Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 02:12 AM EDT

PDB ID	:	5JHG
Title	:	Crystal structure of the complex between the human RhoA and the DH/PH domain of human ARHGEF11
Authors	:	Wang, R.; Chen, Q.; Zhang, H.; Yan, Z.; Li, J.; Miao, L.; Wang, F.
Deposited on	:	2016-04-21
Resolution	:	2.50 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:

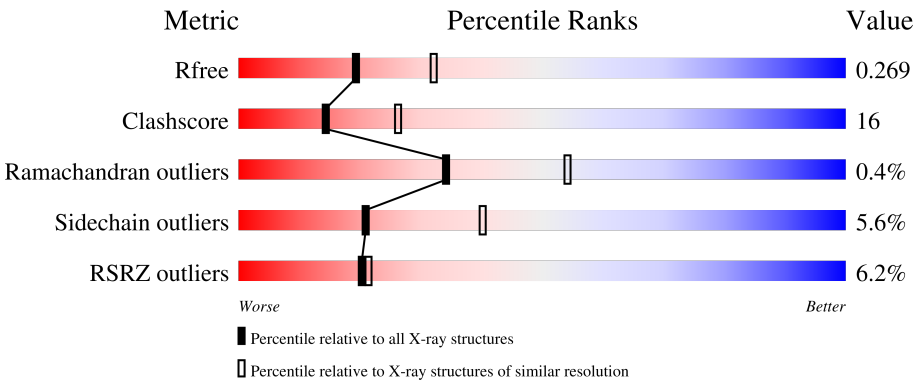
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	369	7% 70% 24%
1	E	369	7% 69% 23%
2	B	181	5% 72% 24%
2	F	181	4% 80% 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8796 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 Rho guanine nucleotide exchange factor 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	356	2916	1843	522	536	15	0	0	0
1	E	358	2931	1852	525	539	15	0	0	0

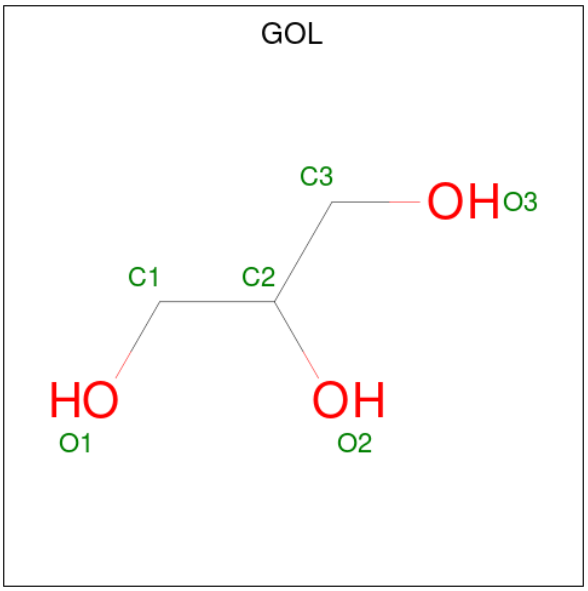
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	713	MET	-	expression tag	UNP O15085
E	713	MET	-	expression tag	UNP O15085

- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	178	1413	894	239	270	10	0	0	0
2	F	178	1413	894	239	270	10	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	E	1	6	3	3	0	0

- Molecule 4 is water.

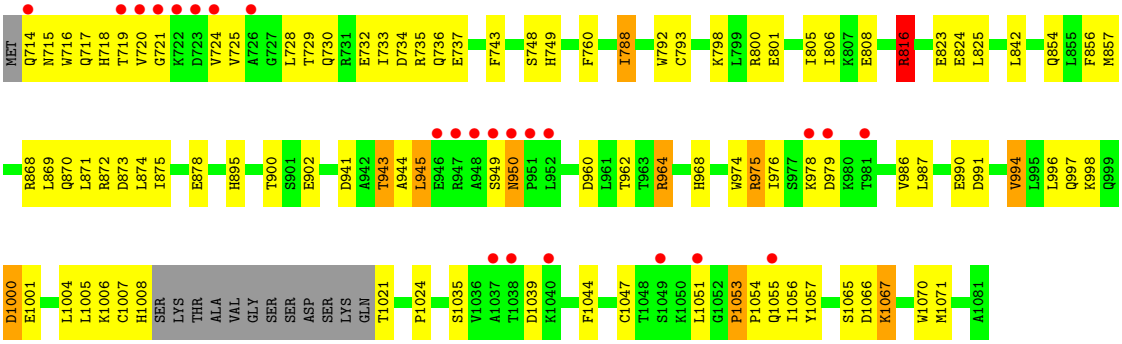
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	41	41	41	0	0
			Total	O		
4	B	23	23	23	0	0
			Total	O		
4	E	26	26	26	0	0
			Total	O		
4	F	9	9	9	0	0

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.

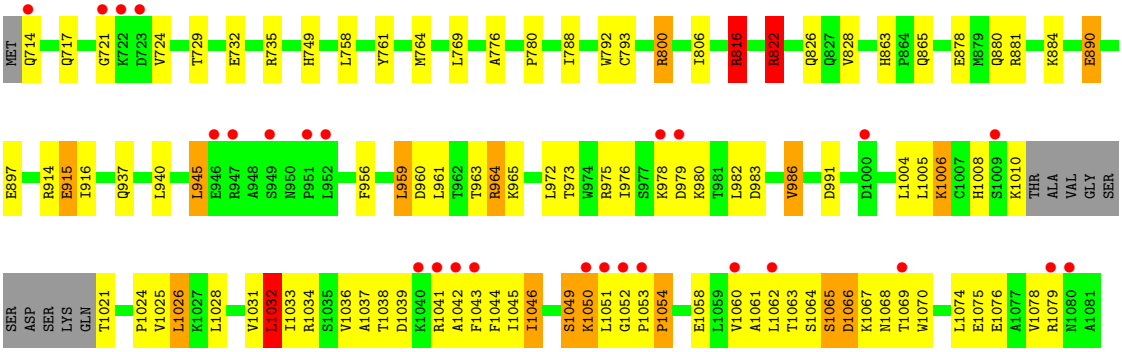
• Molecule 1: Rho guanine nucleotide exchange factor 11

Chain A:



• Molecule 1: Rho guanine nucleotide exchange factor 11

Chain E:

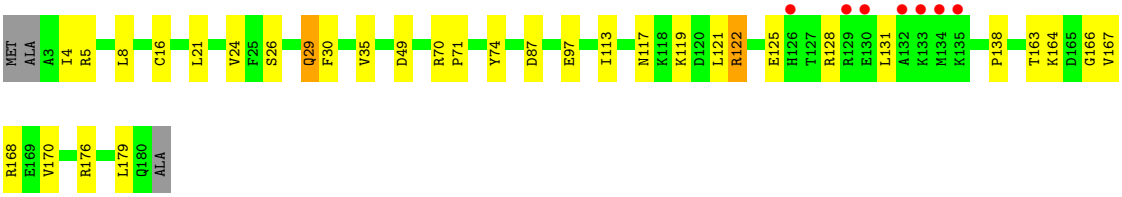


• Molecule 2: Transforming protein RhoA

Chain B:

• Molecule 2: Transforming protein RhoA

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	87.44Å 118.59Å 88.00Å 90.00° 113.00° 90.00°	Depositor
Resolution (Å)	31.13 – 2.50 31.13 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (31.13-2.50) 97.1 (31.13-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	23.99 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.221 , 0.270 0.222 , 0.269	Depositor DCC
R_{free} test set	2814 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8796	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: GOL

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	1.00	1/2961 (0.0%)	0.99	5/3985 (0.1%)
1	E	0.97	1/2976 (0.0%)	0.98	9/4004 (0.2%)
2	B	0.95	0/1441	0.90	1/1949 (0.1%)
2	F	0.94	0/1441	0.94	3/1949 (0.2%)
All	All	0.97	2/8819 (0.0%)	0.96	18/11887 (0.2%)

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	A	0	1
1	E	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	748	SER	CB-OG	-6.14	1.34	1.42
1	E	761	TYR	CB-CG	-5.13	1.44	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	49	ASP	CB-CG-OD1	8.83	126.24	118.30
1	E	816	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	E	816	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	A	1051	LEU	CB-CA-C	-7.19	96.54	110.20
1	E	1052	GLY	C-N-CD	6.42	141.88	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	718	HIS	CB-CA-C	-6.26	97.89	110.40
1	A	816	ARG	NE-CZ-NH1	6.15	123.37	120.30
2	F	49	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	A	735	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	E	822	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	E	1065	SER	N-CA-C	5.46	125.75	111.00
1	E	822	ARG	NE-CZ-NH1	-5.13	117.74	120.30
1	E	1032	LEU	CA-CB-CG	5.11	127.05	115.30
2	B	68	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	1053	PRO	C-N-CD	5.07	139.04	128.40
2	F	122	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	E	800	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	E	735	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	714	GLN	Peptide
1	E	965	LYS	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	2916	0	3003	97	2
1	E	2931	0	3020	125	0
2	B	1413	0	1405	37	0
2	F	1413	0	1405	22	2
3	A	12	0	16	1	0
3	B	6	0	8	2	0
3	E	6	0	8	1	0
4	A	41	0	0	5	0
4	B	23	0	0	0	0
4	E	26	0	0	3	0
4	F	9	0	0	2	0
All	All	8796	0	8865	273	2

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 16.

All (273) 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:E:1042:ALA:H	1:E:1067:LYS:CD	1.24	1.45
1:E:1042:ALA:N	1:E:1067:LYS:HD2	1.39	1.33
1:E:1039:ASP:O	1:E:1067:LYS:NZ	1.60	1.32
1:E:1066:ASP:HA	1:E:1069:THR:CG2	1.62	1.29
1:E:1042:ALA:O	1:E:1067:LYS:HE3	1.11	1.25
1:A:715:ASN:O	1:A:719:THR:HG23	1.16	1.24
1:E:1042:ALA:H	1:E:1067:LYS:CE	1.54	1.21
1:A:715:ASN:O	1:A:719:THR:CG2	1.86	1.20
1:E:1066:ASP:C	1:E:1069:THR:HG22	1.67	1.15
1:E:1042:ALA:N	1:E:1067:LYS:CD	2.01	1.14
1:E:1042:ALA:O	1:E:1067:LYS:CE	1.97	1.12
1:A:964:ARG:NH1	1:A:991:ASP:OD2	1.83	1.11
1:E:964:ARG:NH1	1:E:991:ASP:OD2	1.83	1.11
1:E:1065:SER:OG	2:F:97:GLU:O	1.67	1.10
1:E:1066:ASP:CA	1:E:1069:THR:HG22	1.83	1.08
1:E:1066:ASP:CA	1:E:1069:THR:CG2	2.32	1.08
1:E:1066:ASP:O	1:E:1069:THR:HG22	1.49	1.08
1:E:1041:ARG:CA	1:E:1067:LYS:HD2	1.84	1.08
1:E:1042:ALA:C	1:E:1067:LYS:HE3	1.73	1.08
1:E:1066:ASP:O	1:E:1069:THR:CG2	2.02	1.07
1:E:1041:ARG:C	1:E:1067:LYS:HD2	1.75	1.07
1:E:1066:ASP:HA	1:E:1069:THR:HG21	1.34	1.05
1:A:1008:HIS:CD2	1:A:1021:THR:HG22	1.94	1.01
1:E:973:THR:HG22	1:E:983:ASP:OD1	1.60	1.01
1:E:978:LYS:NZ	1:E:979:ASP:OD2	1.93	1.00
1:E:976:ILE:HD12	1:E:980:LYS:HE3	1.44	0.98
1:E:1042:ALA:N	1:E:1067:LYS:CE	2.20	0.98
1:E:937:GLN:NE2	1:E:961:LEU:H	1.60	0.98
1:A:870:GLN:OE1	1:A:872:ARG:NH2	1.98	0.97
1:E:1004:LEU:HD12	1:E:1004:LEU:O	1.66	0.95
1:A:1044:PHE:CD1	1:A:1056:ILE:HG21	2.03	0.94
1:A:872:ARG:NH1	4:A:1201:HOH:O	2.00	0.93
1:A:975:ARG:NH2	1:A:1039:ASP:OD2	2.05	0.90
1:A:1008:HIS:HB2	1:A:1021:THR:CG2	2.00	0.90
1:A:721:GLY:HA2	1:A:724:VAL:HG12	1.54	0.89
1:E:945:LEU:HD23	1:E:956:PHE:O	1.70	0.89
1:E:973:THR:OG1	1:E:1060:VAL:HB	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1041:ARG:HA	1:E:1067:LYS:HD2	1.56	0.87
1:E:717:GLN:O	1:E:721:GLY:O	1.92	0.86
1:A:816:ARG:O	1:A:816:ARG:HD3	1.76	0.85
1:E:1070:TRP:O	1:E:1074:LEU:HG	1.77	0.85
1:A:950:ASN:ND2	1:A:950:ASN:O	2.10	0.84
1:E:890:GLU:OE2	1:E:914:ARG:NH2	2.11	0.83
1:A:1054:PRO:HA	1:E:1034:ARG:HH11	1.45	0.82
1:A:1008:HIS:HD2	1:A:1021:THR:HG22	1.40	0.82
1:A:1008:HIS:HB2	1:A:1021:THR:HB	1.60	0.81
1:E:937:GLN:HE22	1:E:961:LEU:H	1.25	0.80
1:E:964:ARG:HG2	1:E:964:ARG:HH11	1.47	0.79
1:E:1066:ASP:O	1:E:1069:THR:N	2.14	0.79
1:A:1008:HIS:HB2	1:A:1021:THR:CB	2.13	0.78
2:F:5:ARG:NE	4:F:201:HOH:O	2.13	0.78
1:E:1042:ALA:N	1:E:1067:LYS:HE3	2.01	0.76
1:E:945:LEU:CD2	1:E:956:PHE:O	2.33	0.76
1:A:964:ARG:HH11	1:A:964:ARG:HG2	1.52	0.75
1:E:816:ARG:O	1:E:816:ARG:HD3	1.85	0.75
1:E:976:ILE:CD1	1:E:980:LYS:HE3	2.16	0.75
1:E:1042:ALA:CA	1:E:1067:LYS:HE3	2.16	0.74
2:B:168:ARG:HG3	2:B:168:ARG:HH21	1.53	0.74
1:E:964:ARG:NH1	1:E:991:ASP:CG	2.41	0.74
1:E:1006:LYS:O	1:E:1008:HIS:CD2	2.41	0.73
1:E:1049:SER:OG	1:E:1050:LYS:N	2.20	0.73
1:E:1044:PHE:HE1	1:E:1058:GLU:HB2	1.52	0.73
2:B:128:ARG:NH1	2:B:128:ARG:HB2	2.03	0.73
1:E:976:ILE:HD11	1:E:982:LEU:HD12	1.72	0.72
2:B:15:ALA:HA	3:B:201:GOL:O2	1.90	0.71
1:A:871:LEU:C	1:A:871:LEU:HD13	2.12	0.70
1:E:1041:ARG:HA	1:E:1067:LYS:CD	2.22	0.70
1:A:1044:PHE:CD1	1:A:1056:ILE:CG2	2.74	0.69
1:E:1042:ALA:H	1:E:1067:LYS:HE3	1.50	0.69
1:E:884:LYS:NZ	4:E:1201:HOH:O	2.27	0.68
1:A:1008:HIS:CG	1:A:1021:THR:HG22	2.27	0.68
1:E:1043:PHE:CZ	1:E:1074:LEU:HD11	2.29	0.68
1:E:1066:ASP:O	1:E:1069:THR:HG23	1.91	0.68
1:A:871:LEU:HD13	1:A:871:LEU:O	1.95	0.67
1:E:937:GLN:NE2	1:E:961:LEU:N	2.41	0.67
1:E:1006:LYS:O	1:E:1008:HIS:NE2	2.28	0.67
1:A:1006:LYS:O	1:A:1024:PRO:HG3	1.95	0.67
1:A:1008:HIS:CB	1:A:1021:THR:CG2	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1028:LEU:O	1:E:1078:VAL:HG23	1.94	0.66
1:E:1066:ASP:C	1:E:1069:THR:CG2	2.44	0.66
1:A:749:HIS:HD2	4:A:1238:HOH:O	1.79	0.66
2:B:128:ARG:HB2	2:B:128:ARG:HH11	1.59	0.66
1:E:975:ARG:NH2	1:E:1039:ASP:OD2	2.27	0.66
1:E:822:ARG:HH21	1:E:826:GLN:HE22	1.44	0.65
1:A:1044:PHE:HD1	1:A:1056:ILE:CG2	2.10	0.65
1:E:1041:ARG:HG3	1:E:1041:ARG:O	1.98	0.64
1:A:724:VAL:HG21	1:A:805:ILE:HD11	1.79	0.64
1:A:941:ASP:HB3	1:A:1004:LEU:HD23	1.80	0.64
1:A:964:ARG:NH1	1:A:991:ASP:CG	2.50	0.64
1:A:716:TRP:O	1:A:720:VAL:O	2.15	0.64
1:A:724:VAL:CG2	1:A:805:ILE:HD11	2.28	0.64
2:F:131:LEU:HD12	2:F:138:PRO:HD3	1.79	0.64
1:A:978:LYS:HE2	1:E:1037:ALA:O	1.98	0.63
1:E:1044:PHE:HE1	1:E:1058:GLU:CB	2.12	0.62
1:A:943:THR:HG22	1:A:944:ALA:N	2.13	0.62
1:A:721:GLY:HA2	1:A:724:VAL:CG1	2.30	0.62
1:A:798:LYS:O	1:A:801:GLU:HB2	1.99	0.62
1:E:729:THR:HG23	1:E:732:GLU:H	1.63	0.62
1:E:1010:LYS:HE3	1:E:1021:THR:CA	2.29	0.62
1:E:1033:ILE:C	1:E:1034:ARG:HG2	2.21	0.62
1:A:1008:HIS:HB2	1:A:1021:THR:HG22	1.79	0.61
1:A:716:TRP:HA	1:A:719:THR:OG1	2.00	0.61
1:A:870:GLN:OE1	1:A:872:ARG:CZ	2.50	0.60
1:A:854:GLN:HG3	4:A:1235:HOH:O	2.02	0.60
2:F:21:LEU:HD22	2:F:117:ASN:HD21	1.67	0.60
1:A:964:ARG:HH11	1:A:964:ARG:CG	2.16	0.59
2:F:163:THR:O	2:F:164:LYS:HB2	2.02	0.59
1:A:724:VAL:O	1:A:724:VAL:HG22	2.02	0.58
2:F:163:THR:O	2:F:164:LYS:CB	2.51	0.58
1:A:871:LEU:O	1:A:874:LEU:HB2	2.03	0.58
1:E:822:ARG:HG2	1:E:916:ILE:HD11	1.85	0.58
1:E:964:ARG:HH11	1:E:964:ARG:CG	2.15	0.57
1:A:871:LEU:C	1:A:871:LEU:CD1	2.72	0.57
1:E:1066:ASP:O	1:E:1070:TRP:N	2.31	0.57
1:A:1053:PRO:C	1:A:1055:GLN:H	2.08	0.57
1:E:959:LEU:HD12	1:E:1005:LEU:HD11	1.86	0.57
2:B:113:ILE:HD11	2:B:115:VAL:HG22	1.87	0.56
1:E:1004:LEU:HD12	1:E:1004:LEU:C	2.25	0.56
1:A:1053:PRO:HB2	1:A:1055:GLN:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1043:PHE:HE1	1:E:1045:ILE:HD11	1.71	0.56
1:A:736:GLN:NE2	1:A:806:ILE:O	2.32	0.56
1:E:1041:ARG:HG3	1:E:1060:VAL:HG13	1.87	0.55
1:E:973:THR:HG1	1:E:1060:VAL:HB	1.72	0.55
1:E:1053:PRO:O	1:E:1054:PRO:O	2.25	0.55
2:B:168:ARG:HG3	2:B:168:ARG:NH2	2.20	0.55
1:A:873:ASP:OD1	2:B:58:TRP:HZ2	1.89	0.55
1:E:800:ARG:HG2	4:E:1203:HOH:O	2.07	0.55
2:B:24:VAL:HG12	2:B:30:PHE:HA	1.89	0.55
1:A:760:PHE:CD1	1:A:871:LEU:HD23	2.42	0.54
1:E:960:ASP:OD2	1:E:963:THR:HG23	2.07	0.54
1:E:1010:LYS:HE3	1:E:1021:THR:N	2.22	0.54
1:E:964:ARG:HH12	1:E:991:ASP:CG	2.03	0.54
2:F:24:VAL:HG12	2:F:30:PHE:HA	1.89	0.54
1:E:1004:LEU:HD13	1:E:1006:LYS:HD3	1.90	0.54
1:A:960:ASP:OD1	1:A:962:THR:HB	2.08	0.54
1:A:1008:HIS:CB	1:A:1021:THR:HG22	2.35	0.54
1:E:1074:LEU:O	1:E:1078:VAL:HG12	2.07	0.54
1:E:880:GLN:O	1:E:884:LYS:HG2	2.09	0.53
1:A:732:GLU:OE2	1:A:736:GLN:HG2	2.09	0.53
1:A:760:PHE:CG	1:A:871:LEU:HD23	2.43	0.53
2:F:4:ILE:HD11	2:F:179:LEU:HD21	1.91	0.52
1:A:1007:CYS:O	1:A:1008:HIS:C	2.46	0.52
1:E:1041:ARG:O	1:E:1042:ALA:HB2	2.08	0.52
1:A:715:ASN:O	1:A:719:THR:HG21	1.98	0.52
1:A:968:HIS:HD2	4:A:1233:HOH:O	1.92	0.52
1:A:743:PHE:HB3	1:A:800:ARG:HH21	1.75	0.52
1:A:816:ARG:HD3	1:A:816:ARG:C	2.29	0.51
1:A:1056:ILE:HG22	1:A:1057:TYR:N	2.26	0.51
1:E:1036:VAL:HG12	1:E:1039:ASP:H	1.75	0.51
1:E:1026:LEU:CD1	1:E:1026:LEU:N	2.73	0.51
2:F:70:ARG:N	2:F:71:PRO:CD	2.74	0.51
1:A:1067:LYS:HE2	1:A:1071:MET:HG3	1.93	0.51
2:F:4:ILE:O	2:F:4:ILE:HG13	2.11	0.50
2:F:122:ARG:O	2:F:128:ARG:NH2	2.43	0.50
1:E:1033:ILE:O	1:E:1034:ARG:HG2	2.12	0.50
1:A:1007:CYS:O	1:A:1008:HIS:O	2.29	0.50
1:A:1065:SER:OG	2:B:97:GLU:O	2.28	0.50
1:E:1043:PHE:CZ	1:E:1074:LEU:CD1	2.95	0.50
1:A:1008:HIS:HD2	1:A:1021:THR:CG2	2.20	0.49
1:E:792:TRP:HB2	3:E:1101:GOL:O3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:THR:HG23	1:A:732:GLU:H	1.76	0.49
2:F:4:ILE:CD1	2:F:179:LEU:HD21	2.42	0.49
1:A:1056:ILE:CG2	1:A:1057:TYR:N	2.76	0.49
1:E:881:ARG:O	1:E:884:LYS:HB2	2.13	0.49
1:A:1054:PRO:HA	1:E:1034:ARG:NH1	2.20	0.48
1:E:937:GLN:OE1	1:E:940:LEU:HD23	2.13	0.48
1:E:1043:PHE:CE1	1:E:1074:LEU:CD1	2.96	0.48
1:A:1008:HIS:CD2	1:A:1021:THR:CG2	2.82	0.48
1:E:1042:ALA:CA	1:E:1067:LYS:CE	2.83	0.48
1:A:724:VAL:HG21	1:A:805:ILE:CD1	2.44	0.48
1:E:937:GLN:HE21	1:E:961:LEU:H	1.52	0.48
2:B:24:VAL:HG23	2:B:167:VAL:HG11	1.96	0.48
1:A:792:TRP:HD1	3:A:1101:GOL:H11	1.79	0.47
1:E:1031:VAL:O	1:E:1032:LEU:HD13	2.15	0.47
1:A:964:ARG:NH1	1:A:964:ARG:CG	2.73	0.47
1:A:1053:PRO:C	1:A:1055:GLN:N	2.67	0.47
1:E:1067:LYS:O	1:E:1068:ASN:C	2.50	0.47
2:F:24:VAL:HG23	2:F:167:VAL:HG11	1.97	0.47
1:A:728:LEU:HB2	1:A:733:ILE:HD11	1.97	0.47
1:A:868:ARG:HB3	2:B:5:ARG:HH22	1.79	0.47
1:A:987:LEU:HB2	1:A:994:VAL:HG22	1.96	0.47
1:A:900:THR:CG2	1:A:902:GLU:HB3	2.45	0.47
1:E:1010:LYS:HG3	1:E:1021:THR:HA	1.96	0.47
1:E:972:LEU:HD23	1:E:1061:ALA:HA	1.95	0.47
1:E:822:ARG:HH21	1:E:826:GLN:NE2	2.11	0.46
1:A:721:GLY:CA	1:A:724:VAL:HG12	2.36	0.46
1:E:816:ARG:HD3	1:E:816:ARG:C	2.34	0.46
1:A:749:HIS:HE1	1:A:878:GLU:OE1	1.99	0.46
1:A:854:GLN:CG	4:A:1235:HOH:O	2.61	0.46
1:E:964:ARG:NH1	1:E:964:ARG:CG	2.74	0.46
2:B:16:CYS:O	2:B:16:CYS:SG	2.74	0.46
2:B:179:LEU:O	2:B:180:GLN:C	2.54	0.46
1:E:1010:LYS:HE3	1:E:1021:THR:C	2.36	0.45
1:A:1047:CYS:HB2	1:A:1053:PRO:HD2	1.97	0.45
1:A:869:LEU:HB3	1:A:873:ASP:HB2	1.97	0.45
1:A:734:ASP:HB3	1:A:895:HIS:CE1	2.52	0.45
1:A:856:PHE:CD1	1:A:856:PHE:C	2.89	0.45
1:E:1044:PHE:CE1	1:E:1058:GLU:CB	2.98	0.45
1:A:996:LEU:HD23	1:A:1005:LEU:HD13	1.98	0.45
1:E:1067:LYS:C	1:E:1069:THR:N	2.68	0.45
2:B:15:ALA:O	2:B:118:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:LYS:HG2	2:B:135:LYS:O	2.17	0.45
1:E:1061:ALA:CB	1:E:1067:LYS:HB2	2.47	0.45
1:A:944:ALA:O	1:A:945:LEU:HD12	2.17	0.45
1:E:1053:PRO:O	1:E:1054:PRO:C	2.52	0.45
1:E:1066:ASP:O	1:E:1069:THR:CA	2.64	0.45
2:F:29:GLN:HE21	2:F:29:GLN:HB2	1.61	0.44
2:B:168:ARG:NH2	2:B:168:ARG:CG	2.77	0.44
1:E:1075:GLU:O	1:E:1079:ARG:HD3	2.17	0.44
1:E:915:GLU:HG3	4:E:1208:HOH:O	2.16	0.44
2:F:5:ARG:CD	4:F:201:HOH:O	2.63	0.44
2:B:70:ARG:N	2:B:71:PRO:CD	2.80	0.44
2:B:128:ARG:HH11	2:B:128:ARG:CB	2.26	0.44
1:A:941:ASP:OD1	1:A:943:THR:HB	2.18	0.43
1:A:717:GLN:HG3	1:A:737:GLU:OE2	2.19	0.43
1:A:868:ARG:HB3	2:B:5:ARG:NH2	2.33	0.43
1:A:1005:LEU:HD12	1:A:1005:LEU:HA	1.73	0.43
1:E:764:MET:HA	1:E:769:LEU:HD12	2.01	0.43
1:E:788:ILE:HD12	1:E:828:VAL:HG11	2.01	0.43
2:B:119:LYS:C	2:B:121:LEU:H	2.21	0.43
2:B:131:LEU:O	2:B:136:GLN:N	2.48	0.43
1:E:776:ALA:O	1:E:780:PRO:HA	2.19	0.43
1:E:1042:ALA:H	1:E:1067:LYS:CG	2.14	0.43
2:F:166:GLY:O	2:F:170:VAL:HG23	2.19	0.43
2:B:122:ARG:NH1	2:B:139:VAL:O	2.44	0.43
1:E:749:HIS:HE1	1:E:878:GLU:OE1	2.02	0.43
1:E:1025:VAL:C	1:E:1026:LEU:HD12	2.38	0.43
1:A:788:ILE:HD11	1:A:824:GLU:HG2	2.00	0.42
1:E:1041:ARG:O	1:E:1060:VAL:HG13	2.20	0.42
2:B:122:ARG:NH2	2:B:158:GLU:OE1	2.45	0.42
2:F:16:CYS:O	2:F:16:CYS:SG	2.76	0.42
2:B:113:ILE:O	2:B:113:ILE:HG13	2.17	0.42
1:A:724:VAL:HG22	1:A:805:ILE:HD11	2.01	0.42
1:A:816:ARG:HD2	1:A:825:LEU:HD22	2.00	0.42
2:B:10:ILE:HG21	2:B:22:LEU:HD11	2.00	0.42
2:B:87:ASP:OD1	2:B:87:ASP:C	2.58	0.42
1:A:721:GLY:O	1:A:725:VAL:HB	2.19	0.42
1:A:856:PHE:CE1	1:A:857:MET:CE	3.02	0.42
1:A:974:TRP:O	1:A:976:ILE:N	2.52	0.42
2:F:71:PRO:HA	2:F:74:TYR:CD2	2.55	0.42
1:A:729:THR:OG1	1:A:730:GLN:N	2.53	0.42
2:B:93:GLU:OE1	2:B:93:GLU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:THR:O	2:B:164:LYS:HB2	2.20	0.42
2:B:71:PRO:HA	2:B:74:TYR:CD2	2.54	0.42
1:E:1062:LEU:O	1:E:1063:THR:HG23	2.20	0.42
2:F:87:ASP:OD1	2:F:87:ASP:C	2.59	0.42
2:B:126:HIS:ND1	2:B:126:HIS:C	2.73	0.41
1:E:1044:PHE:CD1	1:E:1058:GLU:HA	2.55	0.41
2:B:126:HIS:ND1	2:B:126:HIS:O	2.52	0.41
1:E:1041:ARG:O	1:E:1041:ARG:CG	2.64	0.41
1:E:1067:LYS:O	1:E:1069:THR:N	2.53	0.41
2:F:117:ASN:HD22	2:F:117:ASN:HA	1.71	0.41
1:A:943:THR:O	1:A:943:THR:HG23	2.19	0.41
1:E:863:HIS:HD2	1:E:865:GLN:H	1.68	0.41
1:E:991:ASP:OD1	1:E:991:ASP:N	2.47	0.41
1:A:1000:ASP:HB3	1:A:1001:GLU:H	1.58	0.41
1:E:1005:LEU:HD22	1:E:1024:PRO:HG2	2.02	0.41
2:B:17:GLY:CA	3:B:201:GOL:H2	2.51	0.41
2:F:119:LYS:C	2:F:121:LEU:H	2.24	0.41
2:B:142:GLU:O	2:B:146:ASP:OD2	2.38	0.41
2:B:35:VAL:HA	2:B:36:PRO:HD3	1.92	0.41
2:B:85:SER:OG	2:B:118:LYS:HD2	2.21	0.41
1:E:986:VAL:HG22	1:E:1070:TRP:CH2	2.55	0.41
1:E:1031:VAL:HA	1:E:1046:ILE:O	2.20	0.41
1:E:1078:VAL:HG13	1:E:1079:ARG:N	2.36	0.41
2:B:6:LYS:HD2	2:B:178:ALA:HB1	2.03	0.41
2:B:129:ARG:O	2:B:130:GLU:C	2.59	0.40
1:E:1041:ARG:HG3	1:E:1060:VAL:CG1	2.50	0.40
2:F:8:LEU:C	2:F:8:LEU:HD23	2.42	0.40
1:E:822:ARG:NH2	1:E:826:GLN:HE22	2.16	0.40
1:E:976:ILE:CD1	1:E:982:LEU:HD12	2.48	0.40
1:A:986:VAL:HG22	1:A:1070:TRP:CH2	2.57	0.40
1:A:872:ARG:HA	1:A:875:ILE:HG22	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:GLU:OE1	2:F:176:ARG:NH1[1_455]	2.05	0.15
1:A:823:GLU:OE2	2:F:176:ARG:NH1[1_455]	2.10	0.10

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	352/369 (95%)	324 (92%)	26 (7%)	2 (1%)	25	43
1	E	354/369 (96%)	327 (92%)	25 (7%)	2 (1%)	25	43
2	B	176/181 (97%)	167 (95%)	9 (5%)	0	100	100
2	F	176/181 (97%)	169 (96%)	7 (4%)	0	100	100
All	All	1058/1100 (96%)	987 (93%)	67 (6%)	4 (0%)	34	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	1049	SER
1	A	975	ARG
1	A	979	ASP
1	E	1054	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	324/335 (97%)	306 (94%)	18 (6%)	21	40
1	E	326/335 (97%)	302 (93%)	24 (7%)	13	27
2	B	156/157 (99%)	150 (96%)	6 (4%)	33	58
2	F	156/157 (99%)	150 (96%)	6 (4%)	33	58
All	All	962/984 (98%)	908 (94%)	54 (6%)	21	40

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	788	ILE
1	A	793	CYS
1	A	808	GLU
1	A	816	ARG
1	A	842	LEU
1	A	943	THR
1	A	945	LEU
1	A	949	SER
1	A	950	ASN
1	A	964	ARG
1	A	990	GLU
1	A	994	VAL
1	A	997	GLN
1	A	998	LYS
1	A	1000	ASP
1	A	1035	SER
1	A	1066	ASP
1	A	1067	LYS
2	B	41	ASN
2	B	101	PRO
2	B	113	ILE
2	B	125	GLU
2	B	142	GLU
2	B	168	ARG
1	E	714	GLN
1	E	724	VAL
1	E	758	LEU
1	E	793	CYS
1	E	806	ILE
1	E	816	ARG
1	E	822	ARG
1	E	890	GLU
1	E	897	GLU
1	E	915	GLU
1	E	945	LEU
1	E	959	LEU
1	E	964	ARG
1	E	986	VAL
1	E	1006	LYS
1	E	1026	LEU
1	E	1032	LEU
1	E	1038	THR

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Mol	Chain	Res	Type
1	E	1046	ILE
1	E	1050	LYS
1	E	1051	LEU
1	E	1064	SER
1	E	1066	ASP
1	E	1076	GLU
2	F	26	SER
2	F	29	GLN
2	F	35	VAL
2	F	113	ILE
2	F	125	GLU
2	F	168	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	715	ASN
1	A	749	HIS
1	A	880	GLN
1	A	895	HIS
1	A	950	ASN
1	A	968	HIS
1	A	1008	HIS
1	A	1068	ASN
2	B	41	ASN
1	E	718	HIS
1	E	749	HIS
1	E	826	GLN
1	E	880	GLN
1	E	895	HIS
1	E	926	GLN
1	E	937	GLN
1	E	997	GLN
1	E	1055	GLN
2	F	29	GLN
2	F	41	ASN
2	F	117	ASN

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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	1101	-	5,5,5	0.52	0	5,5,5	0.81	0
3	GOL	E	1101	-	5,5,5	0.24	0	5,5,5	0.79	0
3	GOL	A	1102	-	5,5,5	1.13	0	5,5,5	1.30	1 (20%)
3	GOL	B	201	-	5,5,5	0.54	0	5,5,5	1.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1101	-	-	0/4/4/4	-
3	GOL	E	1101	-	-	2/4/4/4	-
3	GOL	A	1102	-	-	2/4/4/4	-
3	GOL	B	201	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1102	GOL	O3-C3-C2	-2.11	100.10	110.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	GOL	O1-C1-C2-C3
3	B	201	GOL	O1-C1-C2-C3
3	A	1102	GOL	O1-C1-C2-O2
3	E	1101	GOL	O2-C2-C3-O3
3	B	201	GOL	O1-C1-C2-O2
3	E	1101	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	GOL	1	0
3	E	1101	GOL	1	0
3	B	201	GOL	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 (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	356/369 (96%)	0.22	24 (6%)	17	18	22, 47, 99, 135	0
1	E	358/369 (97%)	0.23	26 (7%)	15	15	25, 49, 108, 127	0
2	B	178/181 (98%)	0.06	9 (5%)	28	29	24, 42, 80, 110	0
2	F	178/181 (98%)	0.02	7 (3%)	39	42	25, 44, 80, 100	0
All	All	1070/1100 (97%)	0.16	66 (6%)	20	21	22, 46, 97, 135	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	949	SER	6.4
1	A	947	ARG	5.8
1	E	1051	LEU	5.7
2	F	132	ALA	5.4
1	E	979	ASP	5.2
2	F	134	MET	4.9
1	A	951	PRO	4.7
2	B	135	LYS	4.7
1	A	952	LEU	4.7
1	A	720	VAL	4.6
1	E	952	LEU	4.5
1	A	1038	THR	4.2
1	A	726	ALA	4.2
1	E	946	GLU	4.0
1	A	1051	LEU	3.9
1	A	714	GLN	3.8
1	E	1050	LYS	3.7
1	A	723	ASP	3.7
1	E	1053	PRO	3.7
1	E	722	LYS	3.6
1	E	1041	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	948	ALA	3.5
1	A	1055	GLN	3.5
2	F	133	LYS	3.4
1	A	722	LYS	3.4
1	A	950	ASN	3.3
2	B	132	ALA	3.3
1	A	979	ASP	3.3
1	E	723	ASP	3.3
1	E	1009	SER	3.3
1	E	1062	LEU	3.3
1	E	1080	ASN	3.2
1	E	1040	LYS	3.2
1	E	949	SER	3.0
2	F	135	LYS	3.0
2	B	3	ALA	2.9
1	A	721	GLY	2.9
1	E	721	GLY	2.8
1	E	1079	ARG	2.8
1	A	719	THR	2.7
1	A	946	GLU	2.7
2	F	126	HIS	2.7
2	F	129	ARG	2.6
1	E	1060	VAL	2.6
1	E	1069	THR	2.6
1	A	981	THR	2.6
2	B	134	MET	2.5
1	E	951	PRO	2.5
1	A	978	LYS	2.5
1	A	724	VAL	2.5
1	E	714	GLN	2.4
2	B	123	ASN	2.4
1	A	1040	LYS	2.4
1	E	1000	ASP	2.4
1	A	1037	ALA	2.4
1	E	1043	PHE	2.3
2	F	130	GLU	2.3
1	A	1049	SER	2.3
1	E	947	ARG	2.2
2	B	125	GLU	2.2
1	E	1042	ALA	2.2
2	B	124	ASP	2.2
2	B	129	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	32	GLU	2.1
1	E	1052	GLY	2.0
1	E	978	LYS	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
3	GOL	B	201	6/6	0.89	0.17	42,50,57,66	0
3	GOL	A	1102	6/6	0.93	0.15	29,32,34,35	0
3	GOL	E	1101	6/6	0.94	0.14	40,49,50,57	0
3	GOL	A	1101	6/6	0.98	0.10	39,41,45,46	0

6.5 Other polymers (i)

There are no such residues in this entry.