



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:03 PM UTC

PDB ID : 3M0V / pdb_00003m0v
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

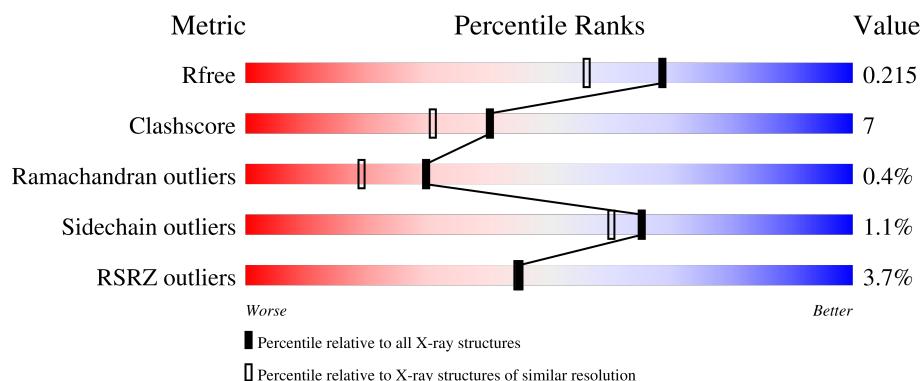
1 Overall quality at a glance

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 $\leq 5\%$. 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	
1	B	438	
1	C	438	
1	D	438	

2 Entry composition

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

Continued on next page...

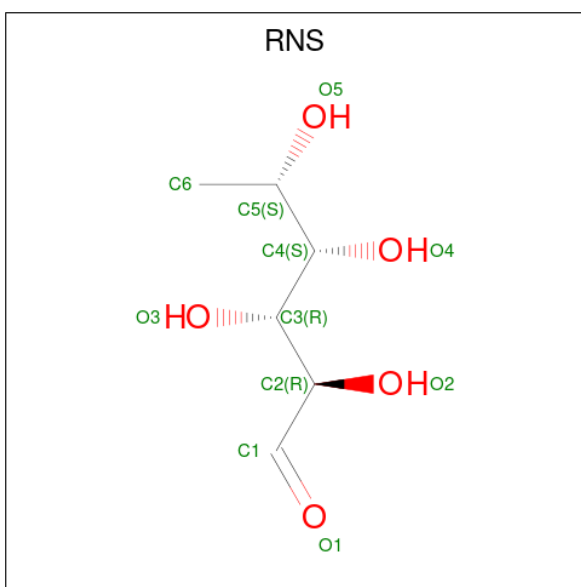
Continued from previous page...

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 (CCD ID: 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 (CCD ID: RNS) (formula: C₆H₁₂O₅).



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

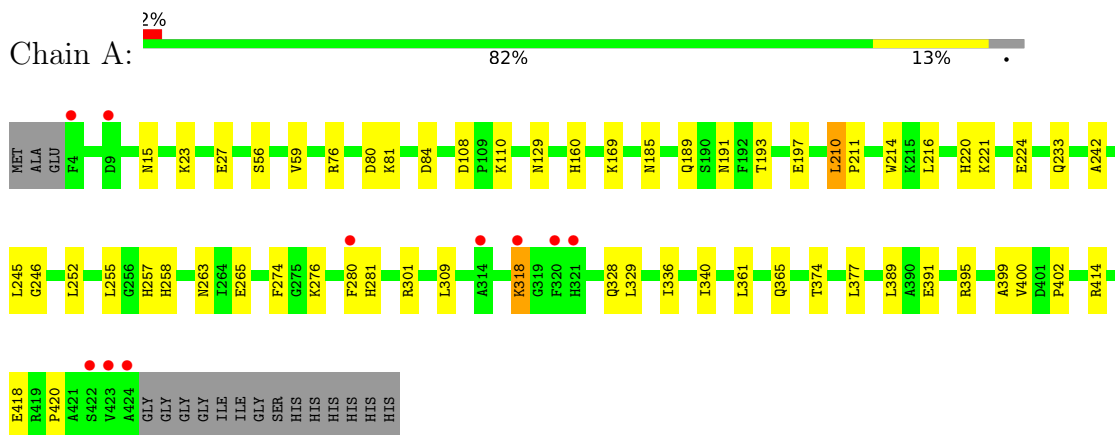
- Molecule 4 is water.

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

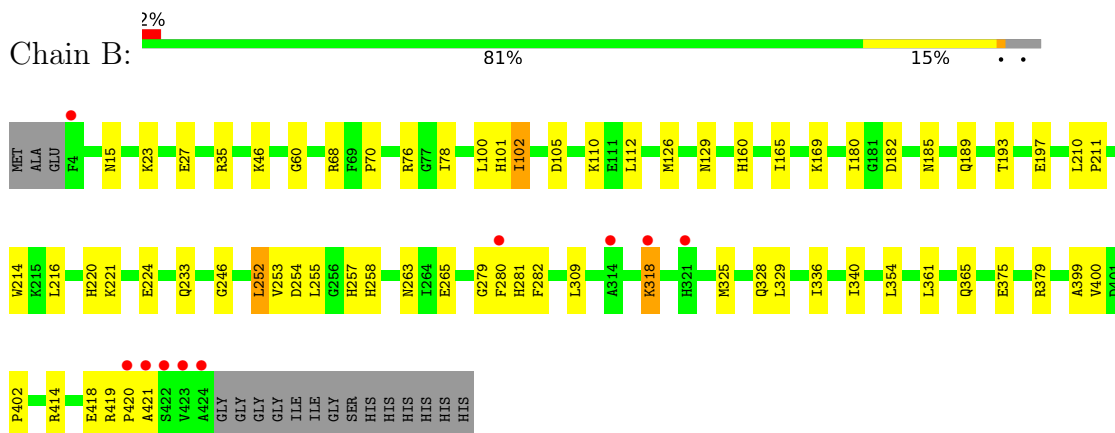
3 Residue-property plots [i](#)

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.

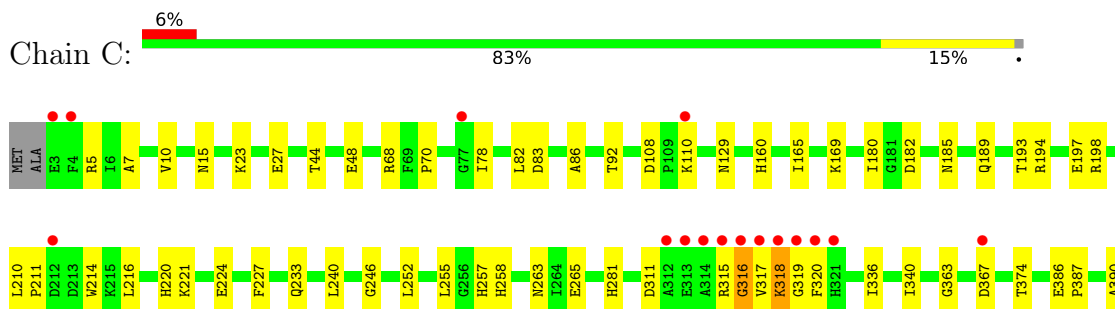
- Molecule 1: L-rhamnose isomerase

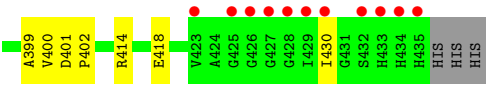


- Molecule 1: L-rhamnose isomerase

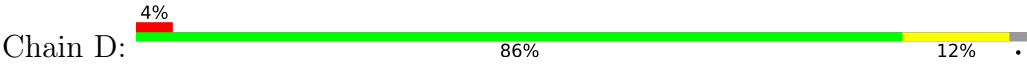


- Molecule 1: L-rhamnose isomerase





● Molecule 1: L-rhamnose isomerase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	5.40 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.216 0.183 , 0.215	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)	0.38 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MN, RNS

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	0.34	0/3334	0.83	6/4521 (0.1%)
1	B	0.34	0/3334	0.82	4/4521 (0.1%)
1	C	0.32	0/3418	0.82	7/4633 (0.2%)
1	D	0.34	0/3379	0.82	3/4580 (0.1%)
All	All	0.34	0/13465	0.82	20/18255 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	246	GLY	CA-C-N	6.76	127.31	119.47
1	C	246	GLY	C-N-CA	6.76	127.31	119.47
1	A	191	ASN	N-CA-C	-6.08	98.62	108.41
1	D	233	GLN	N-CA-C	5.84	119.59	112.23
1	A	255	LEU	N-CA-C	5.68	118.21	111.33
1	B	246	GLY	CA-C-N	5.55	125.91	119.47
1	B	246	GLY	C-N-CA	5.55	125.91	119.47
1	C	401	ASP	CA-C-N	5.53	124.99	119.24
1	C	401	ASP	C-N-CA	5.53	124.99	119.24
1	D	245	LEU	N-CA-C	5.43	117.28	111.36
1	C	227	PHE	N-CA-C	5.40	119.56	112.92
1	B	233	GLN	N-CA-C	5.35	118.97	112.23
1	D	191	ASN	N-CA-C	-5.32	99.84	108.41
1	B	60	GLY	N-CA-C	-5.32	104.57	113.02
1	C	255	LEU	N-CA-C	5.27	117.71	111.33
1	A	233	GLN	N-CA-C	5.16	118.73	112.23
1	A	245	LEU	N-CA-C	5.13	116.69	111.14
1	A	246	GLY	CA-C-N	5.09	125.12	119.32
1	A	246	GLY	C-N-CA	5.09	125.12	119.32
1	C	233	GLN	N-CA-C	5.03	118.57	112.23

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	52	0
1	C	3343	0	3240	46	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
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	173	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 (173) 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:102:ILE:HD11	1:B:126:MET:HE3	1.52	0.90
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:328:GLN:C	1:B:329:LEU:HD22	2.23	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: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:D:328:GLN:C	1:D:329:LEU:HD22	2.25	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:328:GLN:C	1:A:329:LEU:HD22	2.31	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:B:102:ILE:CD1	1:B:126:MET:HE3	2.31	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:C:193:THR:O	1:C:197:GLU:HG3	2.08	0.53
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: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:252:LEU:HD13	1:B:279:GLY:C	2.37	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:252:LEU:HD12	1:B:252:LEU:C	2.39	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
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:C:180:ILE:HD12	1:C:182:ASP:CG	2.41	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:B:180:ILE:HD12	1:B:182:ASP:CG	2.42	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:180:ILE:HD12	1:D:182:ASP:CG	2.43	0.44
1:A:414:ARG:O	1:A:418:GLU:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:101:HIS:C	1:B:102:ILE:HD12	2.41	0.43
1:C:129:ASN:N	1:C:160:HIS:HE1	2.01	0.43
1:C:315:ARG:O	1:C:316:GLY:C	2.61	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: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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	43	31
1	B	419/438 (96%)	408 (97%)	10 (2%)	1 (0%)	43	31
1	C	431/438 (98%)	416 (96%)	11 (3%)	4 (1%)	14	5
1	D	427/438 (98%)	417 (98%)	9 (2%)	1 (0%)	43	31
All	All	1696/1752 (97%)	1651 (97%)	38 (2%)	7 (0%)	30	19

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%)	325 (98%)	5 (2%)	57	49
1	B	330/341 (97%)	324 (98%)	6 (2%)	51	43
1	C	337/341 (99%)	336 (100%)	1 (0%)	86	86
1	D	333/341 (98%)	331 (99%)	2 (1%)	78	77
All	All	1330/1364 (98%)	1316 (99%)	14 (1%)	65	60

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	A	389	LEU
1	B	100	LEU
1	B	102	ILE
1	B	252	LEU
1	B	318	LYS
1	B	325	MET
1	B	354	LEU
1	C	374	THR
1	D	374	THR
1	D	389	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) 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	328	GLN
1	A	344	ASN
1	B	15	ASN
1	B	160	HIS
1	B	189	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	250	GLN
1	B	258	HIS
1	B	344	ASN
1	C	8	GLN
1	C	15	ASN
1	C	127	ASN
1	C	150	ASN
1	C	160	HIS
1	C	189	GLN
1	C	258	HIS
1	C	328	GLN
1	C	330	HIS
1	C	344	ASN
1	D	15	ASN
1	D	150	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	2002	2	9,10,10	0.48	0	12,13,13	0.85	0
3	RNS	D	2004	2	9,10,10	0.46	0	12,13,13	0.82	1 (8%)
3	RNS	C	2003	2	9,10,10	0.44	0	12,13,13	0.94	2 (16%)
3	RNS	A	2001	2	9,10,10	0.48	0	12,13,13	0.86	1 (8%)

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	B	2002	2	-	1/13/14/14	-
3	RNS	D	2004	2	-	1/13/14/14	-
3	RNS	C	2003	2	-	1/13/14/14	-
3	RNS	A	2001	2	-	1/13/14/14	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2003	RNS	C6-C5-C4	-2.28	109.32	112.11
3	D	2004	RNS	C6-C5-C4	-2.26	109.34	112.11
3	A	2001	RNS	C6-C5-C4	-2.15	109.49	112.11
3	C	2003	RNS	C3-C4-C5	-2.08	110.36	113.21

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	RNS	O1-C1-C2-C3
3	B	2002	RNS	O1-C1-C2-C3
3	C	2003	RNS	O1-C1-C2-C3
3	D	2004	RNS	O1-C1-C2-C3

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	421/438 (96%)	0.06	10 (2%) 59 60	6, 12, 23, 40	0
1	B	421/438 (96%)	0.13	10 (2%) 59 60	7, 13, 25, 49	0
1	C	433/438 (98%)	0.43	27 (6%) 26 25	7, 16, 34, 53	0
1	D	429/438 (97%)	0.13	16 (3%) 45 45	7, 13, 26, 46	0
All	All	1704/1752 (97%)	0.19	63 (3%) 45 45	6, 13, 28, 53	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	317	VAL	7.3
1	B	424	ALA	7.2
1	D	427	GLY	6.5
1	C	427	GLY	6.2
1	C	320	PHE	6.0
1	B	421	ALA	5.6
1	C	319	GLY	5.5
1	D	429	ILE	5.3
1	B	423	VAL	5.3
1	A	424	ALA	5.0
1	D	428	GLY	4.7
1	C	318	LYS	4.7
1	D	423	VAL	4.6
1	B	422	SER	4.2
1	C	314	ALA	4.1
1	D	424	ALA	4.0
1	A	320	PHE	3.9
1	A	423	VAL	3.8
1	C	3	GLU	3.4
1	C	316	GLY	3.4
1	D	430	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	435	HIS	3.3
1	D	3	GLU	3.2
1	C	426	GLY	3.0
1	C	4	PHE	3.0
1	C	428	GLY	3.0
1	D	4	PHE	3.0
1	C	315	ARG	2.9
1	C	321	HIS	2.9
1	A	318	LYS	2.8
1	C	432	SER	2.8
1	C	433	HIS	2.7
1	D	136	GLY	2.7
1	D	431	GLY	2.6
1	C	367	ASP	2.6
1	C	430	ILE	2.5
1	C	425	GLY	2.4
1	A	314	ALA	2.3
1	C	110	LYS	2.3
1	C	429	ILE	2.3
1	C	313	GLU	2.3
1	A	9	ASP	2.3
1	C	423	VAL	2.3
1	A	4	PHE	2.2
1	C	77	GLY	2.2
1	A	321	HIS	2.2
1	C	312	ALA	2.2
1	D	426	GLY	2.2
1	D	110	LYS	2.2
1	C	212	ASP	2.2
1	D	8	GLN	2.2
1	C	434	HIS	2.2
1	B	4	PHE	2.2
1	B	314	ALA	2.1
1	B	321	HIS	2.1
1	A	422	SER	2.1
1	B	280	PHE	2.1
1	B	318	LYS	2.1
1	D	421	ALA	2.1
1	B	420	PRO	2.1
1	D	135	PRO	2.0
1	D	425	GLY	2.0
1	A	280	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	RNS	D	2004	11/11	0.90	0.12	11,13,19,20	0
3	RNS	B	2002	11/11	0.92	0.09	10,13,17,19	0
3	RNS	C	2003	11/11	0.93	0.09	14,16,20,21	0
3	RNS	A	2001	11/11	0.94	0.08	13,14,17,19	0
2	MN	D	508	1/1	0.99	0.02	11,11,11,11	0
2	MN	B	503	1/1	0.99	0.02	12,12,12,12	0
2	MN	B	504	1/1	0.99	0.02	12,12,12,12	0
2	MN	C	505	1/1	0.99	0.02	12,12,12,12	0
2	MN	D	507	1/1	0.99	0.01	9,9,9,9	0
2	MN	A	502	1/1	1.00	0.03	11,11,11,11	0
2	MN	A	501	1/1	1.00	0.02	12,12,12,12	0
2	MN	C	506	1/1	1.00	0.02	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.