Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 02:56 PM EDT

PDB ID	:	3M0V
Title	:	Crystal structure of Pseudomonas stutzeri L-rhamnose isomerase mutant S329L in complex with L-rhamnose
Authors	:	Yoshida, H.; Takeda, K.; Izumori, K.; Kamitori, S.
Deposited on	:	2010-03-03
Resolution	:	1.79 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

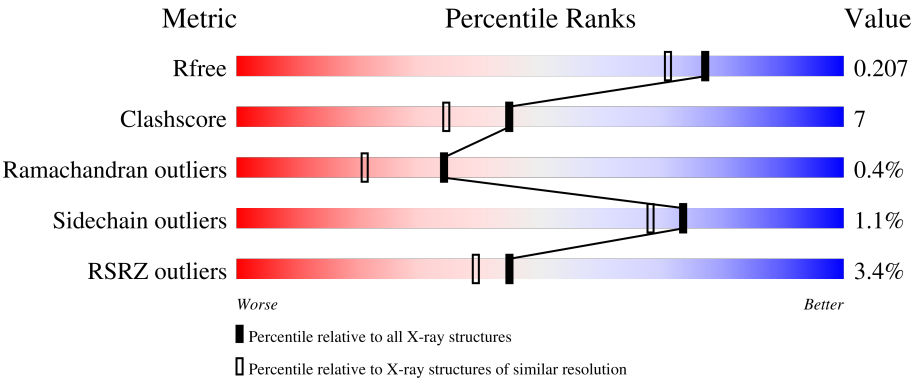
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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% 84% 12% ·
1	B	438	2% 81% 14% ·
1	C	438	6% 84% 14% ·
1	D	438	3% 87% 11% ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14971 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	0	0
			3262	2051	584	618	9			
1	B	421	Total	C	N	O	S	0	0	0
			3262	2051	584	618	9			
1	C	433	Total	C	N	O	S	0	0	0
			3343	2099	602	633	9			
1	D	429	Total	C	N	O	S	0	0	0
			3307	2078	592	628	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	ASN	ASP	engineered mutation	UNP Q75WH8
A	329	LEU	SER	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	150	ASN	ASP	engineered mutation	UNP Q75WH8
B	329	LEU	SER	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	150	ASN	ASP	engineered mutation	UNP Q75WH8

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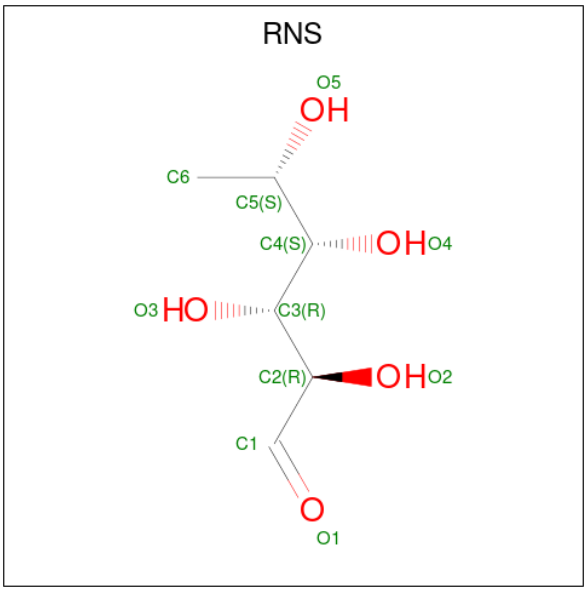
Chain	Residue	Modelled	Actual	Comment	Reference
C	329	LEU	SER	engineered mutation	UNP Q75WH8
C	431	GLY	-	expression tag	UNP Q75WH8
C	432	SER	-	expression tag	UNP Q75WH8
C	433	HIS	-	expression tag	UNP Q75WH8
C	434	HIS	-	expression tag	UNP Q75WH8
C	435	HIS	-	expression tag	UNP Q75WH8
C	436	HIS	-	expression tag	UNP Q75WH8
C	437	HIS	-	expression tag	UNP Q75WH8
C	438	HIS	-	expression tag	UNP Q75WH8
D	150	ASN	ASP	engineered mutation	UNP Q75WH8
D	329	LEU	SER	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 MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is L-RHAMNOSE (three-letter code: RNS) (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 water.

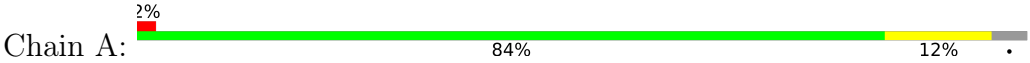
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	471	Total O 471 471	0	0
4	B	437	Total O 437 437	0	0
4	C	403	Total O 403 403	0	0
4	D	434	Total O 434 434	0	0

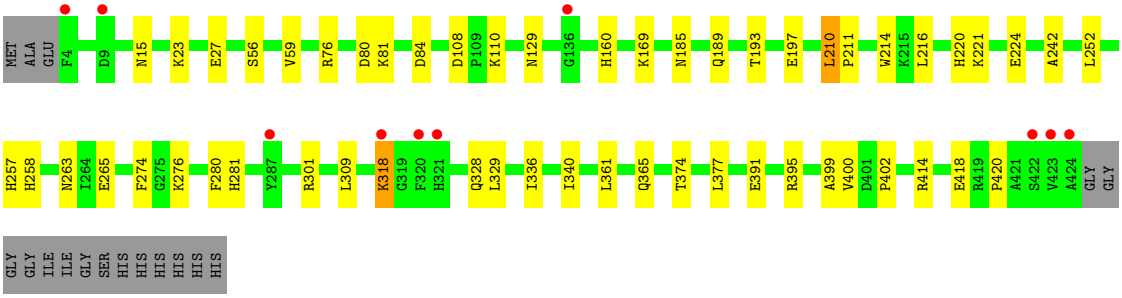
3 Residue-property plots (i)

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

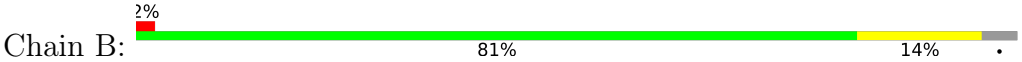
Chain A:

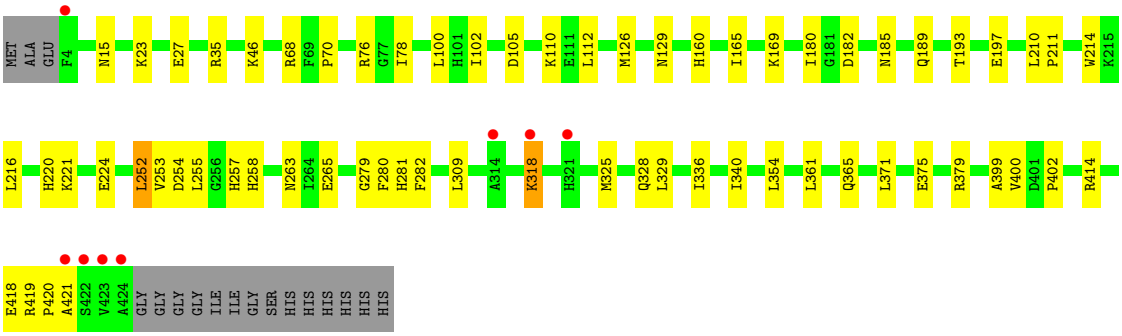




• Molecule 1: L-rhamnose isomerase

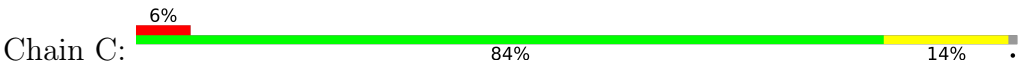
Chain B:

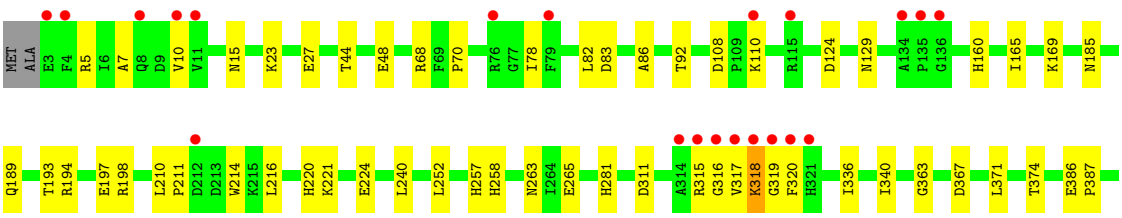


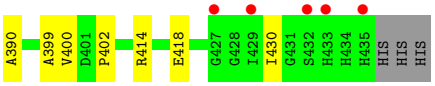


• Molecule 1: L-rhamnose isomerase

Chain C:

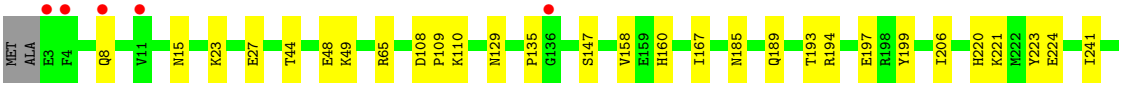


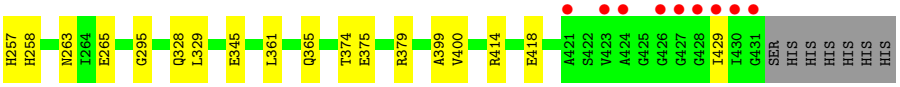




• Molecule 1: L-rhamnose isomerase

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	74.64Å 104.49Å 111.62Å 90.00° 106.15° 90.00°	Depositor
Resolution (Å)	47.70 – 1.79 47.70 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.70-1.79) 98.6 (47.70-1.79)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.40 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.216 0.175 , 0.207	Depositor DCC
R_{free} test set	15156 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14971	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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, 0.333 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: RNS, 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	0.30	0/3334	0.55	0/4521
1	B	0.30	0/3334	0.54	0/4521
1	C	0.29	0/3418	0.53	0/4633
1	D	0.29	0/3379	0.54	0/4580
All	All	0.30	0/13465	0.54	0/18255

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	3262	0	3171	39	0
1	B	3262	0	3171	51	0
1	C	3343	0	3240	44	0
1	D	3307	0	3214	37	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	11	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	11	0	0
3	C	11	0	10	1	0
3	D	11	0	10	1	0
4	A	471	0	0	1	0
4	B	437	0	0	3	0
4	C	403	0	0	2	0
4	D	434	0	0	5	0
All	All	14971	0	12837	170	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 7.

All (170) 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:B:78:ILE:HD12	1:B:105:ASP:HB3	1.40	1.01
1:A:129:ASN:H	1:A:160:HIS:HE1	1.09	0.92
1:B:129:ASN:H	1:B:160:HIS:HE1	1.19	0.86
1:C:129:ASN:H	1:C:160:HIS:HE1	1.20	0.86
1:A:129:ASN:H	1:A:160:HIS:CE1	1.95	0.85
1:C:317:VAL:HG22	1:C:318:LYS:HG2	1.62	0.80
1:A:56:SER:O	1:A:59:VAL:HG12	1.82	0.79
1:C:129:ASN:H	1:C:160:HIS:CE1	2.00	0.79
1:B:129:ASN:H	1:B:160:HIS:CE1	2.03	0.77
1:C:317:VAL:HG13	1:C:320:PHE:HB2	1.67	0.76
1:B:255:LEU:H	1:B:255:LEU:HD22	1.53	0.74
1:B:255:LEU:HD23	1:B:282:PHE:HA	1.70	0.74
1:B:102:ILE:HD12	1:B:102:ILE:N	2.02	0.74
1:A:76:ARG:HD2	1:A:420:PRO:HD2	1.72	0.71
1:C:23:LYS:O	1:C:27:GLU:HG3	1.90	0.71
1:D:129:ASN:H	1:D:160:HIS:HE1	1.36	0.71
1:B:23:LYS:O	1:B:27:GLU:HG3	1.93	0.69
1:A:220:HIS:HE2	1:A:258:HIS:CE1	2.11	0.69
1:B:102:ILE:HD11	1:B:126:MET:CE	2.22	0.69
1:C:68:ARG:HH12	1:C:70:PRO:HB3	1.58	0.69
1:B:220:HIS:HE2	1:B:258:HIS:CE1	2.12	0.68
1:C:220:HIS:HE2	1:C:258:HIS:CE1	2.12	0.68
1:D:129:ASN:H	1:D:160:HIS:CE1	2.12	0.68
1:A:210:LEU:HD21	1:A:216:LEU:HB2	1.77	0.67
1:B:252:LEU:HD12	1:B:253:VAL:N	2.10	0.66
1:D:220:HIS:HE2	1:D:258:HIS:CE1	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASN:ND2	1:A:400:VAL:H	1.93	0.66
1:A:185:ASN:H	1:A:189:GLN:HE22	1.43	0.64
1:C:185:ASN:H	1:C:189:GLN:HE22	1.43	0.64
1:C:210:LEU:HD11	1:C:216:LEU:HB2	1.80	0.63
1:B:414:ARG:O	1:B:418:GLU:HG3	1.98	0.63
1:C:363:GLY:O	1:C:367:ASP:HB2	1.99	0.63
1:A:220:HIS:HE2	1:A:258:HIS:HE1	1.47	0.62
1:B:102:ILE:HD11	1:B:126:MET:HE3	1.81	0.62
1:D:23:LYS:O	1:D:27:GLU:HG3	2.01	0.61
1:D:158:VAL:HA	1:D:206:ILE:HD11	1.82	0.61
1:B:220:HIS:HE2	1:B:258:HIS:HE1	1.47	0.60
1:D:185:ASN:H	1:D:189:GLN:NE2	2.00	0.60
1:D:185:ASN:H	1:D:189:GLN:HE22	1.49	0.60
1:D:220:HIS:HE2	1:D:258:HIS:HE1	1.49	0.60
1:B:185:ASN:H	1:B:189:GLN:NE2	2.01	0.59
1:B:328:GLN:C	1:B:329:LEU:HD22	2.23	0.59
1:C:44:THR:O	1:C:48:GLU:HG3	2.03	0.59
1:C:185:ASN:H	1:C:189:GLN:NE2	2.01	0.59
1:D:221:LYS:HA	1:D:257:HIS:HB3	1.84	0.59
1:B:185:ASN:H	1:B:189:GLN:HE22	1.49	0.58
1:D:158:VAL:HG13	1:D:206:ILE:HD13	1.84	0.58
1:A:15:ASN:HD21	1:A:400:VAL:H	1.48	0.58
1:C:15:ASN:ND2	1:C:400:VAL:H	2.02	0.58
1:B:46:LYS:HE3	4:B:1485:HOH:O	2.03	0.57
1:B:15:ASN:HD21	1:B:399:ALA:HA	1.70	0.57
1:A:185:ASN:H	1:A:189:GLN:NE2	2.02	0.57
1:B:110:LYS:HD2	4:B:1342:HOH:O	2.05	0.56
1:D:328:GLN:C	1:D:329:LEU:HD22	2.25	0.56
1:D:44:THR:O	1:D:48:GLU:HG2	2.06	0.56
1:A:263:ASN:OD1	1:A:265:GLU:HG2	2.06	0.56
1:C:15:ASN:HD21	1:C:399:ALA:HA	1.70	0.56
1:B:15:ASN:ND2	1:B:400:VAL:H	2.04	0.55
1:A:193:THR:O	1:A:197:GLU:HG3	2.07	0.55
1:C:220:HIS:HE2	1:C:258:HIS:HE1	1.54	0.55
1:B:375:GLU:O	1:B:379:ARG:HG3	2.07	0.55
1:C:317:VAL:HG13	1:C:320:PHE:CB	2.34	0.55
1:A:76:ARG:HD3	1:A:80:ASP:OD2	2.07	0.55
1:C:5:ARG:HD2	1:C:83:ASP:O	2.06	0.54
1:D:15:ASN:ND2	1:D:400:VAL:H	2.06	0.54
1:B:102:ILE:HD11	1:B:126:MET:HE1	1.89	0.54
1:C:193:THR:O	1:C:197:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:PRO:HG3	1:D:167:ILE:HD12	1.91	0.53
1:D:15:ASN:HD21	1:D:399:ALA:HA	1.74	0.53
1:C:68:ARG:NH1	1:C:70:PRO:HB3	2.23	0.52
1:B:78:ILE:HD13	1:B:112:LEU:CD2	2.38	0.52
1:A:59:VAL:HG11	1:A:81:LYS:HG2	1.91	0.52
1:C:15:ASN:HD21	1:C:400:VAL:H	1.57	0.52
1:C:165:ILE:O	1:C:169:LYS:HG3	2.09	0.52
1:A:361:LEU:O	1:A:365:GLN:HG3	2.10	0.52
1:C:340:ILE:HG21	1:C:402:PRO:HB2	1.91	0.52
1:B:263:ASN:OD1	1:B:265:GLU:HG2	2.10	0.51
1:A:328:GLN:C	1:A:329:LEU:HD22	2.31	0.51
1:A:15:ASN:HD21	1:A:399:ALA:HA	1.76	0.51
1:D:263:ASN:OD1	1:D:265:GLU:HG2	2.10	0.51
1:A:59:VAL:CG1	1:A:81:LYS:HG2	2.41	0.51
1:A:391:GLU:O	1:A:395:ARG:HG3	2.10	0.51
1:A:23:LYS:O	1:A:27:GLU:HG3	2.12	0.50
1:D:65:ARG:O	1:D:429:ILE:HG23	2.11	0.50
1:B:102:ILE:N	1:B:102:ILE:CD1	2.73	0.50
1:A:301:ARG:HD3	4:A:503:HOH:O	2.12	0.49
1:A:129:ASN:N	1:A:160:HIS:HE1	1.92	0.49
1:C:414:ARG:O	1:C:418:GLU:HG3	2.13	0.49
1:B:68:ARG:HH12	1:B:70:PRO:HB3	1.78	0.49
1:C:263:ASN:OD1	1:C:265:GLU:HG2	2.13	0.49
1:A:221:LYS:HA	1:A:257:HIS:HB3	1.94	0.48
1:D:414:ARG:O	1:D:418:GLU:HG3	2.12	0.48
1:A:318:LYS:O	1:A:318:LYS:HD3	2.14	0.48
1:B:210:LEU:HD11	1:B:216:LEU:HB2	1.95	0.48
1:B:15:ASN:HD21	1:B:400:VAL:H	1.60	0.48
1:D:65:ARG:HD2	1:D:429:ILE:HG22	1.95	0.48
1:C:221:LYS:HA	1:C:257:HIS:HB3	1.95	0.48
1:D:49:LYS:HE2	4:D:585:HOH:O	2.14	0.48
1:B:78:ILE:HD13	1:B:112:LEU:HD22	1.95	0.47
1:B:361:LEU:O	1:B:365:GLN:HG3	2.14	0.47
1:D:158:VAL:HG13	1:D:206:ILE:CD1	2.43	0.47
1:B:255:LEU:H	1:B:255:LEU:CD2	2.26	0.47
1:B:340:ILE:HG21	1:B:402:PRO:HB2	1.96	0.47
1:C:311:ASP:O	1:C:315:ARG:HG2	2.14	0.47
1:B:419:ARG:HA	1:B:420:PRO:HD3	1.79	0.47
1:D:375:GLU:O	1:D:379:ARG:HG3	2.15	0.47
1:A:59:VAL:HG11	1:A:81:LYS:CG	2.45	0.47
1:B:221:LYS:HA	1:B:257:HIS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PHE:CE2	1:C:240:LEU:HD13	2.51	0.46
1:C:110:LYS:HE2	4:C:717:HOH:O	2.16	0.46
1:D:361:LEU:O	1:D:365:GLN:HG3	2.16	0.46
1:B:255:LEU:CD2	1:B:282:PHE:HA	2.42	0.46
1:A:280:PHE:CE2	1:A:309:LEU:HD21	2.51	0.46
1:D:160:HIS:HD2	4:D:1219:HOH:O	1.98	0.46
1:A:108:ASP:OD2	1:A:110:LYS:HB2	2.16	0.46
1:D:193:THR:O	1:D:197:GLU:HG3	2.16	0.46
1:B:211:PRO:HD2	1:B:214:TRP:CG	2.50	0.45
1:B:252:LEU:HD13	1:B:279:GLY:C	2.37	0.45
1:D:135:PRO:HA	4:D:1724:HOH:O	2.17	0.45
1:D:194:ARG:HG2	1:D:194:ARG:HH11	1.82	0.45
1:C:108:ASP:OD2	1:C:110:LYS:HB2	2.16	0.45
1:D:65:ARG:HB2	1:D:429:ILE:HG23	1.98	0.45
1:A:169:LYS:HD3	1:A:211:PRO:CG	2.46	0.45
1:D:15:ASN:HD21	1:D:400:VAL:H	1.64	0.44
1:D:257:HIS:HE1	3:D:2004:RNS:H2	1.82	0.44
1:D:108:ASP:OD1	1:D:110:LYS:NZ	2.46	0.44
1:A:414:ARG:O	1:A:418:GLU:HG3	2.18	0.44
1:B:255:LEU:HD22	1:B:255:LEU:N	2.27	0.43
1:C:430:ILE:HG22	4:D:1417:HOH:O	2.18	0.43
1:C:129:ASN:N	1:C:160:HIS:HE1	2.01	0.43
1:B:318:LYS:O	1:B:318:LYS:HD3	2.18	0.43
1:C:5:ARG:HG3	1:C:86:ALA:HB3	2.00	0.43
1:D:108:ASP:OD2	1:D:110:LYS:HB2	2.18	0.43
1:D:147:SER:HB3	1:D:199:TYR:HB2	2.01	0.43
1:A:242:ALA:HB1	1:A:276:LYS:HD2	1.99	0.43
1:B:221:LYS:HG3	1:B:257:HIS:CG	2.54	0.43
1:C:257:HIS:HE1	3:C:2003:RNS:H2	1.83	0.43
1:C:211:PRO:HD2	1:C:214:TRP:CG	2.52	0.43
1:C:336:ILE:O	1:C:340:ILE:HG13	2.19	0.43
1:C:7:ALA:HB3	1:C:10:VAL:HG23	2.01	0.43
1:C:390:ALA:HB1	1:C:400:VAL:HG13	2.00	0.42
1:C:386:GLU:N	1:C:387:PRO:CD	2.82	0.42
1:B:336:ILE:O	1:B:340:ILE:HG13	2.19	0.42
1:B:165:ILE:O	1:B:169:LYS:HG3	2.19	0.42
1:C:160:HIS:HD2	4:C:1169:HOH:O	2.03	0.42
1:B:252:LEU:HD12	1:B:252:LEU:C	2.39	0.42
1:D:221:LYS:HE2	1:D:223:TYR:O	2.19	0.42
1:A:211:PRO:HD2	1:A:214:TRP:CG	2.54	0.42
1:A:336:ILE:O	1:A:340:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:THR:CG2	1:C:340:ILE:HG23	2.50	0.41
1:B:68:ARG:NH1	1:B:70:PRO:HB3	2.35	0.41
1:C:78:ILE:O	1:C:82:LEU:HG	2.21	0.41
1:A:340:ILE:HG21	1:A:402:PRO:HB2	2.02	0.41
1:B:76:ARG:HH22	1:B:421:ALA:HA	1.86	0.41
1:B:280:PHE:CE2	1:B:309:LEU:HD21	2.55	0.41
1:C:318:LYS:O	1:C:320:PHE:N	2.53	0.41
1:C:252:LEU:HD21	1:C:281:HIS:CG	2.56	0.41
1:A:59:VAL:HG21	1:A:84:ASP:HB2	2.03	0.40
1:C:194:ARG:O	1:C:198:ARG:HG3	2.22	0.40
1:D:199:TYR:CE1	1:D:241:ILE:HD13	2.56	0.40
1:B:78:ILE:HD13	1:B:112:LEU:HD21	2.02	0.40
1:B:180:ILE:HD12	1:B:182:ASP:CG	2.42	0.40
1:B:35:ARG:HG3	4:B:1704:HOH:O	2.21	0.40
1:B:254:ASP:HA	1:B:281:HIS:HB2	2.02	0.40
1:A:252:LEU:HD21	1:A:281:HIS:CG	2.57	0.40
1:A:257:HIS:HE1	3:A:2001:RNS:H2	1.87	0.40
1:D:295:GLY:HA3	1:D:345:GLU:HG2	2.03	0.40
1:A:169:LYS:HD3	1:A:211:PRO:HG3	2.04	0.40
1:B:193:THR:O	1:B:197:GLU:HG3	2.22	0.40
1:D:8:GLN:HG3	4:D:1074:HOH: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	419/438 (96%)	410 (98%)	8 (2%)	1 (0%)	47 33
1	B	419/438 (96%)	408 (97%)	10 (2%)	1 (0%)	47 33
1	C	431/438 (98%)	416 (96%)	11 (3%)	4 (1%)	17 6
1	D	427/438 (98%)	417 (98%)	9 (2%)	1 (0%)	47 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1696/1752 (97%)	1651 (97%)	38 (2%)	7 (0%)	34 21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	316	GLY
1	C	318	LYS
1	A	224	GLU
1	B	224	GLU
1	C	224	GLU
1	C	319	GLY
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	330/341 (97%)	326 (99%)	4 (1%)	71 65
1	B	330/341 (97%)	324 (98%)	6 (2%)	59 48
1	C	337/341 (99%)	334 (99%)	3 (1%)	78 75
1	D	333/341 (98%)	332 (100%)	1 (0%)	92 91
All	All	1330/1364 (98%)	1316 (99%)	14 (1%)	73 68

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	LEU
1	A	318	LYS
1	A	374	THR
1	A	377	LEU
1	B	100	LEU
1	B	252	LEU
1	B	318	LYS
1	B	325	MET

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Mol	Chain	Res	Type
1	B	354	LEU
1	B	371	LEU
1	C	124	ASP
1	C	371	LEU
1	C	374	THR
1	D	374	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	15	ASN
1	A	150	ASN
1	A	160	HIS
1	A	189	GLN
1	A	258	HIS
1	A	344	ASN
1	B	15	ASN
1	B	160	HIS
1	B	189	GLN
1	B	258	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	344	ASN

5.3.3 RNA

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	RNS	D	2004	2	8,10,10	0.46	0	9,13,13	0.56	0
3	RNS	C	2003	2	8,10,10	0.45	0	9,13,13	0.75	1 (11%)
3	RNS	B	2002	2	8,10,10	0.49	0	9,13,13	0.70	0
3	RNS	A	2001	2	8,10,10	0.48	0	9,13,13	0.68	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	RNS	D	2004	2	-	0/12/14/14	-
3	RNS	C	2003	2	-	0/12/14/14	-
3	RNS	B	2002	2	-	0/12/14/14	-
3	RNS	A	2001	2	-	0/12/14/14	-

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	C	2003	RNS	C3-C4-C5	-2.05	110.36	113.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2004	RNS	1	0
3	C	2003	RNS	1	0
3	A	2001	RNS	1	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%)	0.26	10 (2%)	59 54	6, 12, 23, 40	0
1	B	421/438 (96%)	0.24	8 (1%)	66 63	7, 13, 25, 49	0
1	C	433/438 (98%)	0.58	26 (6%)	21 17	7, 16, 34, 53	0
1	D	429/438 (97%)	0.31	14 (3%)	46 40	7, 13, 26, 46	0
All	All	1704/1752 (97%)	0.35	58 (3%)	45 39	6, 13, 28, 53	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	423	VAL	8.6
1	B	423	VAL	7.5
1	C	317	VAL	6.9
1	C	319	GLY	6.5
1	D	427	GLY	6.2
1	B	424	ALA	6.0
1	C	3	GLU	5.9
1	D	3	GLU	5.9
1	D	424	ALA	5.5
1	D	4	PHE	5.4
1	C	318	LYS	5.2
1	C	427	GLY	4.8
1	C	320	PHE	4.7
1	C	4	PHE	4.4
1	C	314	ALA	4.3
1	B	422	SER	4.2
1	D	428	GLY	4.2
1	A	4	PHE	3.9
1	C	321	HIS	3.9
1	D	429	ILE	3.6
1	B	314	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	318	LYS	3.4
1	A	424	ALA	3.4
1	C	110	LYS	3.4
1	C	136	GLY	3.3
1	C	316	GLY	3.3
1	C	8	GLN	3.1
1	A	320	PHE	3.0
1	B	421	ALA	2.9
1	C	315	ARG	2.9
1	C	432	SER	2.9
1	A	423	VAL	2.8
1	C	135	PRO	2.8
1	B	4	PHE	2.8
1	C	435	HIS	2.7
1	B	318	LYS	2.7
1	C	76	ARG	2.6
1	C	79	PHE	2.6
1	A	321	HIS	2.6
1	D	431	GLY	2.5
1	D	8	GLN	2.5
1	C	115	ARG	2.5
1	C	11	VAL	2.5
1	C	212	ASP	2.4
1	B	321	HIS	2.4
1	D	11	VAL	2.3
1	D	136	GLY	2.2
1	C	433	HIS	2.2
1	C	10	VAL	2.2
1	D	430	ILE	2.2
1	A	422	SER	2.1
1	D	421	ALA	2.1
1	C	429	ILE	2.1
1	A	287	TYR	2.1
1	C	134	ALA	2.0
1	A	136	GLY	2.0
1	D	426	GLY	2.0
1	A	9	ASP	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	RNS	B	2002	11/11	0.90	0.13	10,13,17,19	0
3	RNS	D	2004	11/11	0.90	0.14	11,13,19,20	0
3	RNS	C	2003	11/11	0.92	0.12	14,16,20,21	0
3	RNS	A	2001	11/11	0.92	0.11	13,14,17,19	0
2	MN	D	508	1/1	0.99	0.05	11,11,11,11	0
2	MN	B	504	1/1	0.99	0.05	12,12,12,12	0
2	MN	C	505	1/1	0.99	0.06	12,12,12,12	0
2	MN	C	506	1/1	0.99	0.04	12,12,12,12	0
2	MN	D	507	1/1	0.99	0.06	9,9,9,9	0
2	MN	A	501	1/1	1.00	0.05	12,12,12,12	0
2	MN	A	502	1/1	1.00	0.04	11,11,11,11	0
2	MN	B	503	1/1	1.00	0.05	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.