH:O	2.18	0.43
1:A:233:ASP:HB2	4:A:332:HOH:O	2.17	0.43
1:D:274:ARG:O	1:D:274:ARG:NH1	2.49	0.43
1:A:203:GLN:HG3	1:A:208:ARG:HE	1.84	0.43
1:B:99:LEU:O	1:B:103:GLN:HB2	2.19	0.43
1:B:28:ILE:O	1:B:31:TRP:CE3	2.72	0.43
1:C:245:ILE:HB	1:C:280:VAL:HG12	2.00	0.43
1:D:139:VAL:HG22	1:D:147:VAL:HG23	2.01	0.43
1:C:142:THR:O	1:C:144:SER:N	2.50	0.42
1:B:221:ILE:HD11	1:B:274:ARG:HG2	2.01	0.42
1:D:152:LEU:HA	1:D:155:GLN:NE2	2.34	0.42
1:D:165:LEU:O	1:D:169:GLY:HA2	2.19	0.42
1:B:79:GLU:HG2	1:B:146:ALA:HB2	2.00	0.42
1:C:161:ASN:HB3	1:C:164:ILE:HG23	2.00	0.42
1:A:77:LYS:HG2	1:A:239:SER:HB2	2.00	0.42
1:C:60:VAL:O	1:C:63:SER:HB3	2.19	0.42
1:D:99:LEU:O	1:D:103:GLN:HB2	2.20	0.42
1:A:125:LEU:HD11	1:A:160:MET:HB3	2.01	0.42
1:B:55:THR:HA	1:B:58:LEU:HD12	2.02	0.42
1:A:248:HIS:HA	1:A:283:HIS:O	2.19	0.42
1:A:131:LEU:HD22	1:A:135:GLN:HG3	2.01	0.42
1:C:14:ILE:HA	1:C:17:THR:HG22	2.00	0.42
1:D:59:VAL:HG11	1:D:82:ALA:HB2	2.02	0.42
1:B:41:ALA:C	1:B:43:LEU:H	2.23	0.41
1:C:11:ARG:NH1	1:C:144:SER:HB2	2.35	0.41
1:D:79:GLU:HG2	1:D:146:ALA:HB2	2.02	0.41
1:D:225:TRP:CZ2	1:D:266:GLN:HB3	2.54	0.41
1:D:55:THR:HA	1:D:58:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:LEU:HG	1:C:236:THR:HB	2.02	0.41
1:C:246:GLN:HB3	1:C:281:ILE:HG23	2.02	0.41
1:B:23:LEU:C	1:B:25:LEU:H	2.23	0.41
1:D:108:PRO:HB2	1:D:109:THR:H	1.61	0.41
1:D:263:VAL:O	1:D:267:VAL:HG23	2.21	0.41
1:A:60:VAL:HA	1:A:63:SER:HB3	2.02	0.41
1:D:232:HIS:CD2	1:D:233:ASP:H	2.38	0.41
1:A:245:ILE:HB	1:A:280:VAL:HG12	2.02	0.41
1:C:104:HIS:C	1:C:106:ILE:N	2.73	0.41
1:C:125:LEU:O	1:C:129:ILE:HG12	2.21	0.41
1:C:191:LEU:O	1:C:195:LEU:HB2	2.21	0.41
1:A:82:ALA:O	1:A:86:GLN:HG3	2.21	0.41
1:A:104:HIS:C	1:A:106:ILE:N	2.74	0.40
1:B:152:LEU:HA	1:B:155:GLN:NE2	2.36	0.40
1:B:233:ASP:O	1:B:247:ILE:HA	2.21	0.40
1:C:286:PRO:HB2	1:C:287:CYS:H	1.70	0.40
1:B:31:TRP:CE3	1:B:31:TRP:O	2.74	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	281/283 (99%)	240 (85%)	33 (12%)	8 (3%)	5 19
1	B	281/283 (99%)	243 (86%)	30 (11%)	8 (3%)	5 19
1	C	281/283 (99%)	237 (84%)	36 (13%)	8 (3%)	5 19
1	D	281/283 (99%)	241 (86%)	32 (11%)	8 (3%)	5 19
All	All	1124/1132 (99%)	961 (86%)	131 (12%)	32 (3%)	5 19

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	LEU
1	A	286	PRO
1	C	170	LEU
1	C	286	PRO
1	A	108	PRO
1	A	117	GLY
1	A	143	GLN
1	B	108	PRO
1	B	286	PRO
1	C	108	PRO
1	C	117	GLY
1	C	143	GLN
1	D	108	PRO
1	D	286	PRO
1	A	144	SER
1	B	144	SER
1	C	144	SER
1	D	144	SER
1	D	226	PRO
1	B	117	GLY
1	B	226	PRO
1	A	110	PRO
1	C	110	PRO
1	D	117	GLY
1	A	241	PRO
1	C	241	PRO
1	B	37	VAL
1	D	37	VAL
1	B	110	PRO
1	D	110	PRO
1	D	116	VAL
1	B	116	VAL

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	234/234 (100%)	187 (80%)	47 (20%)	1 4
1	B	234/234 (100%)	198 (85%)	36 (15%)	2 8
1	C	234/234 (100%)	184 (79%)	50 (21%)	1 3
1	D	234/234 (100%)	199 (85%)	35 (15%)	3 9
All	All	936/936 (100%)	768 (82%)	168 (18%)	2 5

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	11	ARG
1	A	14	ILE
1	A	17	THR
1	A	21	SER
1	A	23	LEU
1	A	24	LEU
1	A	25	LEU
1	A	28	ILE
1	A	31	TRP
1	A	32	TRP
1	A	53	SER
1	A	64	LEU
1	A	68	ASP
1	A	70	ASN
1	A	72	SER
1	A	81	LEU
1	A	105	LEU
1	A	109	THR
1	A	119	ILE
1	A	125	LEU
1	A	131	LEU
1	A	138	VAL
1	A	142	THR
1	A	145	GLN
1	A	159	MET
1	A	193	SER
1	A	195	LEU
1	A	196	ARG
1	A	202	VAL
1	A	204	SER
1	A	206	LEU
1	A	212	ASP

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Mol	Chain	Res	Type
1	A	228	VAL
1	A	234	LEU
1	A	235	ARG
1	A	237	ARG
1	A	249	LEU
1	A	253	ASP
1	A	257	LEU
1	A	262	MET
1	A	263	VAL
1	A	272	LEU
1	A	273	ARG
1	A	278	SER
1	A	284	GLN
1	A	289	VAL
1	B	8	LEU
1	B	9	VAL
1	B	11	ARG
1	B	14	ILE
1	B	28	ILE
1	B	31	TRP
1	B	43	LEU
1	B	61	ARG
1	B	64	LEU
1	B	91	SER
1	B	105	LEU
1	B	109	THR
1	B	118	VAL
1	B	119	ILE
1	B	142	THR
1	B	196	ARG
1	B	206	LEU
1	B	212	ASP
1	B	213	GLU
1	B	219	ILE
1	B	226	PRO
1	B	228	VAL
1	B	234	LEU
1	B	237	ARG
1	B	239	SER
1	B	242	THR
1	B	246	GLN
1	B	253	ASP

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Mol	Chain	Res	Type
1	B	257	LEU
1	B	263	VAL
1	B	265	ASP
1	B	272	LEU
1	B	273	ARG
1	B	280	VAL
1	B	287	CYS
1	B	289	VAL
1	C	8	LEU
1	C	9	VAL
1	C	11	ARG
1	C	14	ILE
1	C	17	THR
1	C	21	SER
1	C	23	LEU
1	C	24	LEU
1	C	25	LEU
1	C	28	ILE
1	C	31	TRP
1	C	32	TRP
1	C	53	SER
1	C	64	LEU
1	C	68	ASP
1	C	70	ASN
1	C	72	SER
1	C	81	LEU
1	C	105	LEU
1	C	109	THR
1	C	119	ILE
1	C	125	LEU
1	C	131	LEU
1	C	138	VAL
1	C	142	THR
1	C	145	GLN
1	C	159	MET
1	C	193	SER
1	C	195	LEU
1	C	196	ARG
1	C	202	VAL
1	C	204	SER
1	C	206	LEU
1	C	212	ASP

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Mol	Chain	Res	Type
1	C	228	VAL
1	C	234	LEU
1	C	235	ARG
1	C	237	ARG
1	C	239	SER
1	C	249	LEU
1	C	253	ASP
1	C	257	LEU
1	C	262	MET
1	C	263	VAL
1	C	268	GLU
1	C	272	LEU
1	C	273	ARG
1	C	278	SER
1	C	284	GLN
1	C	289	VAL
1	D	8	LEU
1	D	9	VAL
1	D	11	ARG
1	D	14	ILE
1	D	28	ILE
1	D	31	TRP
1	D	43	LEU
1	D	61	ARG
1	D	64	LEU
1	D	91	SER
1	D	105	LEU
1	D	109	THR
1	D	118	VAL
1	D	119	ILE
1	D	142	THR
1	D	206	LEU
1	D	212	ASP
1	D	213	GLU
1	D	219	ILE
1	D	226	PRO
1	D	228	VAL
1	D	234	LEU
1	D	237	ARG
1	D	239	SER
1	D	242	THR
1	D	246	GLN

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Mol	Chain	Res	Type
1	D	253	ASP
1	D	257	LEU
1	D	263	VAL
1	D	265	ASP
1	D	272	LEU
1	D	273	ARG
1	D	280	VAL
1	D	287	CYS
1	D	289	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	135	GLN
1	A	155	GLN
1	A	246	GLN
1	A	259	GLN
1	A	284	GLN
1	B	56	ASN
1	B	155	GLN
1	C	104	HIS
1	C	135	GLN
1	C	155	GLN
1	C	246	GLN
1	C	284	GLN
1	D	56	ASN
1	D	155	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	283/283 (100%)	0.68	28 (9%)	7	5	-5, 54, 201, 289	0
1	B	283/283 (100%)	0.83	30 (10%)	6	4	-3, 43, 195, 257	0
1	C	283/283 (100%)	0.81	37 (13%)	3	2	-4, 51, 209, 281	0
1	D	283/283 (100%)	0.89	35 (12%)	4	3	-4, 45, 208, 267	0
All	All	1132/1132 (100%)	0.81	130 (11%)	4	3	-5, 47, 204, 289	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	TRP	18.5
1	D	173	TYR	16.6
1	C	172	TRP	16.1
1	B	173	TYR	13.6
1	C	175	TRP	11.9
1	B	169	GLY	11.4
1	B	166	LEU	11.2
1	C	173	TYR	9.7
1	D	112	THR	9.4
1	C	112	THR	9.3
1	A	174	GLY	9.0
1	D	175	TRP	8.1
1	C	171	SER	8.0
1	C	176	HIS	7.5
1	D	172	TRP	7.3
1	D	174	GLY	7.3
1	B	168	LEU	6.8
1	B	167	ALA	6.7
1	B	171	SER	6.7
1	D	8	LEU	6.6
1	D	35	GLY	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	167	ALA	6.4
1	D	102	ILE	6.4
1	B	172	TRP	6.3
1	C	183	ALA	6.2
1	A	112	THR	5.8
1	A	166	LEU	5.5
1	A	172	TRP	5.4
1	D	37	VAL	5.3
1	C	111	MET	5.0
1	B	106	ILE	4.9
1	C	167	ALA	4.9
1	A	111	MET	4.9
1	A	29	PHE	4.9
1	B	177	ARG	4.7
1	D	29	PHE	4.7
1	B	33	TYR	4.6
1	A	171	SER	4.6
1	B	112	THR	4.4
1	B	34	THR	4.3
1	B	170	LEU	4.3
1	B	178	ALA	4.2
1	C	97	LEU	4.2
1	B	109	THR	4.1
1	B	110	PRO	4.0
1	A	114	PRO	4.0
1	B	176	HIS	3.9
1	A	189	TYR	3.8
1	B	107	SER	3.6
1	A	162	GLY	3.6
1	C	109	THR	3.5
1	C	114	PRO	3.5
1	D	140	ARG	3.5
1	D	119	ILE	3.5
1	C	8	LEU	3.5
1	B	104	HIS	3.4
1	C	155	GLN	3.4
1	D	171	SER	3.4
1	A	164	ILE	3.4
1	D	147	VAL	3.3
1	C	117	GLY	3.3
1	C	29	PHE	3.3
1	A	183	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	168	LEU	3.3
1	B	205	LEU	3.2
1	C	164	ILE	3.1
1	A	155	GLN	3.1
1	D	43	LEU	3.1
1	D	105	LEU	3.1
1	D	26	ILE	3.1
1	A	186	ILE	3.0
1	D	120	VAL	3.0
1	D	167	ALA	3.0
1	A	126	ILE	2.9
1	C	148	ARG	2.9
1	A	39	ILE	2.8
1	D	148	ARG	2.8
1	B	108	PRO	2.8
1	C	119	ILE	2.8
1	B	77	LYS	2.8
1	D	36	SER	2.7
1	C	182	PHE	2.7
1	D	166	LEU	2.7
1	A	61	ARG	2.7
1	A	58	LEU	2.7
1	B	29	PHE	2.6
1	B	140	ARG	2.6
1	C	166	LEU	2.6
1	C	116	VAL	2.6
1	C	110	PRO	2.6
1	D	239	SER	2.5
1	A	161	ASN	2.5
1	C	42	ALA	2.5
1	C	290	VAL	2.5
1	A	9	VAL	2.4
1	D	279	ASP	2.4
1	A	176	HIS	2.4
1	B	81	LEU	2.4
1	B	43	LEU	2.3
1	B	31	TRP	2.3
1	A	158	VAL	2.3
1	C	99	LEU	2.3
1	D	88	MET	2.3
1	C	61	ARG	2.3
1	D	118	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	41	ALA	2.2
1	D	137	TRP	2.2
1	C	160	MET	2.2
1	D	143	GLN	2.2
1	B	126	ILE	2.2
1	D	139	VAL	2.2
1	C	161	ASN	2.2
1	A	222	VAL	2.2
1	D	188	ILE	2.2
1	C	39	ILE	2.1
1	C	158	VAL	2.1
1	A	182	PHE	2.1
1	D	121	THR	2.1
1	C	255	LEU	2.1
1	B	25	LEU	2.1
1	C	57	LEU	2.1
1	C	260	ALA	2.1
1	D	19	MET	2.1
1	D	240	GLY	2.1
1	A	8	LEU	2.0
1	C	168	LEU	2.0
1	D	31	TRP	2.0
1	A	106	ILE	2.0
1	C	19	MET	2.0
1	B	95	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HG	A	2	1/1	0.82	0.12	176,176,176,176	0
2	HG	C	6	1/1	0.90	0.17	175,175,175,175	0
2	HG	B	4	1/1	0.96	0.21	80,80,80,80	0
2	HG	D	7	1/1	0.96	0.24	92,92,92,92	0
3	ZN	B	291	1/1	0.96	0.23	42,42,42,42	0
3	ZN	A	4	1/1	0.97	0.18	69,69,69,69	0
2	HG	D	291	1/1	0.97	0.24	81,81,81,81	0
3	ZN	C	291	1/1	0.97	0.10	69,69,69,69	0
3	ZN	D	292	1/1	0.97	0.32	8,8,8,8	0
3	ZN	B	292	1/1	0.98	0.29	17,17,17,17	0
2	HG	C	5	1/1	0.98	0.18	92,92,92,92	0
3	ZN	D	6	1/1	0.98	0.28	20,20,20,20	0
2	HG	A	1	1/1	0.98	0.20	88,88,88,88	0
3	ZN	D	293	1/1	0.98	0.24	51,51,51,51	0
3	ZN	C	1	1/1	0.99	0.31	2,2,2,2	0
2	HG	B	3	1/1	0.99	0.22	86,86,86,86	0
3	ZN	D	5	1/1	0.99	0.28	12,12,12,12	0
3	ZN	A	293	1/1	0.99	0.30	10,10,10,10	0
3	ZN	B	293	1/1	0.99	0.26	21,21,21,21	0
3	ZN	B	294	1/1	0.99	0.28	9,9,9,9	0
3	ZN	A	292	1/1	1.00	0.26	26,26,26,26	0
3	ZN	C	2	1/1	1.00	0.29	23,23,23,23	0
3	ZN	C	3	1/1	1.00	0.31	5,5,5,5	0
3	ZN	A	291	1/1	1.00	0.28	5,5,5,5	0

6.5 Other polymers (i)

There are no such residues in this entry.