Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:36 AM GMT

PDB ID	:	2HT1
Title	:	The closed ring structure of the Rho transcription termination factor in complex with nucleic acid in the motor domains
Authors	:	Skordalakes, E.; Berger, J.M.
Deposited on	:	2006-07-24
Resolution	:	3.51 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

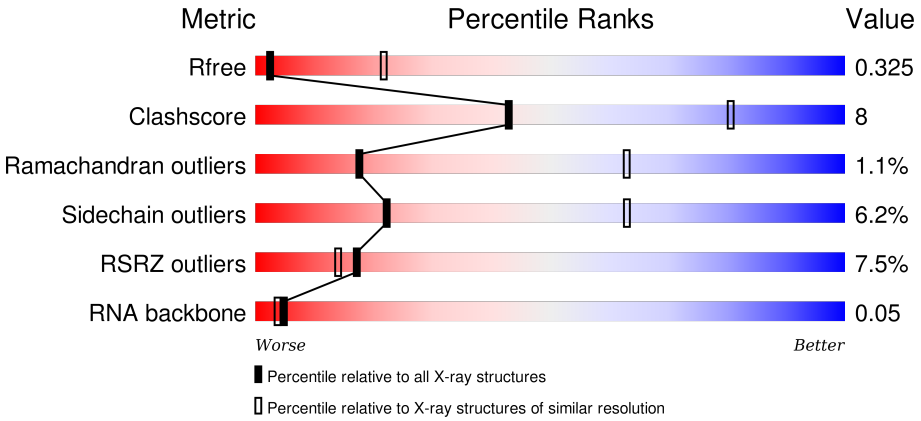
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.51 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}	91344	1089 (3.64-3.40)
Clashscore	102246	1197 (3.64-3.40)
Ramachandran outliers	100387	1159 (3.64-3.40)
Sidechain outliers	100360	1160 (3.64-3.40)
RSRZ outliers	91569	1096 (3.64-3.40)
RNA backbone	2183	1051 (4.22-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	J	2	100% 50% 50%
1	K	2	100% 50% 50%
2	M	5	100% 100%
3	A	433	6% 59% 14% • 25%

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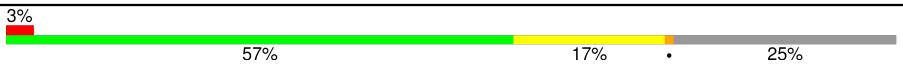
Mol	Chain	Length	Quality of chain
3	B	433	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5223 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 RNA chain called 5'-R(*UP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	2	Total	C	N	O	P	0	0	0
			37	18	5	13	1			
1	K	2	Total	C	N	O	P	0	0	0
			37	18	5	13	1			

- Molecule 2 is a RNA chain called 5'-R(*UP*CP*UP*CP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	5	Total	C	N	O	P	0	0	0
			97	45	12	36	4			

- Molecule 3 is a protein called Transcription termination factor rho.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	324	Total	C	N	O	S	0	0	0
			2521	1585	454	474	8			
3	B	324	Total	C	N	O	S	0	0	0
			2521	1585	454	474	8			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	INITIATING METHIONINE	UNP P0AG30
A	-20	GLY	-	CLONING ARTIFACT	UNP P0AG30
A	-19	SER	-	CLONING ARTIFACT	UNP P0AG30
A	-18	SER	-	CLONING ARTIFACT	UNP P0AG30
A	-17	HIS	-	EXPRESSION TAG	UNP P0AG30
A	-16	HIS	-	EXPRESSION TAG	UNP P0AG30
A	-15	HIS	-	EXPRESSION TAG	UNP P0AG30
A	-14	HIS	-	EXPRESSION TAG	UNP P0AG30
A	-13	HIS	-	EXPRESSION TAG	UNP P0AG30
A	-12	HIS	-	EXPRESSION TAG	UNP P0AG30

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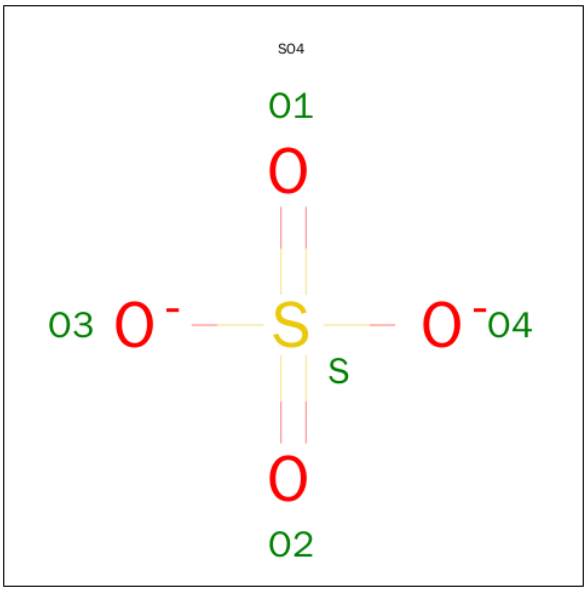
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	SER	-	CLONING ARTIFACT	UNP P0AG30
A	-10	SER	-	CLONING ARTIFACT	UNP P0AG30
A	-9	GLY	-	CLONING ARTIFACT	UNP P0AG30
A	-8	GLU	-	CLONING ARTIFACT	UNP P0AG30
A	-7	ASN	-	CLONING ARTIFACT	UNP P0AG30
A	-6	LEU	-	CLONING ARTIFACT	UNP P0AG30
A	-5	TYR	-	CLONING ARTIFACT	UNP P0AG30
A	-4	PHE	-	CLONING ARTIFACT	UNP P0AG30
A	-3	GLN	-	CLONING ARTIFACT	UNP P0AG30
A	-2	ALA	-	CLONING ARTIFACT	UNP P0AG30
A	-1	GLY	-	CLONING ARTIFACT	UNP P0AG30
A	0	HIS	-	CLONING ARTIFACT	UNP P0AG30
B	-21	MET	-	INITIATING METHIONINE	UNP P0AG30
B	-20	GLY	-	CLONING ARTIFACT	UNP P0AG30
B	-19	SER	-	CLONING ARTIFACT	UNP P0AG30
B	-18	SER	-	CLONING ARTIFACT	UNP P0AG30
B	-17	HIS	-	EXPRESSION TAG	UNP P0AG30
B	-16	HIS	-	EXPRESSION TAG	UNP P0AG30
B	-15	HIS	-	EXPRESSION TAG	UNP P0AG30
B	-14	HIS	-	EXPRESSION TAG	UNP P0AG30
B	-13	HIS	-	EXPRESSION TAG	UNP P0AG30
B	-12	HIS	-	EXPRESSION TAG	UNP P0AG30
B	-11	SER	-	CLONING ARTIFACT	UNP P0AG30
B	-10	SER	-	CLONING ARTIFACT	UNP P0AG30
B	-9	GLY	-	CLONING ARTIFACT	UNP P0AG30
B	-8	GLU	-	CLONING ARTIFACT	UNP P0AG30
B	-7	ASN	-	CLONING ARTIFACT	UNP P0AG30
B	-6	LEU	-	CLONING ARTIFACT	UNP P0AG30
B	-5	TYR	-	CLONING ARTIFACT	UNP P0AG30
B	-4	PHE	-	CLONING ARTIFACT	UNP P0AG30
B	-3	GLN	-	CLONING ARTIFACT	UNP P0AG30
B	-2	ALA	-	CLONING ARTIFACT	UNP P0AG30
B	-1	GLY	-	CLONING ARTIFACT	UNP P0AG30
B	0	HIS	-	CLONING ARTIFACT	UNP P0AG30

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	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 errors 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'-R(*UP*C)-3'

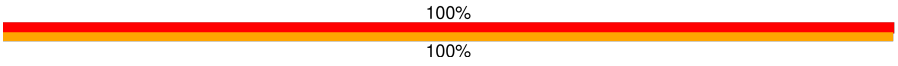
Chain J:

- Molecule 1: 5'-R(*UP*C)-3'

Chain K:

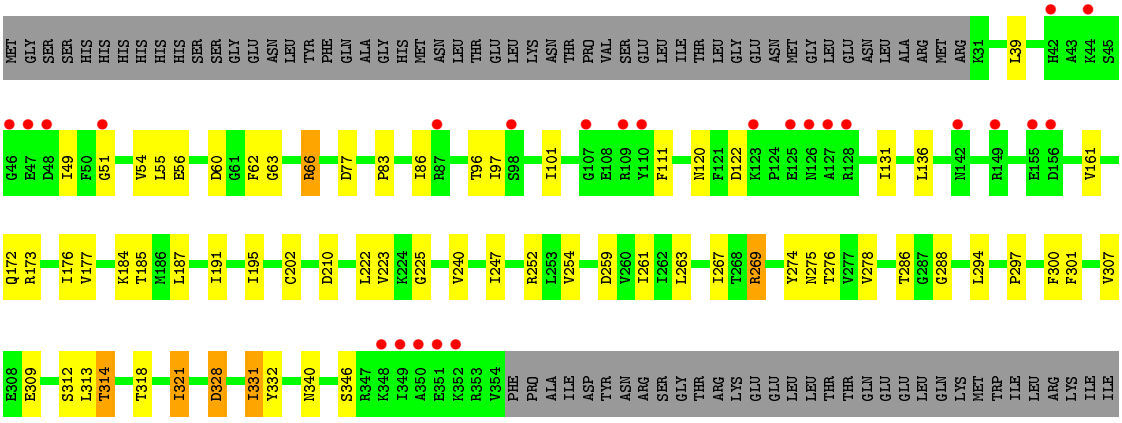
- Molecule 2: 5'-R(*UP*CP*UP*CP*U)-3'

Chain M:



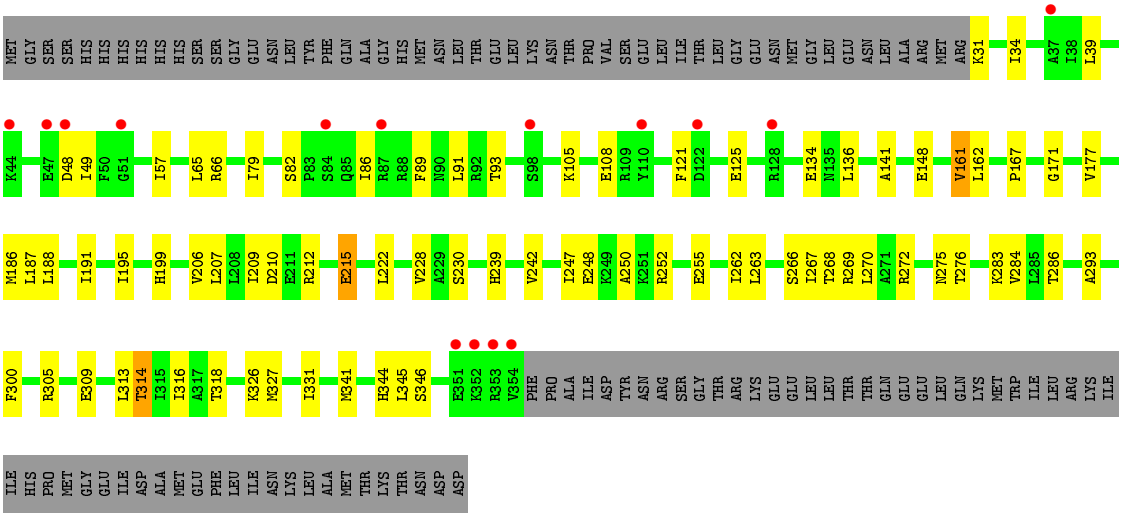
- Molecule 3: Transcription termination factor rho

Chain A:



• Molecule 3: Transcription termination factor rho

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α, β, γ	257.69Å 257.69Å 257.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.51 20.00 – 3.51	Depositor EDS
% Data completeness (in resolution range)	91.9 (20.00-3.51) 90.3 (20.00-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.294 , 0.328 0.275 , 0.325	Depositor DCC
R_{free} test set	854 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	108.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 114.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 16675 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5223	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4

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	J	0.71	0/40	1.37	0/60
1	K	0.74	0/40	1.24	0/60
2	M	0.72	0/106	1.27	0/162
3	A	0.33	0/2559	0.51	0/3450
3	B	0.33	0/2559	0.51	0/3450
All	All	0.35	0/5304	0.56	0/7182

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	37	0	23	1	0
1	K	37	0	23	0	0
2	M	97	0	54	12	0
3	A	2521	0	2580	35	0
3	B	2521	0	2580	41	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
All	All	5223	0	5260	86	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 8.

All (86) 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:M:3:U:C2'	2:M:4:C:H5"	1.87	1.04
2:M:3:U:C3'	2:M:4:C:H5"	1.93	0.99
2:M:3:U:O2'	2:M:4:C:H5"	1.65	0.94
2:M:2:C:H4'	2:M:3:U:OP1	1.68	0.93
3:A:66:ARG:HH11	3:A:66:ARG:HG2	1.36	0.89
2:M:3:U:C3'	2:M:4:C:C5'	2.58	0.81
2:M:2:C:C4'	2:M:3:U:OP1	2.29	0.79
2:M:3:U:H3'	2:M:4:C:C5'	2.13	0.77
3:B:266:SER:HB2	3:B:269:ARG:HB2	1.69	0.75
3:A:66:ARG:NH1	3:A:66:ARG:HG2	1.99	0.70
3:A:55:LEU:HB2	3:A:97:ILE:HD12	1.74	0.69
3:B:171:GLY:H	3:B:314:THR:HG22	1.58	0.68
3:A:56:GLU:O	3:A:63:GLY:HA3	1.95	0.67
3:B:188:LEU:HD22	3:B:263:LEU:HD21	1.77	0.66
3:A:39:LEU:HD22	3:A:49:ILE:HD12	1.76	0.66
3:B:316:ILE:HG13	3:B:316:ILE:O	1.94	0.66
3:B:161:VAL:HG21	3:B:191:ILE:HD12	1.77	0.66
2:M:1:U:H4'	2:M:2:C:OP1	1.92	0.63
3:A:223:VAL:HG12	3:A:225:GLY:H	1.64	0.61
3:B:89:PHE:HB2	3:B:91:LEU:HG	1.82	0.60
2:M:3:U:H3'	2:M:4:C:H5'	1.86	0.58
3:B:171:GLY:H	3:B:314:THR:CG2	2.16	0.57
3:A:39:LEU:HD12	3:A:111:PHE:CE1	2.40	0.57
3:B:39:LEU:HD22	3:B:49:ILE:HD12	1.87	0.56
3:A:83:PRO:HA	3:A:86:ILE:HD12	1.88	0.55
3:B:210:ASP:HB3	3:B:269:ARG:HG2	1.89	0.55
2:M:3:U:HO2'	2:M:4:C:H5"	1.71	0.55
3:B:263:LEU:HG	3:B:316:ILE:HD11	1.90	0.54
3:B:212:ARG:HB3	3:B:215:GLU:HB2	1.90	0.53
3:A:62:PHE:HB3	3:A:83:PRO:HG3	1.90	0.53
3:A:66:ARG:HH11	3:A:66:ARG:CG	2.16	0.52
3:A:191:ILE:O	3:A:195:ILE:HG12	2.10	0.52
3:A:321:ILE:HD11	3:A:332:TYR:CE2	2.45	0.52
3:B:272:ARG:HD3	3:B:327:MET:SD	2.50	0.51
3:A:254:VAL:HG21	3:A:313:LEU:HB2	1.92	0.51
3:A:261:ILE:HG12	3:A:314:THR:HG23	1.94	0.50
2:M:5:U:O5'	2:M:5:U:H6	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:252:ARG:NH1	3:B:255:GLU:OE2	2.44	0.49
3:B:162:LEU:HD11	3:B:195:ILE:HG13	1.95	0.49
3:B:247:ILE:HB	3:B:300:PHE:CE1	2.48	0.48
3:A:177:VAL:HG13	3:A:321:ILE:HD12	1.94	0.48
3:A:176:ILE:HB	3:A:318:THR:HG22	1.95	0.47
3:B:31:LYS:HA	3:B:34:ILE:HD12	1.95	0.47
1:J:2:C:H42	3:B:66:ARG:HH12	1.62	0.47
3:B:230:SER:OG	3:B:239:HIS:HD2	1.98	0.47
3:B:207:LEU:HA	3:B:228:VAL:O	2.15	0.47
3:B:65:LEU:HB2	3:B:79:ILE:HB	1.97	0.47
3:A:247:ILE:HB	3:A:300:PHE:CE1	2.50	0.46
3:B:136:LEU:HD22	3:B:309:GLU:HG3	1.96	0.46
3:B:268:THR:HA	3:B:331:ILE:HG21	1.98	0.46
3:A:54:VAL:HG22	3:A:96:THR:HA	1.97	0.46
3:A:136:LEU:HD23	3:A:307:VAL:HG21	1.97	0.46
3:B:57:ILE:H	3:B:93:THR:HB	1.80	0.46
3:A:278:VAL:O	3:B:283:LYS:NZ	2.49	0.46
3:B:82:SER:O	3:B:86:ILE:HG12	2.16	0.45
2:M:3:U:HO2'	2:M:4:C:H6	1.63	0.45
3:B:345:LEU:HB3	3:B:346:SER:H	1.68	0.44
3:A:187:LEU:O	3:A:191:ILE:HG12	2.16	0.44
3:A:184:LYS:HG3	3:A:185:THR:N	2.31	0.44
3:B:177:VAL:HB	3:B:344:HIS:HD2	1.83	0.44
3:B:275:ASN:HA	3:B:293:ALA:HB1	2.00	0.44
3:B:248:GLU:OE2	3:B:252:ARG:NH2	2.51	0.44
3:A:39:LEU:HD13	3:A:49:ILE:HG21	1.99	0.44
3:A:210:ASP:HB3	3:A:269:ARG:HG3	2.00	0.43
3:B:209:ILE:HD13	3:B:270:LEU:HB2	2.00	0.43
3:B:187:LEU:O	3:B:191:ILE:HG12	2.18	0.43
3:B:105:LYS:O	3:B:108:GLU:HB2	2.19	0.43
3:B:250:ALA:HB2	3:B:262:ILE:HD11	2.01	0.43
3:B:206:VAL:HG22	3:B:263:LEU:HB3	2.00	0.43
3:A:240:VAL:HG13	3:A:274:TYR:CE1	2.53	0.43
3:A:173:ARG:HB3	3:A:301:PHE:CZ	2.53	0.43
3:B:188:LEU:HD11	3:B:318:THR:HG21	2.01	0.43
3:A:161:VAL:HB	3:A:191:ILE:HD12	2.00	0.43
3:A:307:VAL:HG12	3:A:309:GLU:H	1.83	0.42
3:B:167:PRO:HD3	3:B:199:HIS:CE1	2.54	0.42
3:A:328:ASP:HA	3:A:331:ILE:HG22	2.01	0.41
3:A:294:LEU:O	3:A:297:PRO:HD2	2.21	0.41
3:B:187:LEU:HD11	3:B:191:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:272:ARG:O	3:B:276:THR:HG23	2.21	0.41
3:B:171:GLY:N	3:B:314:THR:HG22	2.32	0.41
3:A:259:ASP:HA	3:A:312:SER:H	1.86	0.41
3:A:321:ILE:HD11	3:A:332:TYR:CD2	2.56	0.40
3:A:172:GLN:H	3:A:314:THR:HB	1.86	0.40
3:A:269:ARG:HD2	3:A:269:ARG:HA	1.90	0.40
3:A:275:ASN:O	3:B:283:LYS:NZ	2.52	0.40
3:B:250:ALA:HB1	3:B:313:LEU:HD13	2.04	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	
3	A	322/433 (74%)	283 (88%)	36 (11%)	3 (1%)	21	67
3	B	322/433 (74%)	295 (92%)	23 (7%)	4 (1%)	16	61
All	All	644/866 (74%)	578 (90%)	59 (9%)	7 (1%)	17	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	121	PHE
3	B	125	GLU
3	B	141	ALA
3	A	346	SER
3	B	48	ASP
3	A	288	GLY
3	A	51	GLY

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
3	A	272/369 (74%)	252 (93%)	20 (7%)	17 56
3	B	272/369 (74%)	258 (95%)	14 (5%)	29 69
All	All	544/738 (74%)	510 (94%)	34 (6%)	22 63

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	60	ASP
3	A	66	ARG
3	A	77	ASP
3	A	101	ILE
3	A	120	ASN
3	A	122	ASP
3	A	131	ILE
3	A	202	CYS
3	A	222	LEU
3	A	252	ARG
3	A	263	LEU
3	A	267	ILE
3	A	269	ARG
3	A	276	THR
3	A	286	THR
3	A	314	THR
3	A	321	ILE
3	A	328	ASP
3	A	331	ILE
3	A	340	ASN
3	B	134	GLU
3	B	148	GLU
3	B	161	VAL
3	B	186	MET
3	B	215	GLU
3	B	222	LEU
3	B	242	VAL

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Mol	Chain	Res	Type
3	B	267	ILE
3	B	284	VAL
3	B	286	THR
3	B	305	ARG
3	B	314	THR
3	B	326	LYS
3	B	341	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	32	GLN
3	B	90	ASN
3	B	198	ASN
3	B	199	HIS
3	B	239	HIS
3	B	344	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	J	1/2 (50%)	0	0
1	K	1/2 (50%)	1 (100%)	0
2	M	5/5 (100%)	4 (80%)	2 (40%)
All	All	7/9 (77%)	5 (71%)	2 (28%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	K	2	C
2	M	2	C
2	M	3	U
2	M	4	C
2	M	5	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	M	1	U
2	M	2	C

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
4	SO4	A	600	-	4,4,4	0.20	0	6,6,6	0.08	0
4	SO4	B	601	-	4,4,4	0.21	0	6,6,6	0.08	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	SO4	A	600	-	-	0/0/0/0	0/0/0/0
4	SO4	B	601	-	-	0/0/0/0	0/0/0/0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	J	2/2 (100%)	4.53	2 (100%)	0	0	198, 198, 198, 216	0
1	K	2/2 (100%)	3.75	2 (100%)	0	0	210, 210, 210, 231	0
2	M	5/5 (100%)	7.67	5 (100%)	0	0	100, 104, 130, 175	5 (100%)
3	A	324/433 (74%)	-0.07	25 (7%)	16	13	66, 115, 211, 266	0
3	B	324/433 (74%)	-0.20	15 (4%)	36	28	66, 89, 204, 247	0
All	All	657/875 (75%)	-0.05	49 (7%)	17	14	66, 101, 210, 266	5 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	4	C	11.1
2	M	1	U	10.4
2	M	2	C	7.1
3	B	354	VAL	6.9
3	A	98	SER	6.2
3	B	48	ASP	6.0
2	M	5	U	5.6
3	A	51	GLY	5.4
3	A	47	GLU	5.2
1	J	1	U	5.1
3	B	51	GLY	4.9
3	A	149	ARG	4.9
3	B	353	ARG	4.3
2	M	3	U	4.2
3	A	156	ASP	4.1
1	K	1	U	4.0
1	J	2	C	3.9
3	A	48	ASP	3.9
3	A	349	ILE	3.8
3	B	122	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
3	A	42	HIS	3.5
1	K	2	C	3.5
3	B	351	GLU	3.2
3	B	47	GLU	3.1
3	A	348	LYS	3.0
3	B	352	LYS	2.9
3	A	125	GLU	2.9
3	A	126	ASN	2.8
3	B	128	ARG	2.8
3	A	352	LYS	2.7
3	A	127	ALA	2.7
3	A	350	ALA	2.6
3	A	155	GLU	2.4
3	A	351	GLU	2.4
3	B	37	ALA	2.4
3	B	98	SER	2.4
3	A	110	TYR	2.4
3	A	142	ASN	2.4
3	A	44	LYS	2.4
3	A	123	LYS	2.2
3	A	107	GLY	2.2
3	B	84	SER	2.2
3	B	110	TYR	2.2
3	A	46	GLY	2.2
3	A	87	ARG	2.1
3	A	128	ARG	2.1
3	A	109	ARG	2.0
3	B	44	LYS	2.0
3	B	87	ARG	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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	B	601	5/5	0.96	0.20	0.43	94,94,94,94	0
4	SO4	A	600	5/5	0.91	0.18	0.39	99,99,99,99	0

6.5 Other polymers

There are no such residues in this entry.