Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 12:29 pm GMT

PDB ID	:	6YMU
Title	:	Imidazole Glycerol Phosphate Synthase
Authors	:	Sterner, R.; Rajendran, C.; Andrea, K.
Deposited on	:	2020-04-09
Resolution	:	2.11 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 (i)) were used in the production of this report:

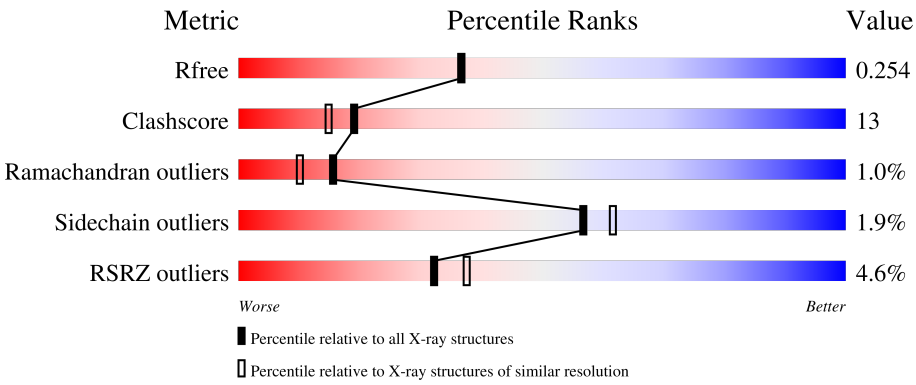
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	253	2%, 74%, 21%
1	C	253	4%, 73%, 25%
1	E	253	7%, 72%, 24%
2	B	201	%, 82%, 16%
2	D	201	%, 79%, 19%

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Mol	Chain	Length	Quality of chain
2	F	201	11% 68% 30%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10918 atoms, of which 14 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 Imidazole glycerol phosphate synthase subunit HisF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	244	1867	1191	314	356	6	0	0	0
1	C	251	1911	1218	319	368	6	0	1	0
1	E	246	1875	1193	317	359	6	0	1	0

- Molecule 2 is a protein called Imidazole glycerol phosphate synthase subunit HisH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	200	1625	1029	14	281	293	8	0	0	0
2	D	200	1614	1030	282	294	8		0	0	0
2	F	199	1581	1013	270	290	8		0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	OZW	TRP	conflict	UNP Q9X0C8
D	123	OZW	TRP	conflict	UNP Q9X0C8
F	123	OZW	TRP	conflict	UNP Q9X0C8

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	88	88	88	0	0
3	B	103	103	103	0	0

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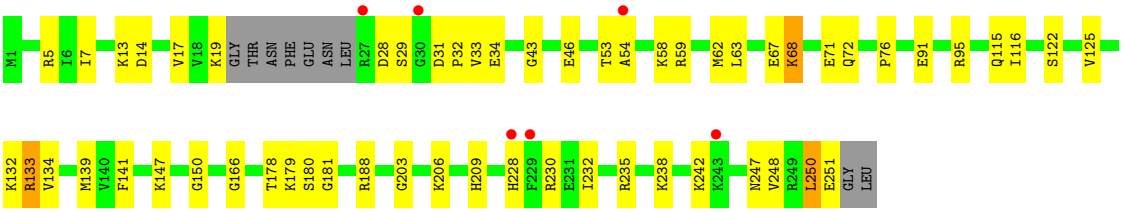
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	C	67	67	67	0	0
			Total	O		
3	D	104	104	104	0	0
			Total	O		
3	E	37	37	37	0	0
			Total	O		
3	F	46	46	46	0	0

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.

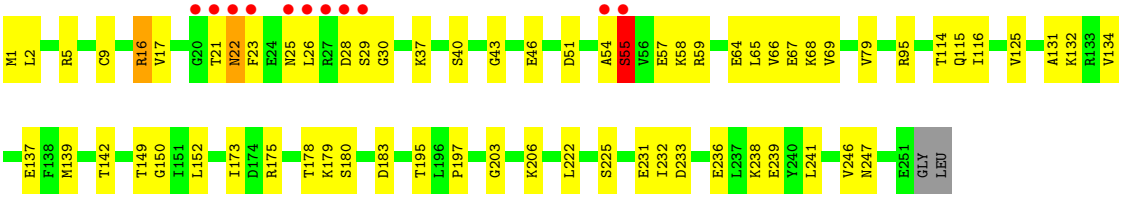
• Molecule 1: Imidazole glycerol phosphate synthase subunit HisF

Chain A:



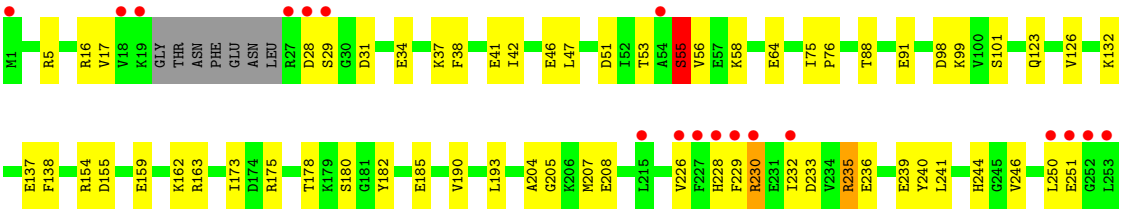
• Molecule 1: Imidazole glycerol phosphate synthase subunit HisF

Chain C:



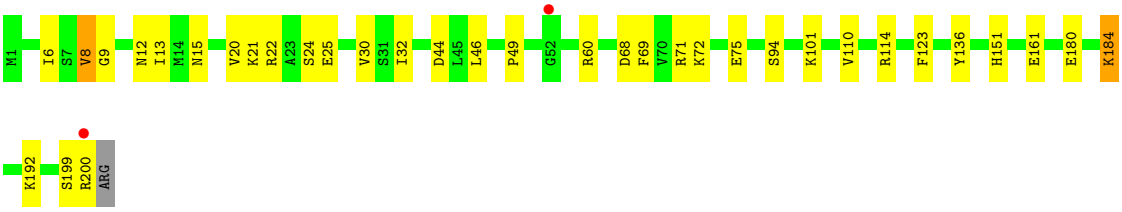
• Molecule 1: Imidazole glycerol phosphate synthase subunit HisF

Chain E:



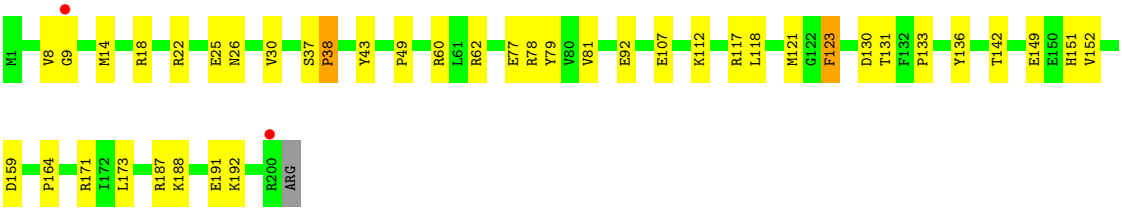
• Molecule 2: Imidazole glycerol phosphate synthase subunit HisH

Chain B:



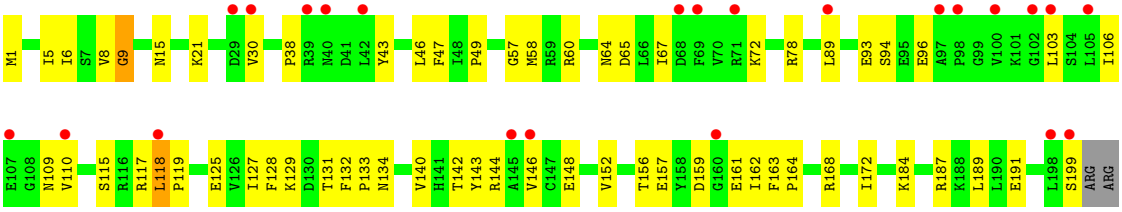
• Molecule 2: Imidazole glycerol phosphate synthase subunit HisH

Chain D:



• Molecule 2: Imidazole glycerol phosphate synthase subunit HisH

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.42Å 85.90Å 128.75Å 90.00° 108.24° 90.00°	Depositor
Resolution (Å)	40.00 – 2.11 47.63 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.00-2.11) 99.4 (47.63-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17	Depositor
R, R_{free}	0.210 , 0.250 0.216 , 0.254	Depositor DCC
R_{free} test set	4764 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10918	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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: OZW

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	0.39	0/1892	0.60	1/2551 (0.0%)
1	C	0.48	0/1938	0.65	2/2618 (0.1%)
1	E	0.47	0/1900	0.63	1/2565 (0.0%)
2	B	0.48	0/1623	0.62	0/2181
2	D	0.52	0/1626	0.64	0/2185
2	F	0.48	0/1593	0.61	1/2145 (0.0%)
All	All	0.47	0/10572	0.62	5/14245 (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
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	117	ARG	N-CA-C	-8.19	88.88	111.00
1	E	55	SER	N-CA-CB	5.58	118.88	110.50
1	C	55	SER	N-CA-CB	5.46	118.68	110.50
1	C	25	ASN	N-CA-C	5.17	124.97	111.00
1	A	250	LEU	CA-CB-CG	-5.10	103.57	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	8	VAL	Peptide
2	D	38	PRO	Mainchain

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	1867	0	1904	46	0
1	C	1911	0	1919	59	0
1	E	1875	0	1888	54	0
2	B	1611	14	1586	31	0
2	D	1614	0	1589	33	0
2	F	1581	0	1538	56	0
3	A	88	0	0	9	0
3	B	103	0	0	4	0
3	C	67	0	0	12	0
3	D	104	0	0	9	0
3	E	37	0	0	8	0
3	F	46	0	0	14	0
All	All	10904	14	10424	271	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 (271) 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)
2:F:118:LEU:HB3	2:F:119:PRO:CD	1.07	1.47
2:F:118:LEU:CB	2:F:119:PRO:HD3	1.29	1.40
2:F:118:LEU:CB	2:F:119:PRO:CD	1.90	1.11
1:E:230:ARG:HG2	1:E:230:ARG:HH11	1.20	1.03
1:C:16:ARG:NH1	3:C:301:HOH:O	1.91	1.02
1:E:235:ARG:NH2	1:E:251:GLU:HB3	1.76	1.01
1:A:29:SER:OG	1:A:228:HIS:NE2	1.97	0.98
1:A:133:ARG:O	3:A:301:HOH:O	1.82	0.97
2:F:157:GLU:HG2	3:F:305:HOH:O	1.63	0.96
1:A:188:ARG:NE	3:A:304:HOH:O	2.01	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLN:OE1	3:A:302:HOH:O	1.86	0.92
2:F:187:ARG:NH1	2:F:191:GLU:OE2	2.04	0.90
2:F:199:SER:N	3:F:302:HOH:O	2.06	0.87
2:F:118:LEU:CB	2:F:119:PRO:HD2	2.01	0.87
1:C:134:VAL:CG1	1:C:139:MET:HG3	2.06	0.85
1:C:195:THR:O	2:D:117:ARG:HG3	1.78	0.84
2:F:58:MET:HG2	2:F:89:LEU:HD22	1.59	0.83
2:F:118:LEU:HB3	2:F:119:PRO:HD2	1.52	0.83
1:C:21:THR:HG1	1:C:23:PHE:HD2	1.26	0.83
1:C:180:SER:O	3:C:303:HOH:O	1.96	0.82
1:A:91:GLU:HB2	3:A:305:HOH:O	1.80	0.81
1:A:251:GLU:O	2:B:184:LYS:NZ	2.14	0.79
1:C:206:LYS:HA	1:C:232:ILE:HD11	1.65	0.78
1:E:235:ARG:HH21	1:E:251:GLU:HB3	1.48	0.78
1:E:64:GLU:OE2	3:E:301:HOH:O	2.01	0.78
1:C:239:GLU:OE1	3:C:305:HOH:O	2.01	0.77
1:E:230:ARG:HG2	1:E:230:ARG:NH1	1.99	0.77
1:A:242:LYS:HZ1	1:A:250:LEU:HG	1.48	0.77
1:A:91:GLU:OE2	3:A:305:HOH:O	2.03	0.76
2:F:30:VAL:HG12	3:F:303:HOH:O	1.84	0.76
1:A:13:LYS:NZ	1:A:14:ASP:OD2	2.18	0.76
1:C:233:ASP:OD2	3:C:304:HOH:O	2.03	0.76
1:E:154:ARG:HD2	1:E:154:ARG:O	1.85	0.76
1:A:115:GLN:NE2	3:A:303:HOH:O	1.90	0.75
1:E:185:GLU:OE1	3:E:302:HOH:O	2.02	0.74
2:F:128:PHE:O	3:F:301:HOH:O	2.04	0.74
1:A:43:GLY:O	1:A:238:LYS:NZ	2.21	0.74
2:B:184:LYS:H	2:B:184:LYS:HD3	1.52	0.74
2:D:136:TYR:OH	3:D:303:HOH:O	2.05	0.74
1:A:242:LYS:NZ	1:A:250:LEU:HG	2.03	0.73
2:F:118:LEU:HB2	2:F:119:PRO:CD	2.12	0.72
1:C:26:LEU:O	3:C:306:HOH:O	2.07	0.72
1:E:154:ARG:NH1	1:E:155:ASP:HA	2.05	0.72
1:C:21:THR:HG22	1:C:29:SER:O	1.91	0.71
2:D:22:ARG:NE	3:D:302:HOH:O	2.04	0.71
1:E:46:GLU:OE2	3:E:304:HOH:O	2.09	0.71
1:A:188:ARG:CD	3:A:304:HOH:O	2.39	0.70
2:D:77:GLU:OE1	3:D:304:HOH:O	2.09	0.70
1:E:31:ASP:HB3	1:E:34:GLU:HG3	1.74	0.70
1:E:41:GLU:OE1	3:E:303:HOH:O	2.08	0.70
2:B:22:ARG:O	2:B:25:GLU:HG2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:GLU:OE1	3:B:301:HOH:O	2.08	0.70
2:B:94:SER:HB2	2:B:110:VAL:HB	1.74	0.69
1:C:1:MET:SD	1:C:247:ASN:ND2	2.66	0.69
1:A:248:VAL:HG23	1:A:250:LEU:CD2	2.23	0.68
1:A:67:GLU:O	1:A:71:GLU:HG2	1.94	0.67
1:A:232:ILE:O	3:A:306:HOH:O	2.10	0.67
2:D:149:GLU:OE2	3:D:305:HOH:O	2.11	0.67
1:C:175:ARG:HG3	1:C:183:ASP:HB2	1.77	0.67
2:F:118:LEU:CG	2:F:119:PRO:HD3	2.20	0.67
1:C:236:GLU:OE2	3:C:307:HOH:O	2.13	0.66
2:F:118:LEU:HB2	2:F:119:PRO:HD2	1.76	0.66
2:B:12:ASN:O	3:B:302:HOH:O	2.14	0.65
1:A:188:ARG:HD2	3:A:304:HOH:O	1.97	0.65
2:F:128:PHE:N	2:F:134:ASN:OD1	2.23	0.65
2:D:25:GLU:OE2	2:D:187:ARG:NH2	2.30	0.64
2:D:117:ARG:NH2	2:D:121:MET:H	1.96	0.64
2:D:117:ARG:HH22	2:D:121:MET:H	1.45	0.64
1:E:154:ARG:HH11	1:E:155:ASP:HA	1.60	0.64
2:B:8:VAL:HG23	2:B:9:GLY:N	2.13	0.64
2:F:199:SER:CB	3:F:302:HOH:O	2.46	0.64
1:A:31:ASP:HB3	1:A:34:GLU:HG2	1.80	0.64
1:A:33:VAL:HG21	1:A:68:LYS:HE3	1.79	0.63
1:C:225:SER:N	3:C:310:HOH:O	2.32	0.63
1:E:154:ARG:NH1	1:E:155:ASP:OD1	2.31	0.63
2:D:187:ARG:NH1	2:D:191:GLU:OE2	2.32	0.63
1:C:134:VAL:HG11	1:C:139:MET:HG3	1.79	0.62
2:D:37:SER:HB2	2:D:38:PRO:HD2	1.81	0.62
2:F:21:LYS:HE3	3:F:304:HOH:O	1.99	0.62
2:F:110:VAL:HG12	2:F:143:TYR:HB3	1.82	0.62
1:C:137:GLU:HG3	1:C:152:LEU:HD21	1.82	0.62
2:F:125:GLU:O	2:F:156:THR:OG1	2.14	0.61
2:B:71:ARG:NH1	2:B:71:ARG:HG3	2.15	0.61
1:E:16:ARG:NE	1:E:28:ASP:OD2	2.23	0.61
1:E:154:ARG:HD2	1:E:154:ARG:C	2.21	0.61
1:A:134:VAL:CG1	1:A:139:MET:HG3	2.30	0.61
1:C:137:GLU:HG3	1:C:152:LEU:CD2	2.31	0.61
2:F:132:PHE:HB3	2:F:189:LEU:CD2	2.31	0.61
2:B:71:ARG:HG3	2:B:71:ARG:HH11	1.64	0.61
1:E:241:LEU:HB3	1:E:246:VAL:HB	1.83	0.60
2:F:58:MET:HG2	2:F:89:LEU:CD2	2.31	0.60
2:F:199:SER:CA	3:F:302:HOH:O	2.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:ILE:CD1	2:B:46:LEU:HD11	2.32	0.59
2:F:57:GLY:H	2:F:60:ARG:HG3	1.67	0.59
1:A:181:GLY:N	1:A:203:GLY:O	2.35	0.59
1:C:21:THR:HG23	1:C:29:SER:HB2	1.84	0.59
2:F:5:ILE:HG12	2:F:47:PHE:HB2	1.83	0.59
2:F:43:TYR:O	2:F:78:ARG:HD2	2.02	0.59
2:F:93:GLU:O	2:F:109:ASN:HB2	2.01	0.59
1:C:67:GLU:HB2	1:C:95:ARG:HH11	1.68	0.59
1:C:66:VAL:HG22	1:C:79:VAL:HG21	1.84	0.59
2:D:22:ARG:HD2	3:D:307:HOH:O	2.02	0.59
1:C:16:ARG:NH2	1:C:30:GLY:HA3	2.17	0.58
1:E:251:GLU:HG3	2:F:184:LYS:HE3	1.84	0.58
1:C:65:LEU:O	1:C:69:VAL:HG23	2.04	0.58
2:F:96:GLU:HG3	2:F:143:TYR:CZ	2.39	0.57
1:C:236:GLU:HG3	3:C:304:HOH:O	2.04	0.57
1:C:197:PRO:HG3	2:D:117:ARG:HH11	1.69	0.57
1:E:232:ILE:HD12	1:E:232:ILE:N	2.19	0.57
1:A:29:SER:OG	1:A:29:SER:O	2.23	0.57
2:B:44:ASP:OD1	2:B:200:ARG:NH1	2.38	0.57
2:F:144:ARG:NH2	2:F:146:VAL:HG22	2.21	0.56
2:B:8:VAL:CG2	2:B:9:GLY:N	2.68	0.56
1:E:17:VAL:HB	1:E:29:SER:HB2	1.88	0.56
2:D:8:VAL:HG23	2:D:9:GLY:N	2.21	0.56
1:E:132:LYS:HB2	1:E:173:ILE:HD12	1.86	0.56
2:F:199:SER:HB2	3:F:302:HOH:O	2.04	0.55
1:E:182:TYR:CZ	1:E:204:ALA:HB2	2.42	0.55
1:E:207:MET:HE3	1:E:240:TYR:CG	2.41	0.55
2:F:94:SER:OG	2:F:110:VAL:HB	2.06	0.55
2:F:58:MET:CG	2:F:89:LEU:HD22	2.33	0.55
2:F:8:VAL:HG23	2:F:9:GLY:N	2.21	0.54
1:E:230:ARG:HH11	1:E:230:ARG:CG	2.05	0.54
2:D:187:ARG:HG3	3:D:356:HOH:O	2.07	0.54
2:F:96:GLU:HG3	2:F:143:TYR:CE1	2.43	0.54
2:B:6:ILE:HD11	2:B:46:LEU:HD11	1.88	0.54
1:E:226:VAL:HB	1:E:232:ILE:HD13	1.90	0.54
2:F:1:MET:O	2:F:30:VAL:HA	2.08	0.54
1:A:247:ASN:OD1	2:B:136:TYR:OH	2.23	0.54
2:D:14:MET:HB3	2:D:18:ARG:NH2	2.23	0.53
2:B:20:VAL:HG12	2:B:32:ILE:HD13	1.90	0.53
1:C:37:LYS:O	1:C:40:SER:HB3	2.08	0.53
1:C:116:ILE:CG2	1:C:125:VAL:HG22	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:ARG:O	1:E:178:THR:HG23	2.08	0.53
1:C:5:ARG:HD2	1:C:46:GLU:OE2	2.09	0.53
1:C:134:VAL:CG1	1:C:139:MET:CG	2.85	0.53
1:E:51:ASP:OD2	1:E:53:THR:OG1	2.27	0.53
2:B:68:ASP:O	2:B:72:LYS:HE3	2.09	0.53
2:D:79:TYR:CE2	2:D:171:ARG:HD3	2.44	0.53
1:C:21:THR:HG23	1:C:29:SER:CB	2.39	0.52
2:D:30:VAL:HG13	2:D:30:VAL:O	2.08	0.52
1:E:55:SER:HA	1:E:58:LYS:HB3	1.91	0.52
1:C:2:LEU:HD12	2:D:123:OZW:O	2.10	0.52
1:C:21:THR:OG1	1:C:23:PHE:CD2	2.60	0.52
1:A:206:LYS:HG2	1:A:209:HIS:CE1	2.45	0.52
2:F:15:ASN:HB2	3:F:310:HOH:O	2.09	0.52
1:A:242:LYS:HZ1	1:A:250:LEU:CG	2.18	0.52
2:D:43:TYR:O	2:D:78:ARG:HD2	2.09	0.51
2:B:184:LYS:H	2:B:184:LYS:CD	2.22	0.51
1:C:179:LYS:HE3	1:C:231:GLU:OE2	2.10	0.51
2:D:62:ARG:NH1	3:D:301:HOH:O	1.83	0.51
2:F:133:PRO:HD2	2:F:189:LEU:HD23	1.91	0.51
2:B:101:LYS:HE2	1:C:114:THR:HG21	1.92	0.51
1:C:21:THR:OG1	1:C:23:PHE:HD2	1.91	0.51
1:E:233:ASP:HB3	1:E:236:GLU:HB2	1.93	0.51
1:E:99[A]:LYS:NZ	1:E:123:GLN:O	2.44	0.50
1:C:21:THR:CG2	1:C:29:SER:HB2	2.41	0.50
1:A:46:GLU:HG2	1:A:76:PRO:HB2	1.94	0.49
1:C:9:CYS:HB2	1:C:222:LEU:HD11	1.92	0.49
1:E:101:SER:HA	1:E:126:VAL:O	2.13	0.49
1:A:116:ILE:CG2	1:A:125:VAL:HG22	2.43	0.49
2:F:163:PHE:HB2	2:F:164:PRO:HD2	1.95	0.49
1:E:47:LEU:CD1	1:E:75:ILE:HG21	2.43	0.49
2:B:13:ILE:C	2:B:13:ILE:HD12	2.33	0.49
2:F:38:PRO:HG3	2:F:65:ASP:O	2.13	0.49
1:A:63:LEU:HD21	1:A:91:GLU:HB3	1.95	0.48
1:A:58:LYS:HE3	1:A:62:MET:HE1	1.95	0.48
2:F:161:GLU:C	3:F:305:HOH:O	2.52	0.48
2:D:81:VAL:HA	2:D:173:LEU:O	2.13	0.48
1:C:22:ASN:O	1:C:22:ASN:ND2	2.38	0.48
2:F:30:VAL:CG1	3:F:303:HOH:O	2.53	0.48
1:E:5:ARG:HD2	1:E:46:GLU:OE2	2.13	0.48
2:F:115:SER:OG	2:F:159:ASP:CB	2.61	0.48
2:D:8:VAL:CG2	2:D:9:GLY:N	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:GLY:O	1:C:238:LYS:NZ	2.38	0.48
1:C:139:MET:HE1	1:C:150:GLY:C	2.34	0.48
2:D:133:PRO:HG3	2:D:188:LYS:HD3	1.96	0.48
1:A:122:SER:O	1:A:166:GLY:HA3	2.14	0.48
2:B:21:LYS:HA	2:B:32:ILE:CD1	2.42	0.48
2:B:24:SER:HB2	2:B:30:VAL:HG11	1.95	0.48
1:E:154:ARG:HD3	1:E:193:LEU:HD22	1.96	0.48
1:E:229:PHE:CD1	1:E:229:PHE:N	2.79	0.47
2:F:6:ILE:HD11	2:F:46:LEU:HD21	1.96	0.47
2:F:94:SER:CB	2:F:110:VAL:HB	2.45	0.47
2:B:71:ARG:HH11	2:B:71:ARG:CG	2.27	0.47
2:B:199:SER:O	2:B:199:SER:OG	2.30	0.47
2:F:199:SER:O	2:F:199:SER:OG	2.28	0.47
2:D:92:GLU:OE2	2:D:107:GLU:HA	2.15	0.47
1:A:178:THR:OG1	1:A:180:SER:HB3	2.15	0.47
1:E:244:HIS:O	3:E:306:HOH:O	2.20	0.47
2:F:162:ILE:HG13	3:F:305:HOH:O	2.14	0.47
1:A:5:ARG:HD2	1:A:46:GLU:OE2	2.14	0.47
1:A:17:VAL:CG2	1:A:32:PRO:HA	2.45	0.47
1:E:235:ARG:HG2	1:E:239:GLU:OE2	2.15	0.46
2:F:67:ILE:HG23	2:F:103:LEU:CD2	2.45	0.46
2:B:114:ARG:HG3	2:B:161:GLU:CD	2.35	0.46
2:D:151:HIS:HD2	3:D:331:HOH:O	1.99	0.46
1:E:190:VAL:HA	1:E:193:LEU:HD12	1.98	0.46
1:C:178:THR:O	1:C:203:GLY:HA2	2.15	0.46
1:C:51:ASP:OD2	1:C:58:LYS:NZ	2.44	0.46
1:C:222:LEU:HD23	1:C:222:LEU:C	2.37	0.46
1:C:233:ASP:HB3	3:C:304:HOH:O	2.14	0.46
1:A:132:LYS:HB3	1:A:141:PHE:CE1	2.51	0.46
1:C:241:LEU:HD22	1:C:246:VAL:HG21	1.97	0.46
1:E:138:PHE:N	3:E:305:HOH:O	2.18	0.45
2:F:142:THR:HG22	2:F:143:TYR:CD1	2.51	0.45
1:C:132:LYS:HB2	1:C:173:ILE:HB	1.98	0.45
1:A:58:LYS:HG2	1:A:62:MET:HE2	1.99	0.45
2:B:9:GLY:HA2	2:B:60:ARG:HD2	1.98	0.45
2:B:15:ASN:HB3	2:B:180:GLU:HG3	1.98	0.45
1:C:5:ARG:NH1	1:C:46:GLU:OE2	2.43	0.45
1:C:21:THR:CG2	1:C:29:SER:O	2.61	0.45
2:B:6:ILE:HD12	2:B:46:LEU:HD11	1.99	0.45
1:A:235:ARG:NH2	1:A:251:GLU:HA	2.32	0.45
2:D:118:LEU:HD13	2:D:142:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:LEU:HA	1:E:250:LEU:HD12	1.50	0.45
1:C:66:VAL:CG2	1:C:79:VAL:HG21	2.47	0.45
2:F:8:VAL:CG2	2:F:9:GLY:N	2.80	0.45
1:C:142:THR:HG23	1:C:149:THR:HG21	1.98	0.45
1:A:139:MET:HE1	1:A:150:GLY:C	2.37	0.44
1:E:208:GLU:HG3	1:E:240:TYR:OH	2.17	0.44
1:E:137:GLU:OE2	1:E:137:GLU:HA	2.18	0.44
1:E:207:MET:HE3	1:E:240:TYR:CB	2.48	0.44
1:C:17:VAL:HG23	1:C:30:GLY:O	2.17	0.44
1:E:76:PRO:HA	1:E:98:ASP:OD2	2.18	0.44
1:E:88:THR:O	1:E:91:GLU:HG2	2.17	0.44
1:A:95:ARG:HA	1:A:95:ARG:HD3	1.88	0.44
2:D:112:LYS:HE3	2:D:118:LEU:CD1	2.48	0.44
2:F:157:GLU:HA	3:F:305:HOH:O	2.18	0.44
2:B:69:PHE:HA	2:B:72:LYS:HE3	2.00	0.44
1:C:16:ARG:NH2	1:C:28:ASP:OD1	2.51	0.43
1:C:26:LEU:N	3:C:306:HOH:O	2.51	0.43
1:E:31:ASP:HB3	1:E:34:GLU:CG	2.45	0.43
1:E:240:TYR:CE1	1:E:244:HIS:CE1	3.06	0.43
1:A:134:VAL:CG1	1:A:139:MET:CG	2.97	0.43
2:D:26:ASN:HB2	3:D:363:HOH:O	2.18	0.43
2:F:1:MET:HG3	2:F:30:VAL:HG23	2.00	0.43
1:C:131:ALA:O	1:C:173:ILE:HG13	2.18	0.43
1:E:37:LYS:NZ	3:E:303:HOH:O	2.52	0.43
1:A:242:LYS:HB3	1:A:242:LYS:HE2	1.71	0.43
2:D:112:LYS:HE3	2:D:118:LEU:HD12	1.99	0.43
2:F:162:ILE:CG1	3:F:305:HOH:O	2.66	0.43
2:B:151:HIS:HD2	3:B:320:HOH:O	2.02	0.43
1:C:197:PRO:HG3	2:D:117:ARG:NH1	2.34	0.42
1:A:7:ILE:HG12	1:A:46:GLU:HB2	2.00	0.42
2:B:199:SER:OG	3:B:303:HOH:O	2.22	0.42
2:F:168:ARG:HA	2:F:172:ILE:O	2.19	0.42
2:B:101:LYS:HB3	2:B:101:LYS:HE3	1.86	0.42
1:C:115:GLN:HG2	3:C:302:HOH:O	2.20	0.42
1:E:154:ARG:HH11	1:E:155:ASP:CA	2.30	0.42
2:F:129:LYS:HD3	2:F:152:VAL:O	2.19	0.42
2:D:9:GLY:HA2	2:D:60:ARG:HD2	2.02	0.41
1:A:141:PHE:HA	1:A:147:LYS:O	2.21	0.41
2:D:130:ASP:OD1	2:D:131:THR:OG1	2.28	0.41
1:E:137:GLU:HA	3:E:305:HOH:O	2.20	0.41
1:E:38:PHE:O	1:E:42:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:127:ILE:HA	2:F:134:ASN:OD1	2.21	0.41
1:C:142:THR:HG23	1:C:149:THR:CG2	2.51	0.41
2:D:152:VAL:HG22	2:D:164:PRO:HB3	2.01	0.41
1:A:53:THR:HG22	1:A:54:ALA:N	2.35	0.41
1:E:159:GLU:O	1:E:163:ARG:HG2	2.21	0.41
2:F:106:ILE:HD11	2:F:172:ILE:HG22	2.02	0.40
1:C:64:GLU:O	1:C:68:LYS:HD3	2.20	0.40
1:A:68:LYS:HD2	1:A:72:GLN:OE1	2.22	0.40
1:C:233:ASP:CB	3:C:304:HOH:O	2.70	0.40
1:E:47:LEU:HD12	1:E:75:ILE:HG21	2.04	0.40
1:E:178:THR:OG1	1:E:180:SER:HB3	2.22	0.40
1:A:58:LYS:HG2	1:A:62:MET:CE	2.52	0.40
1:A:235:ARG:CZ	1:A:251:GLU:HA	2.52	0.40
1:C:57:GLU:OE2	1:C:57:GLU:HA	2.22	0.40
1:E:226:VAL:HB	1:E:232:ILE:CD1	2.51	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	240/253 (95%)	229 (95%)	9 (4%)	2 (1%)	19 14
1	C	250/253 (99%)	236 (94%)	12 (5%)	2 (1%)	19 14
1	E	243/253 (96%)	229 (94%)	12 (5%)	2 (1%)	19 14
2	B	197/201 (98%)	187 (95%)	9 (5%)	1 (0%)	29 25
2	D	197/201 (98%)	189 (96%)	7 (4%)	1 (0%)	29 25
2	F	196/201 (98%)	178 (91%)	13 (7%)	5 (3%)	5 1
All	All	1323/1362 (97%)	1248 (94%)	62 (5%)	13 (1%)	15 10

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	54	ALA
2	F	118	LEU
1	C	55	SER
2	F	131	THR
1	A	28	ASP
2	F	49	PRO
2	D	49	PRO
1	A	230	ARG
2	B	49	PRO
1	E	55	SER
2	F	9	GLY
1	E	205	GLY
2	F	140	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	198/208 (95%)	193 (98%)	5 (2%)	47	50
1	C	200/208 (96%)	196 (98%)	4 (2%)	55	59
1	E	196/208 (94%)	191 (97%)	5 (3%)	46	49
2	B	173/176 (98%)	171 (99%)	2 (1%)	71	77
2	D	174/176 (99%)	172 (99%)	2 (1%)	73	79
2	F	168/176 (96%)	165 (98%)	3 (2%)	59	63
All	All	1109/1152 (96%)	1088 (98%)	21 (2%)	57	61

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	59	ARG
1	A	68	LYS
1	A	133	ARG
1	A	179	LYS
2	B	184	LYS

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Mol	Chain	Res	Type
2	B	192	LYS
1	C	16	ARG
1	C	22	ASN
1	C	55	SER
1	C	59	ARG
2	D	159	ASP
2	D	192	LYS
1	E	56	VAL
1	E	162	LYS
1	E	228	HIS
1	E	230	ARG
1	E	235	ARG
2	F	64	ASN
2	F	72	LYS
2	F	148	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 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	$\#\|Z\| > 2$
2	OZW	D	123	2	19,20,21	0.72	0	22,25,27	1.26	2 (9%)
2	OZW	F	123	2	19,20,21	0.66	0	22,25,27	0.89	0
2	OZW	B	123	2	19,20,21	0.69	0	22,25,27	0.98	2 (9%)

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	OZW	D	123	2	-	1/10/11/13	0/2/2/2
2	OZW	F	123	2	-	3/10/11/13	0/2/2/2
2	OZW	B	123	2	-	2/10/11/13	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	123	OZW	CD2-CG-CD1	2.49	122.08	118.17
2	D	123	OZW	CB-CA-C	-2.47	106.83	111.47
2	B	123	OZW	CB-CA-C	-2.19	107.36	111.47
2	B	123	OZW	CD2-CG-CD1	2.02	121.34	118.17

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	123	OZW	CE1-CZ-N2-N1
2	F	123	OZW	CE2-CZ-N2-N1
2	F	123	OZW	C6-N1-N2-CZ
2	B	123	OZW	C1-C6-N1-N2
2	D	123	OZW	C1-C6-N1-N2
2	B	123	OZW	C2-C6-N1-N2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	123	OZW	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	123:OZW	C	124:ASN	N	1.05

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	244/253 (96%)	0.18	6 (2%)	57	62	27, 46, 72, 90	0
1	C	251/253 (99%)	0.26	11 (4%)	34	40	35, 50, 75, 96	0
1	E	246/253 (97%)	0.47	18 (7%)	15	19	35, 53, 82, 101	0
2	B	199/201 (99%)	0.03	2 (1%)	82	85	30, 39, 58, 85	0
2	D	199/201 (99%)	-0.01	2 (1%)	82	85	29, 39, 55, 86	0
2	F	198/201 (98%)	0.67	23 (11%)	4	6	39, 61, 85, 90	0
All	All	1337/1362 (98%)	0.27	62 (4%)	32	37	27, 48, 77, 101	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	253	LEU	8.8
1	E	229	PHE	6.7
1	C	26	LEU	6.5
1	E	27	ARG	5.9
1	E	54	ALA	5.8
1	A	229	PHE	5.7
1	E	29	SER	5.3
1	E	252	GLY	5.3
2	F	40	ASN	5.2
2	F	199	SER	4.8
2	F	160	GLY	4.4
1	E	19	LYS	4.2
2	F	198	LEU	3.9
2	B	200	ARG	3.7
2	F	30	VAL	3.7
1	E	28	ASP	3.6
1	E	18	VAL	3.6
1	E	251	GLU	3.5
1	C	27	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	23	PHE	3.5
1	A	228	HIS	3.2
1	E	230	ARG	3.2
1	A	54	ALA	3.1
1	C	21	THR	3.1
1	E	226	VAL	3.1
2	F	39	ARG	2.9
2	F	42	LEU	2.7
1	C	25	ASN	2.7
1	E	228	HIS	2.7
1	E	232	ILE	2.6
1	E	227	PHE	2.6
2	F	107	GLU	2.6
1	C	20	GLY	2.6
2	F	98	PRO	2.6
2	F	145	ALA	2.5
2	D	9	GLY	2.5
1	A	30	GLY	2.5
2	F	29	ASP	2.5
1	C	22	ASN	2.5
1	A	243	LYS	2.5
2	F	118	LEU	2.4
2	F	105	LEU	2.4
2	F	146	VAL	2.4
1	C	28	ASP	2.4
2	F	71	ARG	2.4
1	C	54	ALA	2.4
1	A	27	ARG	2.3
2	F	97	ALA	2.3
2	F	100	VAL	2.3
2	F	102	GLY	2.2
2	F	69	PHE	2.2
2	D	200	ARG	2.2
1	C	55	SER	2.1
2	F	89	LEU	2.1
2	F	68	ASP	2.1
1	E	250	LEU	2.1
2	B	52	GLY	2.1
1	C	29	SER	2.0
2	F	103	LEU	2.0
1	E	1	MET	2.0
1	E	215	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	110	VAL	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. 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	OZW	F	123	19/20	0.92	0.15	45,48,55,55	0
2	OZW	D	123	19/20	0.94	0.14	35,41,48,49	0
2	OZW	B	123	19/20	0.97	0.10	34,40,48,52	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.