Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 09:03 AM EDT

PDB ID	:	4GJI
Title	:	Crystal structure of Pseudomonas stutzeri L-rhamnose isomerase mutant H101N in complex with L-rhamnopyranose
Authors	:	Yoshida, H.; Kamitori, S.
Deposited on	:	2012-08-09
Resolution	:	1.70 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:

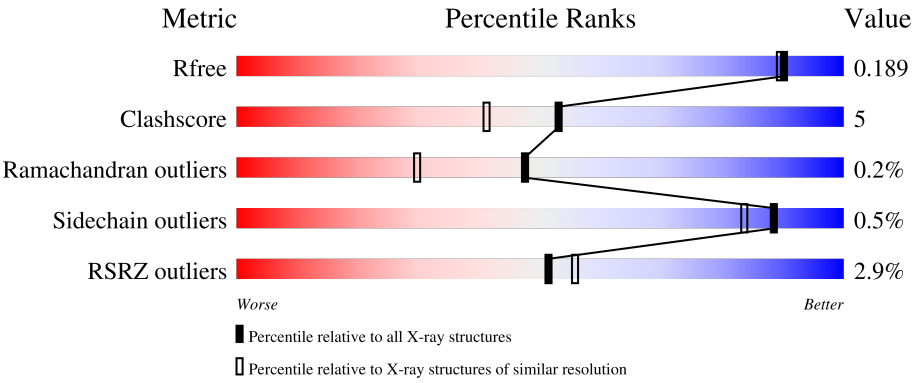
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	438	2% 87% 9% .
1	B	438	2% 84% 12% .
1	C	438	6% 83% 14% .
1	D	438	% 86% 9% .

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15195 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 L-rhamnose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	4	0
			3269	2050	586	623	10			
1	B	421	Total	C	N	O	S	0	4	0
			3269	2050	586	623	10			
1	C	427	Total	C	N	O	S	0	4	0
			3302	2069	592	631	10			
1	D	419	Total	C	N	O	S	0	4	0
			3260	2044	584	622	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	ASN	HIS	engineered mutation	UNP Q75WH8
A	150	ASN	ASP	engineered mutation	UNP Q75WH8
A	431	GLY	-	expression tag	UNP Q75WH8
A	432	SER	-	expression tag	UNP Q75WH8
A	433	HIS	-	expression tag	UNP Q75WH8
A	434	HIS	-	expression tag	UNP Q75WH8
A	435	HIS	-	expression tag	UNP Q75WH8
A	436	HIS	-	expression tag	UNP Q75WH8
A	437	HIS	-	expression tag	UNP Q75WH8
A	438	HIS	-	expression tag	UNP Q75WH8
B	101	ASN	HIS	engineered mutation	UNP Q75WH8
B	150	ASN	ASP	engineered mutation	UNP Q75WH8
B	431	GLY	-	expression tag	UNP Q75WH8
B	432	SER	-	expression tag	UNP Q75WH8
B	433	HIS	-	expression tag	UNP Q75WH8
B	434	HIS	-	expression tag	UNP Q75WH8
B	435	HIS	-	expression tag	UNP Q75WH8
B	436	HIS	-	expression tag	UNP Q75WH8
B	437	HIS	-	expression tag	UNP Q75WH8
B	438	HIS	-	expression tag	UNP Q75WH8
C	101	ASN	HIS	engineered mutation	UNP Q75WH8

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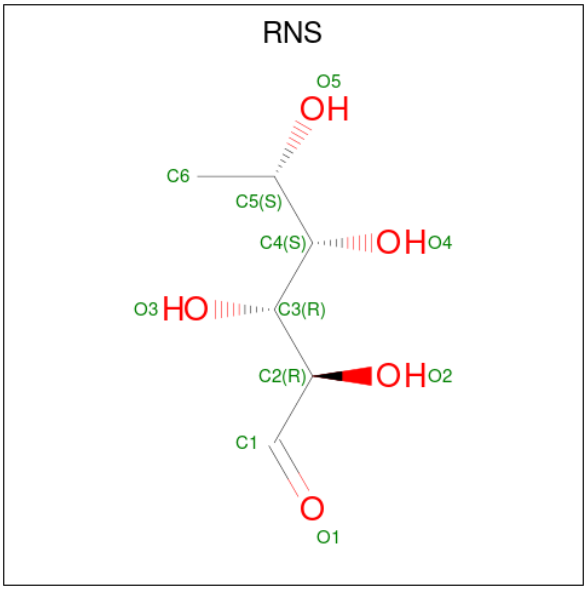
Chain	Residue	Modelled	Actual	Comment	Reference
C	150	ASN	ASP	engineered mutation	UNP Q75WH8
C	431	GLY	-	expression tag	UNP Q75WH8
C	432	SER	-	expression tag	UNP Q75WH8
C	433	HIS	-	expression tag	UNP Q75WH8
C	434	HIS	-	expression tag	UNP Q75WH8
C	435	HIS	-	expression tag	UNP Q75WH8
C	436	HIS	-	expression tag	UNP Q75WH8
C	437	HIS	-	expression tag	UNP Q75WH8
C	438	HIS	-	expression tag	UNP Q75WH8
D	101	ASN	HIS	engineered mutation	UNP Q75WH8
D	150	ASN	ASP	engineered mutation	UNP Q75WH8
D	431	GLY	-	expression tag	UNP Q75WH8
D	432	SER	-	expression tag	UNP Q75WH8
D	433	HIS	-	expression tag	UNP Q75WH8
D	434	HIS	-	expression tag	UNP Q75WH8
D	435	HIS	-	expression tag	UNP Q75WH8
D	436	HIS	-	expression tag	UNP Q75WH8
D	437	HIS	-	expression tag	UNP Q75WH8
D	438	HIS	-	expression tag	UNP Q75WH8

- Molecule 2 is L-RHAMNOSE (three-letter code: RNS) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	1
			11	6	5		

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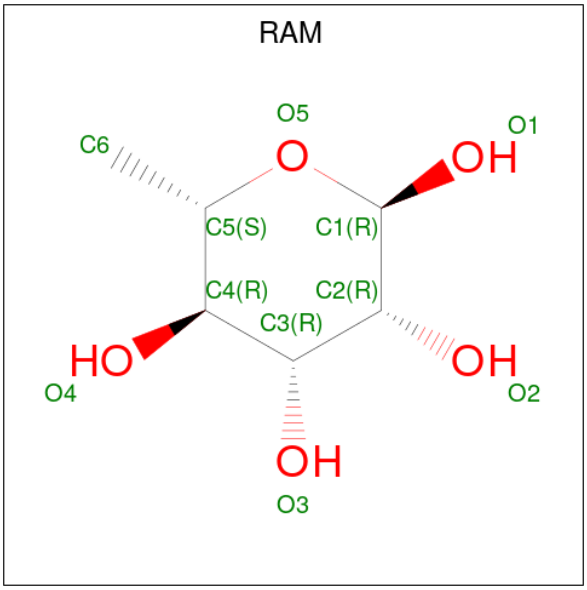
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 11 6 5	0	0
2	D	1	Total C O 11 6 5	0	1

- Molecule 3 is alpha-L-rhamnopyranose (three-letter code: RAM) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	C	1	Total C O 11 6 5	0	0
3	D	1	Total C O 11 6 5	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mn 2 2	0	0
4	B	2	Total Mn 2 2	0	0
4	C	3	Total Mn 3 3	0	0

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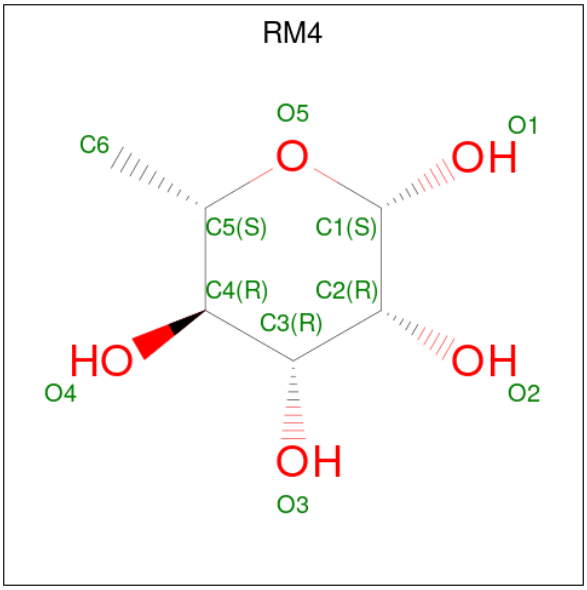
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	3	Total Mn 3 3	0	0

- Molecule 5 is beta-L-rhamnopyranose (three-letter code: RM4) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 11 6 5	0	1
5	B	1	Total C O 11 6 5	0	0
5	D	1	Total C O 11 6 5	0	1

- Molecule 6 is water.

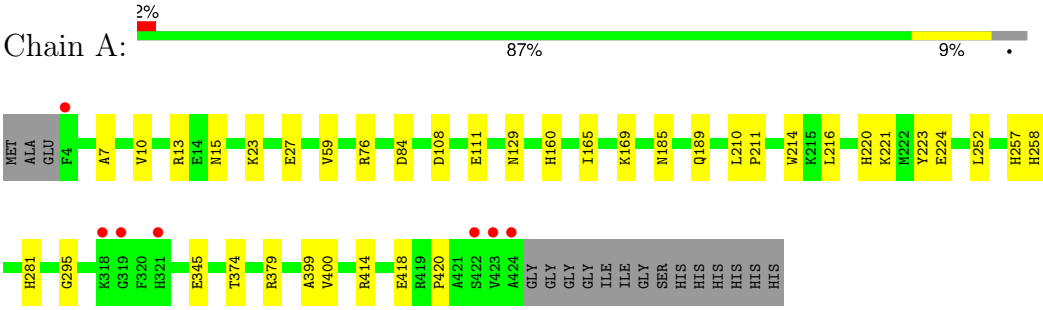
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	493	Total O 493 493	0	0
6	B	529	Total O 529 529	0	0
6	C	430	Total O 430 430	0	0
6	D	512	Total O 512 512	0	0

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.

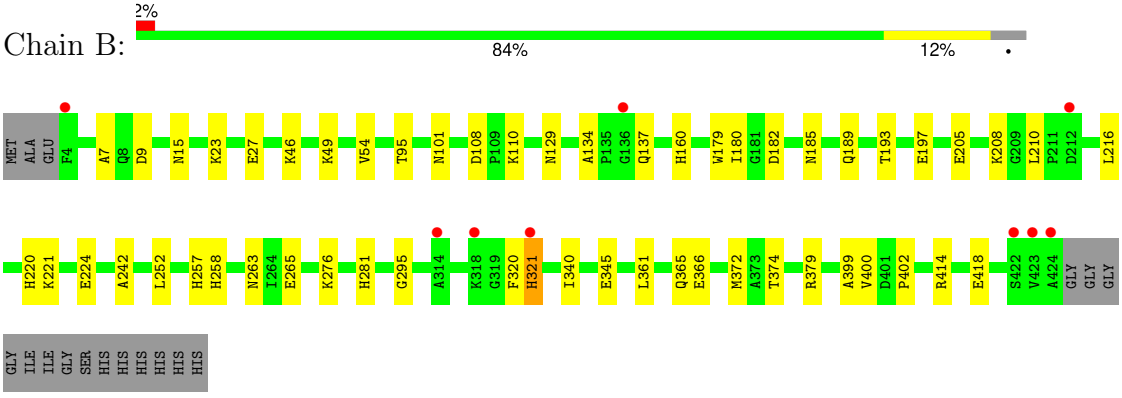
• Molecule 1: L-rhamnose isomerase

Chain A:



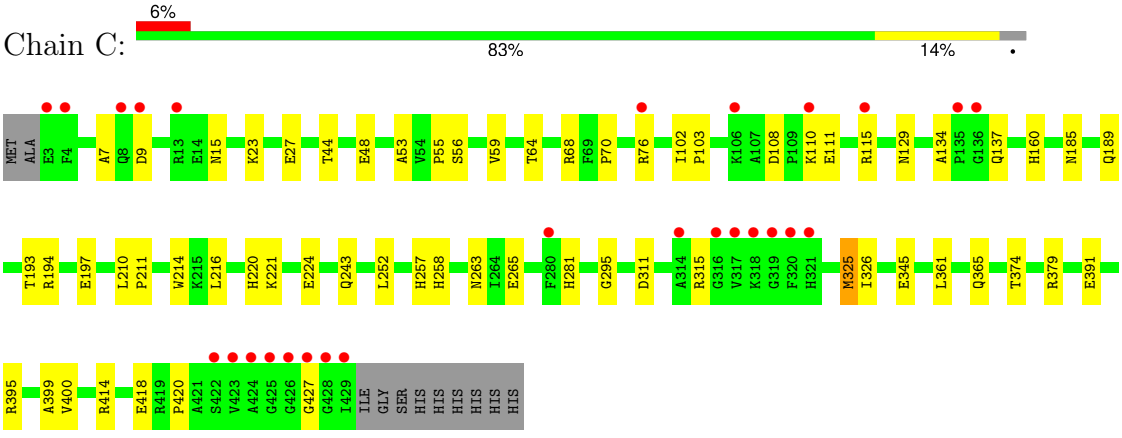
• Molecule 1: L-rhamnose isomerase

Chain B:



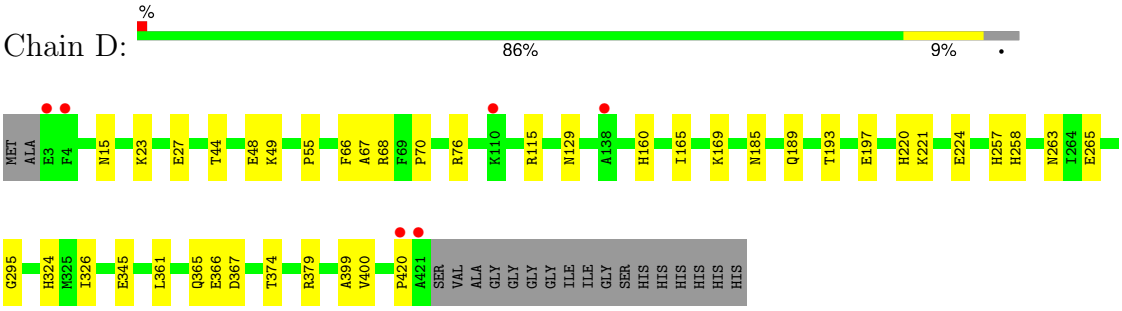
• Molecule 1: L-rhamnose isomerase

Chain C:



• Molecule 1: L-rhamnose isomerase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.12Å 104.92Å 112.38Å 90.00° 106.01° 90.00°	Depositor
Resolution (Å)	31.48 – 1.70 31.48 – 1.69	Depositor EDS
% Data completeness (in resolution range)	94.2 (31.48-1.70) 93.4 (31.48-1.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 1.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.175 , 0.195 0.169 , 0.189	Depositor DCC
R_{free} test set	17191 reflections (9.41%)	wwPDB-VP
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 66.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15195	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: RAM, RNS, RM4, MN

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	0.31	0/3363	0.55	0/4558
1	B	0.31	0/3363	0.55	0/4558
1	C	0.29	0/3396	0.52	0/4601
1	D	0.30	0/3354	0.53	0/4545
All	All	0.30	0/13476	0.54	0/18262

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	A	3269	0	3169	31	0
1	B	3269	0	3169	41	0
1	C	3302	0	3198	40	0
1	D	3260	0	3156	28	0
2	A	11	0	10	0	0
2	B	11	0	10	1	0
2	C	11	0	11	0	0
2	D	11	0	11	1	0
3	A	11	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	12	0	0
3	C	11	0	12	0	0
3	D	11	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	B	22	0	21	2	0
5	D	11	0	9	0	0
6	A	493	0	0	1	0
6	B	529	0	0	8	0
6	C	430	0	0	3	0
6	D	512	0	0	4	0
All	All	15195	0	12812	142	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 5.

All (142) 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:129:ASN:H	1:A:160:HIS:HE1	1.18	0.90
1:B:129:ASN:H	1:B:160:HIS:HE1	1.22	0.86
1:A:76:ARG:HH11	1:A:420:PRO:HD2	1.41	0.85
1:A:129:ASN:H	1:A:160:HIS:CE1	2.01	0.79
1:D:129:ASN:H	1:D:160:HIS:HE1	1.29	0.76
1:B:129:ASN:H	1:B:160:HIS:CE1	2.05	0.74
1:C:129:ASN:H	1:C:160:HIS:HE1	1.34	0.74
1:D:129:ASN:H	1:D:160:HIS:CE1	2.06	0.73
2:D:502[B]:RNS:H61	6:D:1104:HOH:O	1.89	0.72
1:C:129:ASN:H	1:C:160:HIS:CE1	2.09	0.70
1:C:23:LYS:O	1:C:27:GLU:HG3	1.92	0.70
1:A:220:HIS:HE2	1:A:258:HIS:CE1	2.09	0.70
1:C:220:HIS:HE2	1:C:258:HIS:CE1	2.12	0.67
1:D:220:HIS:HE2	1:D:258:HIS:CE1	2.13	0.67
1:C:391:GLU:O	1:C:395:ARG:HG3	1.95	0.67
1:A:185:ASN:H	1:A:189:GLN:HE22	1.40	0.67
1:A:220:HIS:HE2	1:A:258:HIS:HE1	1.44	0.65
1:A:15:ASN:ND2	1:A:400:VAL:H	1.94	0.65
1:A:15:ASN:HD21	1:A:400:VAL:H	1.46	0.64
1:B:220:HIS:HE2	1:B:258:HIS:CE1	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:H	1:A:189:GLN:NE2	1.96	0.63
1:C:210:LEU:HD11	1:C:216:LEU:HB2	1.80	0.63
1:C:15:ASN:ND2	1:C:400:VAL:H	1.96	0.63
1:D:44:THR:O	1:D:48:GLU:HG3	1.99	0.63
1:C:64:THR:O	1:C:427:GLY:HA3	1.98	0.63
1:A:76:ARG:HD3	1:A:420:PRO:HD2	1.79	0.62
1:D:185:ASN:H	1:D:189:GLN:HE22	1.47	0.61
1:D:220:HIS:HE2	1:D:258:HIS:HE1	1.45	0.61
2:B:502[B]:RNS:H61	6:B:1064:HOH:O	2.00	0.60
1:B:185:ASN:H	1:B:189:GLN:HE22	1.49	0.60
1:C:243:GLN:HG3	6:C:1017:HOH:O	2.02	0.59
1:D:15:ASN:ND2	1:D:400:VAL:H	2.00	0.59
1:D:366:GLU:HG2	6:D:788:HOH:O	2.02	0.59
1:A:295:GLY:HA3	1:A:345:GLU:HG2	1.82	0.59
1:B:185:ASN:H	1:B:189:GLN:NE2	2.01	0.59
1:D:185:ASN:H	1:D:189:GLN:NE2	2.01	0.58
1:B:320:PHE:C	1:B:321:HIS:HD2	2.07	0.58
1:B:205:GLU:HA	1:B:208:LYS:HE2	1.85	0.58
1:C:220:HIS:HE2	1:C:258:HIS:HE1	1.48	0.58
1:B:15:ASN:ND2	1:B:400:VAL:H	2.01	0.58
1:B:321:HIS:N	1:B:321:HIS:CD2	2.71	0.58
1:D:68:ARG:HH12	1:D:70:PRO:HB3	1.70	0.57
1:B:361:LEU:O	1:B:365:GLN:HG3	2.04	0.57
1:C:185:ASN:H	1:C:189:GLN:HE22	1.51	0.57
1:C:311:ASP:OD1	1:C:315:ARG:HD2	2.04	0.57
1:A:7:ALA:HB3	1:A:10:VAL:HG23	1.87	0.56
1:B:23:LYS:O	1:B:27:GLU:HG3	2.05	0.56
1:C:15:ASN:HD21	1:C:400:VAL:H	1.51	0.56
1:B:366:GLU:HG2	6:B:851:HOH:O	2.03	0.56
1:B:220:HIS:HE2	1:B:258:HIS:HE1	1.52	0.56
1:A:76:ARG:HH11	1:A:420:PRO:CD	2.17	0.55
1:B:210:LEU:HD11	1:B:216:LEU:HB2	1.89	0.55
1:B:320:PHE:C	1:B:321:HIS:CD2	2.80	0.55
1:A:263:ASN:OD1	1:A:265:GLU:HG2	2.07	0.55
1:C:193:THR:O	1:C:197:GLU:HG3	2.06	0.55
1:B:414:ARG:O	1:B:418:GLU:HG3	2.07	0.55
1:C:185:ASN:H	1:C:189:GLN:NE2	2.04	0.55
1:C:56:SER:O	1:C:59:VAL:HG22	2.07	0.54
1:B:54:VAL:HG23	1:B:95:THR:HB	1.90	0.54
1:D:76:ARG:HD3	1:D:420:PRO:HD2	1.89	0.54
1:A:210:LEU:HD11	1:A:216:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ASP:OD2	1:C:111:GLU:HG3	2.09	0.53
1:C:68:ARG:HH12	1:C:70:PRO:HB3	1.74	0.53
1:B:110:LYS:HG3	6:B:1116:HOH:O	2.09	0.53
1:B:263:ASN:OD1	1:B:265:GLU:HG2	2.10	0.52
1:B:295:GLY:HA3	1:B:345:GLU:HG2	1.92	0.52
1:C:361:LEU:O	1:C:365:GLN:HG3	2.10	0.52
1:C:44:THR:O	1:C:48:GLU:HG3	2.10	0.52
1:D:15:ASN:HD21	1:D:400:VAL:H	1.56	0.52
1:A:76:ARG:CD	1:A:420:PRO:HD2	2.40	0.51
1:B:15:ASN:HD21	1:B:399:ALA:HA	1.76	0.51
1:C:221:LYS:HA	1:C:257:HIS:HB3	1.92	0.51
1:C:55:PRO:HD3	1:C:326:ILE:O	2.10	0.51
1:D:221:LYS:HA	1:D:257:HIS:HB3	1.91	0.51
1:B:108:ASP:OD2	1:B:110:LYS:HB2	2.11	0.50
1:B:221:LYS:HA	1:B:257:HIS:HB3	1.92	0.50
1:B:15:ASN:HD21	1:B:400:VAL:H	1.57	0.50
1:C:48:GLU:CD	1:C:395:ARG:HH21	2.13	0.50
1:D:193:THR:O	1:D:197:GLU:HG3	2.12	0.49
1:B:46:LYS:HE3	6:B:1002:HOH:O	2.13	0.49
1:C:7:ALA:HB1	1:C:9:ASP:OD1	2.13	0.49
1:B:101:ASN:ND2	6:B:1058:HOH:O	2.45	0.49
1:C:68:ARG:NH1	1:C:70:PRO:HB3	2.27	0.48
1:A:211:PRO:HD2	1:A:214:TRP:CG	2.48	0.48
1:C:295:GLY:HA3	1:C:345:GLU:HG2	1.96	0.47
1:A:221:LYS:HA	1:A:257:HIS:HB3	1.96	0.46
1:D:295:GLY:HA3	1:D:345:GLU:HG2	1.96	0.46
1:A:108:ASP:HB3	1:A:111:GLU:HG3	1.97	0.46
1:D:165:ILE:O	1:D:169:LYS:HG3	2.16	0.46
1:D:15:ASN:HD21	1:D:399:ALA:HA	1.81	0.46
1:D:324:HIS:HE1	3:D:503:RAM:O4	1.97	0.46
1:B:193:THR:O	1:B:197:GLU:HG3	2.15	0.45
1:A:414:ARG:O	1:A:418:GLU:HG3	2.17	0.45
1:B:49:LYS:HE2	6:B:691:HOH:O	2.17	0.45
1:D:23:LYS:O	1:D:27:GLU:HG3	2.16	0.45
1:A:23:LYS:O	1:A:27:GLU:HG3	2.17	0.45
1:C:252:LEU:HD11	1:C:281:HIS:CD2	2.51	0.44
1:C:263:ASN:OD1	1:C:265:GLU:HG2	2.18	0.44
1:D:361:LEU:O	1:D:365:GLN:HG3	2.18	0.44
1:A:15:ASN:HD21	1:A:399:ALA:HA	1.83	0.44
1:A:252:LEU:HD21	1:A:281:HIS:CG	2.52	0.44
1:B:252:LEU:HD21	1:B:281:HIS:CG	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ARG:O	1:C:418:GLU:HG3	2.18	0.44
1:B:160:HIS:HD2	6:B:953:HOH:O	2.01	0.43
1:B:7:ALA:HB1	1:B:9:ASP:OD1	2.18	0.43
1:D:68:ARG:NH1	1:D:70:PRO:HB3	2.31	0.43
1:A:160:HIS:HD2	6:A:1399:HOH:O	2.00	0.43
1:C:15:ASN:HD21	1:C:399:ALA:HA	1.84	0.43
1:D:49:LYS:HE2	6:D:724:HOH:O	2.18	0.42
1:C:108:ASP:OD2	1:C:110:LYS:HB2	2.18	0.42
1:C:211:PRO:HD2	1:C:214:TRP:CG	2.54	0.42
1:D:367:ASP:HB2	6:D:1069:HOH:O	2.18	0.42
1:B:179:TRP:CD2	5:B:501[A]:RM4:H1	2.54	0.42
1:A:13:ARG:HG3	1:A:13:ARG:HH11	1.84	0.42
1:A:129:ASN:N	1:A:160:HIS:HE1	2.00	0.42
1:C:379:ARG:HD3	6:C:943:HOH:O	2.20	0.42
1:C:414:ARG:HD2	6:C:1003:HOH:O	2.18	0.42
1:B:179:TRP:CE3	5:B:501[A]:RM4:H1	2.54	0.42
1:D:66:PHE:O	1:D:67:ALA:HB2	2.19	0.42
1:B:340:ILE:HG21	1:B:402:PRO:HB2	2.01	0.42
1:B:134:ALA:O	1:B:137:GLN:HB2	2.20	0.42
1:D:263:ASN:OD1	1:D:265:GLU:HG2	2.20	0.42
1:B:180:ILE:HD12	1:B:182:ASP:CG	2.41	0.41
1:A:252:LEU:HD21	1:A:281:HIS:CD2	2.56	0.41
1:C:76:ARG:HD3	1:C:420:PRO:CD	2.51	0.41
1:C:134:ALA:O	1:C:137:GLN:HB2	2.20	0.41
1:B:321:HIS:HD2	1:B:321:HIS:N	2.15	0.41
1:C:53:ALA:HB3	1:C:325[B]:MET:HG2	2.01	0.41
1:B:242:ALA:HB1	1:B:276:LYS:HD2	2.03	0.41
1:B:372:MET:HE2	6:B:751:HOH:O	2.20	0.41
1:A:221:LYS:HE2	1:A:223:TYR:O	2.21	0.41
1:D:115:ARG:HA	1:D:115:ARG:HD2	1.84	0.41
1:B:320:PHE:N	1:B:321:HIS:HD2	2.20	0.40
1:C:102:ILE:CG2	1:C:103:PRO:HA	2.52	0.40
1:C:115:ARG:HA	1:C:115:ARG:HD2	1.89	0.40
1:A:165:ILE:O	1:A:169:LYS:HG3	2.21	0.40
1:A:59:VAL:HG11	1:A:84:ASP:HB2	2.04	0.40
1:D:55:PRO:HD3	1:D:326:ILE:O	2.22	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	423/438 (97%)	412 (97%)	10 (2%)	1 (0%)	47	30
1	B	423/438 (97%)	413 (98%)	9 (2%)	1 (0%)	47	30
1	C	429/438 (98%)	417 (97%)	11 (3%)	1 (0%)	47	30
1	D	421/438 (96%)	412 (98%)	8 (2%)	1 (0%)	47	30
All	All	1696/1752 (97%)	1654 (98%)	38 (2%)	4 (0%)	47	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	GLU
1	B	224	GLU
1	C	224	GLU
1	D	224	GLU

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	334/341 (98%)	333 (100%)	1 (0%)	92	89
1	B	334/341 (98%)	332 (99%)	2 (1%)	86	80
1	C	336/341 (98%)	332 (99%)	4 (1%)	71	59
1	D	333/341 (98%)	332 (100%)	1 (0%)	92	89
All	All	1337/1364 (98%)	1329 (99%)	8 (1%)	88	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	374	THR
1	B	321	HIS
1	B	374	THR
1	C	194	ARG
1	C	325[A]	MET
1	C	325[B]	MET
1	C	374	THR
1	D	374	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	15	ASN
1	A	160	HIS
1	A	189	GLN
1	A	258	HIS
1	A	324	HIS
1	A	344	ASN
1	A	368	ASN
1	B	15	ASN
1	B	160	HIS
1	B	189	GLN
1	B	258	HIS
1	B	321	HIS
1	B	324	HIS
1	B	344	ASN
1	C	8	GLN
1	C	15	ASN
1	C	160	HIS
1	C	189	GLN
1	C	258	HIS
1	C	344	ASN
1	D	15	ASN
1	D	160	HIS
1	D	189	GLN
1	D	258	HIS
1	D	324	HIS
1	D	344	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)

Of 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
3	RAM	C	502	-	11,11,11	0.40	0	16,16,16	0.40	0
2	RNS	A	1001	4	9,10,10	0.48	0	12,13,13	0.86	1 (8%)
3	RAM	D	503	-	11,11,11	0.36	0	16,16,16	0.43	0
2	RNS	B	502[B]	4	9,10,10	0.44	0	12,13,13	0.93	2 (16%)
2	RNS	C	501	4	9,10,10	0.43	0	12,13,13	0.92	1 (8%)
3	RAM	A	1002	-	11,11,11	0.38	0	16,16,16	0.42	0
2	RNS	D	502[B]	4	9,10,10	0.42	0	12,13,13	0.91	2 (16%)
5	RM4	B	501[A]	4	11,11,11	0.36	0	16,16,16	0.45	0
5	RM4	D	501[A]	4	11,11,11	0.41	0	16,16,16	0.48	0
3	RAM	B	503	-	11,11,11	0.39	0	16,16,16	0.39	0
5	RM4	B	504	-	11,11,11	0.36	0	16,16,16	0.43	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	RAM	C	502	-	-	-	0/1/1/1
2	RNS	A	1001	4	-	1/13/14/14	-
3	RAM	D	503	-	-	-	0/1/1/1
2	RNS	B	502[B]	4	-	1/13/14/14	-
2	RNS	C	501	4	-	1/13/14/14	-
3	RAM	A	1002	-	-	-	0/1/1/1
2	RNS	D	502[B]	4	-	1/13/14/14	-
5	RM4	B	501[A]	4	-	-	0/1/1/1
5	RM4	D	501[A]	4	-	-	0/1/1/1
3	RAM	B	503	-	-	-	0/1/1/1
5	RM4	B	504	-	-	-	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502[B]	RNS	C6-C5-C4	-2.28	109.32	112.11
2	C	501	RNS	C6-C5-C4	-2.21	109.41	112.11
2	A	1001	RNS	C6-C5-C4	-2.14	109.49	112.11
2	D	502[B]	RNS	C3-C4-C5	-2.13	110.29	113.21
2	D	502[B]	RNS	C6-C5-C4	-2.04	109.61	112.11
2	B	502[B]	RNS	C3-C4-C5	-2.04	110.42	113.21

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	RNS	O1-C1-C2-C3
2	B	502[B]	RNS	O1-C1-C2-C3
2	C	501	RNS	O1-C1-C2-C3
2	D	502[B]	RNS	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	503	RAM	1	0
2	B	502[B]	RNS	1	0
2	D	502[B]	RNS	1	0
5	B	501[A]	RM4	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

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	421/438 (96%)	-0.23	7 (1%)	70	74	11, 15, 28, 44	0
1	B	421/438 (96%)	-0.19	9 (2%)	63	67	10, 16, 30, 45	0
1	C	427/438 (97%)	0.18	27 (6%)	20	22	12, 21, 41, 57	0
1	D	419/438 (95%)	-0.16	6 (1%)	75	79	11, 17, 29, 51	0
All	All	1688/1752 (96%)	-0.10	49 (2%)	51	56	10, 17, 33, 57	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	319	GLY	8.3
1	C	317	VAL	7.7
1	C	316	GLY	6.3
1	C	427	GLY	5.6
1	D	4	PHE	5.5
1	D	421	ALA	5.2
1	B	423	VAL	4.5
1	C	426	GLY	4.5
1	C	314	ALA	4.5
1	C	136	GLY	4.4
1	C	320	PHE	4.4
1	C	318	LYS	4.3
1	A	423	VAL	4.2
1	C	4	PHE	4.1
1	C	3	GLU	4.0
1	C	424	ALA	4.0
1	C	135	PRO	3.9
1	D	3	GLU	3.9
1	A	424	ALA	3.8
1	C	76	ARG	3.7
1	C	110	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	321	HIS	3.6
1	A	422	SER	3.5
1	B	424	ALA	3.4
1	C	8	GLN	3.4
1	C	422	SER	3.2
1	B	321	HIS	3.2
1	B	4	PHE	3.0
1	B	314	ALA	2.9
1	B	318	LYS	2.9
1	D	420	PRO	2.9
1	C	9	ASP	2.9
1	A	318	LYS	2.9
1	C	280	PHE	2.8
1	C	106	LYS	2.7
1	C	423	VAL	2.7
1	C	428	GLY	2.7
1	B	422	SER	2.5
1	C	425	GLY	2.5
1	A	4	PHE	2.5
1	C	429	ILE	2.4
1	A	321	HIS	2.4
1	C	13	ARG	2.3
1	A	319	GLY	2.2
1	B	212	ASP	2.1
1	B	136	GLY	2.1
1	D	138	ALA	2.1
1	C	115	ARG	2.1
1	D	110	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, 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
3	RAM	C	502	11/11	0.54	0.22	48,49,49,49	0
5	RM4	B	504	11/11	0.67	0.33	42,45,47,49	0
3	RAM	B	503	11/11	0.72	0.19	38,40,41,42	0
3	RAM	D	503	11/11	0.82	0.15	27,30,31,34	0
3	RAM	A	1002	11/11	0.84	0.15	30,32,33,34	0
2	RNS	C	501	11/11	0.92	0.09	23,26,32,32	0
2	RNS	B	502[B]	11/11	0.92	0.12	13,16,18,18	11
2	RNS	D	502[B]	11/11	0.93	0.14	21,26,27,27	11
5	RM4	B	501[A]	11/11	0.93	0.11	17,19,20,21	11
2	RNS	A	1001	11/11	0.93	0.12	16,19,26,28	0
5	RM4	D	501[A]	11/11	0.93	0.12	10,14,17,19	11
4	MN	D	506	1/1	0.98	0.16	31,31,31,31	0
4	MN	B	506	1/1	0.98	0.08	21,21,21,21	0
4	MN	C	503	1/1	0.98	0.05	20,20,20,20	0
4	MN	C	505	1/1	0.98	0.12	31,31,31,31	0
4	MN	A	1003	1/1	0.99	0.03	15,15,15,15	0
4	MN	A	1004	1/1	0.99	0.07	20,20,20,20	0
4	MN	B	505	1/1	0.99	0.04	16,16,16,16	0
4	MN	D	505	1/1	0.99	0.03	19,19,19,19	0
4	MN	D	504	1/1	1.00	0.06	16,16,16,16	0
4	MN	C	504	1/1	1.00	0.07	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.