Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:26 am BST

PDB ID	:	3FQD
Title	:	Crystal Structure of the S. pombe Rat1-Rai1 Complex
Authors	:	Xiang, S.; Tong, L.
Deposited on	:	2009-01-07
Resolution	:	2.20 Å(reported)

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

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

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

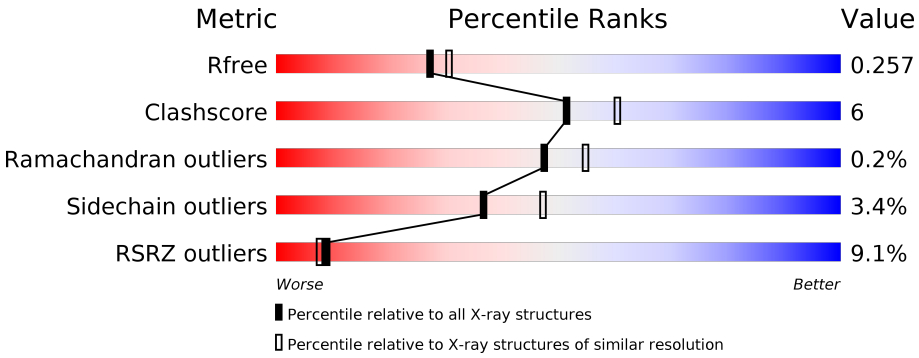
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	899	9% 64% 11% • 24%
2	B	352	3% 77% 16% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8926 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 5'-3' exoribonuclease 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	682	5550	3553	946	1029	7	15	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	EXPRESSION TAG	UNP P40848
A	0	ALA	-	EXPRESSION TAG	UNP P40848
A	0A	SER	-	EXPRESSION TAG	UNP P40848
A	886	ALA	-	EXPRESSION TAG	UNP P40848
A	887	ALA	-	EXPRESSION TAG	UNP P40848
A	888	ALA	-	EXPRESSION TAG	UNP P40848
A	889	LEU	-	EXPRESSION TAG	UNP P40848
A	890	GLU	-	EXPRESSION TAG	UNP P40848
A	891	HIS	-	EXPRESSION TAG	UNP P40848
A	892	HIS	-	EXPRESSION TAG	UNP P40848
A	893	HIS	-	EXPRESSION TAG	UNP P40848
A	894	HIS	-	EXPRESSION TAG	UNP P40848
A	895	HIS	-	EXPRESSION TAG	UNP P40848
A	896	HIS	-	EXPRESSION TAG	UNP P40848

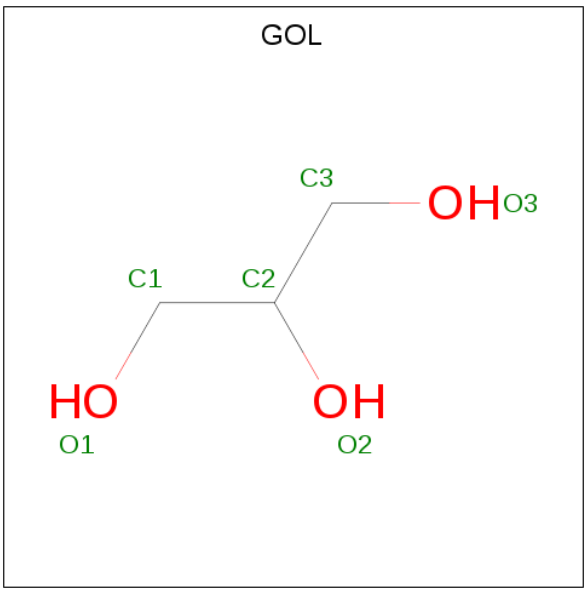
- Molecule 2 is a protein called Protein din1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	332	2721	1755	452	496	7	11	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	B	1	1	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

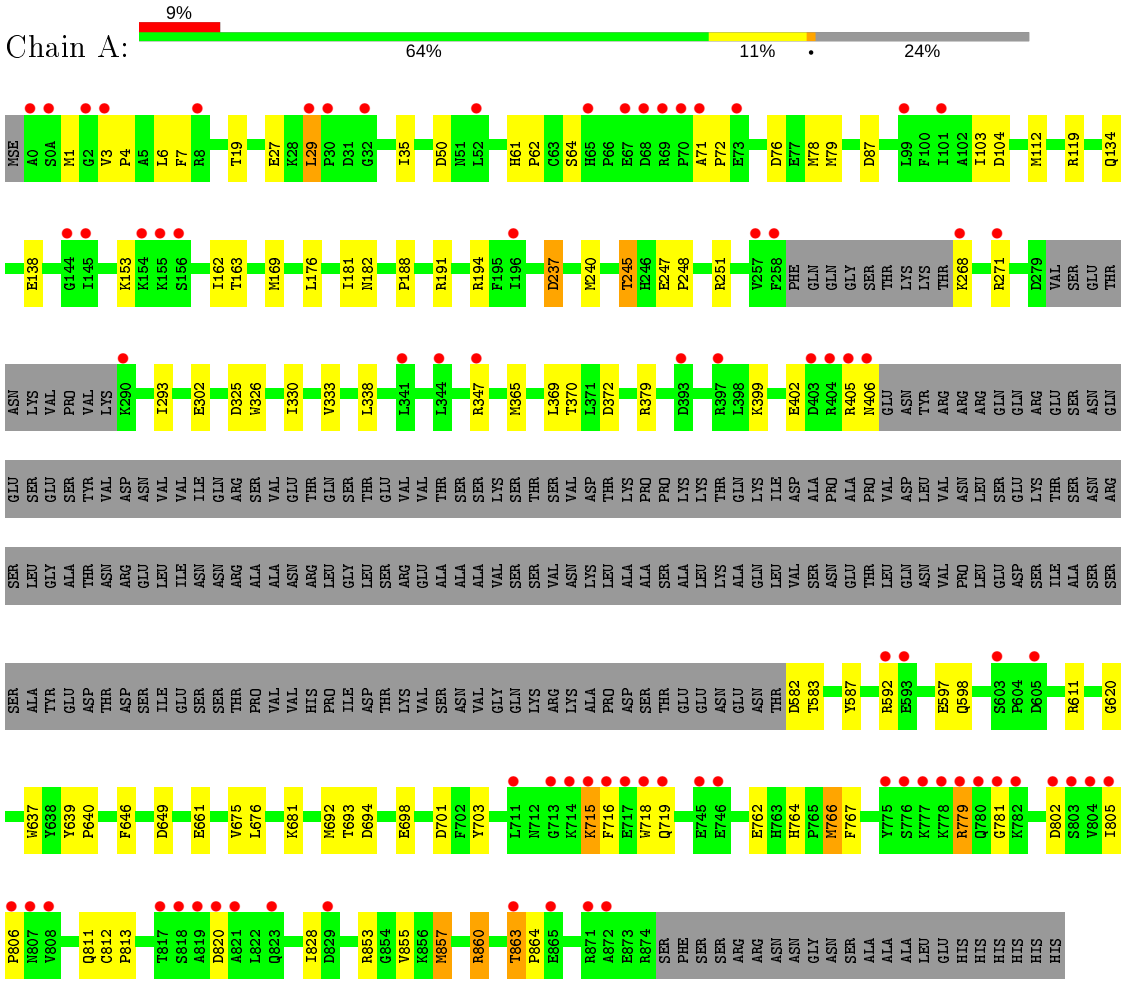
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	387	Total O 387 387	0	0
5	B	261	Total O 261 261	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

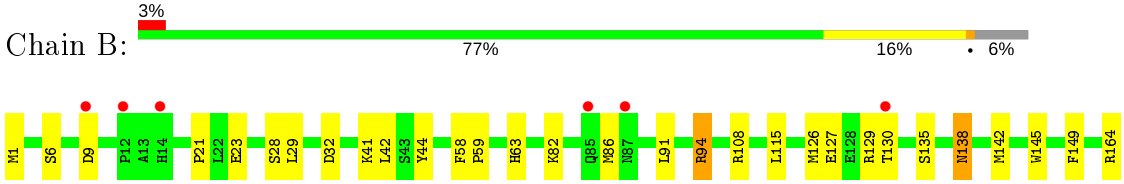
- Molecule 1: 5'-3' exoribonuclease 2

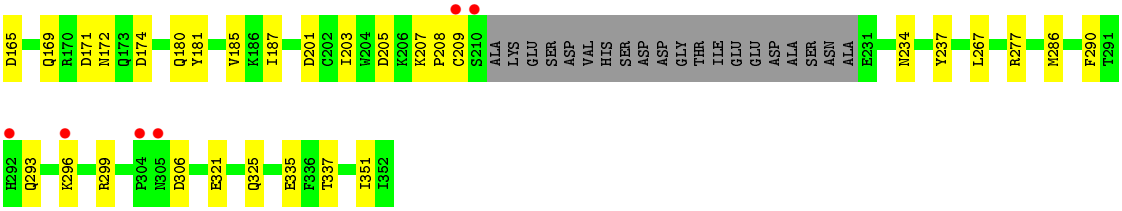
Chain A:



- Molecule 2: Protein din1

Chain B:




D165
Q169
R170
D171
N172
Q173
D174
Q180
Y181
V185
K186
I187
D201
C202
I203
W204
D205
K206
K207
P208
C209
S210
ALA
LYS
GLU
SER
ASP
VAL
HIS
SER
ASP
ASP
GLY
THR
ILE
GLU
GLU
ASP
ALA
SER
ASN
ALA
E231
N234
Y237
L267
R277
M286
F290
T291
H292
Q293
K296
R299
P304
M305
D306
E321
Q325
E335
F336
T337
I351
I352

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	96.69Å 190.87Å 84.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 28.75 – 2.16	Depositor EDS
% Data completeness (in resolution range)	94.3 (30.00-2.20) 90.7 (28.75-2.16)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.218 , 0.258 0.217 , 0.257	Depositor DCC
R_{free} test set	3924 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8926	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.37	1/5675 (0.0%)	0.69	13/7669 (0.2%)
2	B	0.37	0/2787	0.70	4/3767 (0.1%)
All	All	0.37	1/8462 (0.0%)	0.69	17/11436 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	ASN	C-O	7.11	1.36	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	694	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	820	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	701	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	802	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	372	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	582	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	50	ASP	CB-CG-OD2	5.35	123.11	118.30
2	B	201	ASP	CB-CG-OD2	5.27	123.04	118.30
2	B	171	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	76	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	87	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	237	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	649	ASP	CB-CG-OD2	5.03	122.83	118.30
2	B	165	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	369	LEU	CA-CB-CG	5.01	126.83	115.30
2	B	32	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

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	5550	0	5479	62	0
2	B	2721	0	2715	30	0
3	B	1	0	0	0	0
4	B	6	0	8	0	0
5	A	387	0	0	3	0
5	B	261	0	0	3	0
All	All	8926	0	8202	92	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 6.

All (92) 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:194:ARG:HD3	1:A:766:MSE:HE1	1.27	1.10
1:A:194:ARG:HD3	1:A:766:MSE:CE	2.05	0.86
1:A:194:ARG:CD	1:A:766:MSE:HE1	2.06	0.83
1:A:863:THR:HG22	1:A:864:PRO:HD2	1.62	0.81
1:A:857:MSE:HE3	1:A:857:MSE:HA	1.63	0.79
2:B:86:MSE:HE1	2:B:91:LEU:HD22	1.65	0.78
1:A:857:MSE:CE	1:A:857:MSE:HA	2.15	0.76
1:A:855:VAL:HG13	1:A:857:MSE:HE1	1.67	0.76
1:A:78:MSE:HG3	1:A:79:MSE:HE3	1.67	0.76
1:A:681:LYS:HD2	1:A:693:THR:HG21	1.70	0.74
2:B:23:GLU:HB2	2:B:234:ASN:HD21	1.52	0.74
2:B:203:ILE:HG22	2:B:237:TYR:HD2	1.56	0.71
1:A:855:VAL:HG13	1:A:857:MSE:CE	2.20	0.71
2:B:44:TYR:CE2	2:B:203:ILE:HD11	2.26	0.70
2:B:42:LEU:HD11	2:B:203:ILE:HG23	1.75	0.68
1:A:78:MSE:HG3	1:A:79:MSE:CE	2.23	0.68
1:A:692:MSE:HE3	1:A:703:TYR:CE2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLU:HB2	1:A:35:ILE:HB	1.80	0.64
1:A:370:THR:CG2	5:A:906:HOH:O	2.45	0.63
1:A:119:ARG:NH2	1:A:163:THR:OG1	2.32	0.63
1:A:365:MSE:HG2	1:A:379:ARG:HG2	1.80	0.62
2:B:203:ILE:HG22	2:B:237:TYR:CD2	2.34	0.62
2:B:94:ARG:NH2	5:B:1234:HOH:O	2.27	0.62
1:A:764:HIS:CE1	1:A:766:MSE:HE2	2.37	0.60
1:A:79:MSE:HE2	1:A:79:MSE:HA	1.84	0.60
2:B:42:LEU:HD11	2:B:203:ILE:CG2	2.32	0.59
1:A:620:GLY:HA2	1:A:637:TRP:CH2	2.38	0.59
1:A:1:MSE:SE	1:A:6:LEU:HB2	2.52	0.59
1:A:330:ILE:O	1:A:333:VAL:HG22	2.05	0.57
1:A:240:MSE:HE1	1:A:326:TRP:HZ3	1.70	0.57
1:A:857:MSE:CA	1:A:857:MSE:HE3	2.34	0.57
2:B:127:GLU:OE2	2:B:129:ARG:HD2	2.05	0.56
1:A:162:ILE:HA	1:A:169:MSE:HE3	1.88	0.55
2:B:296:LYS:HG2	2:B:299:ARG:HH12	1.71	0.55
1:A:779:ARG:HH11	1:A:781:GLY:HA3	1.71	0.55
1:A:583:THR:HB	1:A:598:GLN:HE22	1.71	0.55
2:B:115:LEU:HG	2:B:126:MSE:HG3	1.90	0.54
1:A:676:LEU:O	1:A:692:MSE:HE1	2.08	0.53
1:A:692:MSE:HE3	1:A:703:TYR:CD2	2.45	0.52
2:B:337:THR:HG22	5:B:900:HOH:O	2.08	0.52
2:B:82:LYS:HE3	5:B:1059:HOH:O	2.10	0.51
1:A:245:THR:HG22	1:A:247:GLU:H	1.76	0.51
1:A:134:GLN:HE22	1:A:153:LYS:HE2	1.77	0.50
1:A:592:ARG:HD3	1:A:646:PHE:CD1	2.46	0.50
2:B:142:MSE:HG2	2:B:145:TRP:CZ3	2.46	0.50
1:A:248:PRO:HG3	1:A:857:MSE:HE1	1.94	0.50
2:B:28:SER:HB3	2:B:41:LYS:HG2	1.94	0.50
1:A:863:THR:CG2	1:A:864:PRO:HD2	2.37	0.49
1:A:240:MSE:HE1	1:A:326:TRP:CZ3	2.47	0.48
2:B:169:GLN:NE2	2:B:172:ASN:HD22	2.11	0.48
1:A:64:SER:HA	1:A:78:MSE:HE1	1.95	0.48
2:B:21:PRO:HG3	2:B:187:ILE:HD12	1.94	0.48
1:A:181:ILE:HG22	1:A:828:ILE:HD13	1.96	0.48
1:A:583:THR:HB	1:A:598:GLN:NE2	2.29	0.47
1:A:399:LYS:HG3	1:A:587:TYR:CD2	2.48	0.47
1:A:3:VAL:HB	1:A:4:PRO:HD3	1.96	0.47
1:A:716:PHE:HD2	1:A:718:TRP:HD1	1.63	0.47
1:A:61:HIS:HB2	1:A:62:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:PHE:HZ	2:B:286:MSE:HE3	1.79	0.47
1:A:698:GLU:HG3	5:A:967:HOH:O	2.14	0.47
1:A:248:PRO:HG3	1:A:857:MSE:CE	2.45	0.47
2:B:149:PHE:CZ	2:B:286:MSE:HE3	2.50	0.47
1:A:762:GLU:HG2	1:A:767:PHE:CZ	2.51	0.46
1:A:112:MSE:HE1	5:A:1529:HOH:O	2.14	0.46
2:B:135:SER:O	2:B:138:ASN:HB2	2.16	0.45
1:A:188:PRO:HA	1:A:191:ARG:HD3	1.98	0.45
2:B:335:GLU:HB3	2:B:351:ILE:HD12	1.99	0.45
1:A:245:THR:CG2	1:A:247:GLU:H	2.30	0.44
2:B:63:HIS:HE1	2:B:174:ASP:OD2	2.00	0.44
1:A:338:LEU:HD21	1:A:620:GLY:HA3	1.99	0.43
2:B:138:ASN:HA	2:B:138:ASN:HD22	1.60	0.43
1:A:268:LYS:HA	1:A:271:ARG:HE	1.83	0.43
2:B:6:SER:HB3	2:B:9:ASP:HB2	2.01	0.43
2:B:29:LEU:HD12	2:B:180:GLN:HG3	2.01	0.43
2:B:58:PHE:HA	2:B:59:PRO:HA	1.71	0.43
2:B:181:TYR:HH	2:B:207:LYS:HZ2	1.62	0.43
1:A:716:PHE:HB3	1:A:718:TRP:CD1	2.54	0.43
1:A:639:TYR:HA	1:A:640:PRO:HD3	1.91	0.42
1:A:7:PHE:HE2	1:A:293:ILE:HD11	1.83	0.42
1:A:29:LEU:HD23	1:A:29:LEU:N	2.34	0.42
2:B:207:LYS:HA	2:B:208:PRO:HD2	1.92	0.42
1:A:812:CYS:HA	1:A:813:PRO:HD3	1.82	0.42
1:A:103:ILE:HD11	1:A:176:LEU:HD12	2.02	0.42
1:A:325:ASP:OD1	1:A:370:THR:HB	2.20	0.42
1:A:302:GLU:OE2	1:A:860:ARG:HG3	2.20	0.41
2:B:321:GLU:HG3	2:B:325:GLN:HE21	1.85	0.41
1:A:805:ILE:HA	1:A:806:PRO:HD3	1.94	0.41
1:A:715:LYS:HG2	1:A:719:GLN:HG3	2.01	0.41
1:A:134:GLN:O	1:A:138:GLU:HG2	2.20	0.41
1:A:71:ALA:HA	1:A:72:PRO:HD2	1.96	0.40
1:A:620:GLY:CA	1:A:637:TRP:CH2	3.04	0.40
2:B:290:PHE:O	2:B:293:GLN:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	674/899 (75%)	650 (96%)	23 (3%)	1 (0%)	51 60
2	B	328/352 (93%)	323 (98%)	4 (1%)	1 (0%)	41 46
All	All	1002/1251 (80%)	973 (97%)	27 (3%)	2 (0%)	47 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	209	CYS
1	A	715	LYS

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	613/791 (78%)	593 (97%)	20 (3%)	38 49
2	B	309/314 (98%)	298 (96%)	11 (4%)	35 45
All	All	922/1105 (83%)	891 (97%)	31 (3%)	37 47

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	29	LEU
1	A	182	ASN
1	A	237	ASP

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Mol	Chain	Res	Type
1	A	245	THR
1	A	251	ARG
1	A	347	ARG
1	A	402	GLU
1	A	405	ARG
1	A	597	GLU
1	A	611	ARG
1	A	661	GLU
1	A	675	VAL
1	A	766	MSE
1	A	779	ARG
1	A	811	GLN
1	A	853	ARG
1	A	857	MSE
1	A	860	ARG
1	A	863	THR
2	B	1	MSE
2	B	94	ARG
2	B	108	ARG
2	B	130	THR
2	B	138	ASN
2	B	164	ARG
2	B	185	VAL
2	B	205	ASP
2	B	267	LEU
2	B	277	ARG
2	B	306	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	134	GLN
1	A	182	ASN
1	A	598	GLN
1	A	682	ASN
2	B	63	HIS
2	B	138	ASN
2	B	169	GLN
2	B	173	GLN
2	B	234	ASN
2	B	318	HIS

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Mol	Chain	Res	Type
2	B	325	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	B	1001	-	5,5,5	0.40	0	5,5,5	0.10	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
4	GOL	B	1001	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1001	GOL	O1-C1-C2-C3

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	667/899 (74%)	0.50	78 (11%) 4 4	22, 45, 85, 119	0
2	B	321/352 (91%)	-0.05	12 (3%) 41 39	20, 31, 54, 66	0
All	All	988/1251 (78%)	0.32	90 (9%) 9 8	20, 39, 81, 119	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	806	PRO	10.3
1	A	716	PHE	8.2
1	A	805	ILE	7.9
2	B	210	SER	7.4
1	A	719	GLN	7.4
1	A	807	ASN	7.3
1	A	780	GLN	7.0
1	A	68	ASP	6.5
1	A	718	TRP	6.4
1	A	808	VAL	6.3
1	A	30	PRO	5.9
2	B	209	CYS	5.8
1	A	69	ARG	5.8
1	A	3	VAL	5.7
1	A	818	SER	5.6
1	A	714	LYS	5.5
1	A	715	LYS	4.9
1	A	802	ASP	4.7
1	A	829	ASP	4.6
1	A	404	ARG	4.6
1	A	779	ARG	4.5
1	A	605	ASP	4.3
1	A	778	LYS	4.3
1	A	405	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	781	GLY	4.2
1	A	154	LYS	4.2
1	A	820	ASP	4.1
1	A	67	GLU	4.1
1	A	713	GLY	3.9
1	A	872	ALA	3.9
2	B	304	PRO	3.9
1	A	341	LEU	3.7
1	A	268	LYS	3.6
1	A	865	GLU	3.5
1	A	155	LYS	3.5
1	A	0(A)	SER	3.5
2	B	87	ASN	3.4
1	A	777	LYS	3.4
1	A	70	PRO	3.4
2	B	305	ASN	3.3
1	A	803	SER	3.3
1	A	258	PHE	3.2
1	A	403	ASP	3.2
1	A	271	ARG	3.2
1	A	406	ASN	3.2
1	A	804	VAL	3.1
1	A	817	THR	3.1
1	A	290	LYS	3.1
1	A	821	ALA	3.1
1	A	196	ILE	3.0
1	A	71	ALA	3.0
1	A	257	VAL	3.0
2	B	12	PRO	3.0
1	A	32	GLY	2.9
1	A	397	ARG	2.9
1	A	145	ILE	2.8
1	A	745	GLU	2.8
1	A	819	ALA	2.8
2	B	14	HIS	2.8
1	A	863	THR	2.8
1	A	8	ARG	2.7
1	A	823	GLN	2.6
1	A	156	SER	2.6
1	A	871	ARG	2.6
2	B	85	GLN	2.6
1	A	782	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	717	GLU	2.5
1	A	2	GLY	2.4
1	A	344	LEU	2.4
1	A	603	SER	2.4
1	A	52	LEU	2.4
1	A	776	SER	2.4
1	A	347	ARG	2.3
2	B	296	LYS	2.3
1	A	775	TYR	2.3
1	A	29	LEU	2.2
1	A	99	LEU	2.2
1	A	393	ASP	2.1
1	A	593	GLU	2.1
2	B	292	HIS	2.1
1	A	144	GLY	2.1
1	A	65	HIS	2.1
2	B	9	ASP	2.1
1	A	592	ARG	2.1
1	A	101	ILE	2.0
1	A	73	GLU	2.0
1	A	746	GLU	2.0
2	B	130	THR	2.0
1	A	0	ALA	2.0
1	A	711	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	1001	6/6	0.84	0.13	59,59,60,60	0
3	MG	B	1000	1/1	0.95	0.07	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.