



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:59 AM UTC

PDB ID : 3ITO / pdb_00003ito
Title : Crystal structure of Pseudomonas stutzeri L-rhamnose isomerase mutant D327N in complex with D-psicose
Authors : Yoshida, H.; Yamaji, M.; Ishii, T.; Izumori, K.; Kamitori, S.
Deposited on : 2009-08-28
Resolution : 1.90 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

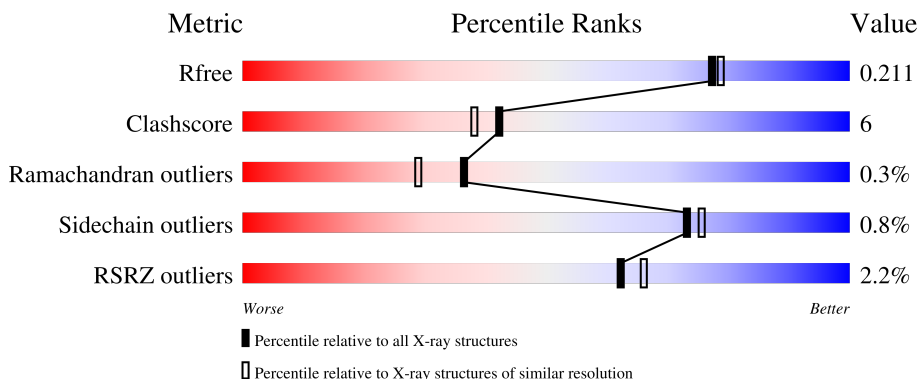
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	% 83% 13% .
1	B	438	3% 82% 14% .
1	C	438	4% 82% 15% .
1	D	438	% 81% 14% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14564 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
			3260	2048	585	618	9			
1	B	421	Total	C	N	O	S	0	0	0
			3260	2048	585	618	9			
1	C	428	Total	C	N	O	S	0	0	0
			3301	2073	592	627	9			
1	D	419	Total	C	N	O	S	0	0	0
			3251	2042	583	617	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	327	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	150	ASN	ASP	engineered mutation	UNP Q75WH8
B	327	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	150	ASN	ASP	engineered mutation	UNP Q75WH8

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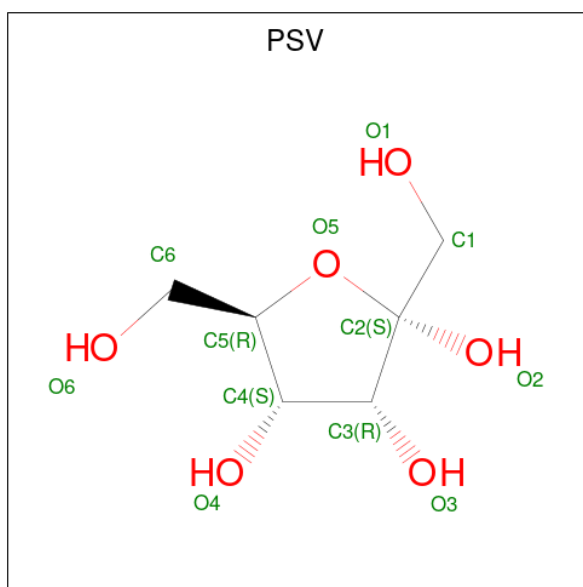
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Chain	Residue	Modelled	Actual	Comment	Reference
C	327	ASN	ASP	engineered mutation	UNP Q75WH8
C	431	GLY	-	expression tag	UNP Q75WH8
C	432	SER	-	expression tag	UNP Q75WH8
C	433	HIS	-	expression tag	UNP Q75WH8
C	434	HIS	-	expression tag	UNP Q75WH8
C	435	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	150	ASN	ASP	engineered mutation	UNP Q75WH8
D	327	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 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 alpha-D-psicofuranose (CCD ID: PSV) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		

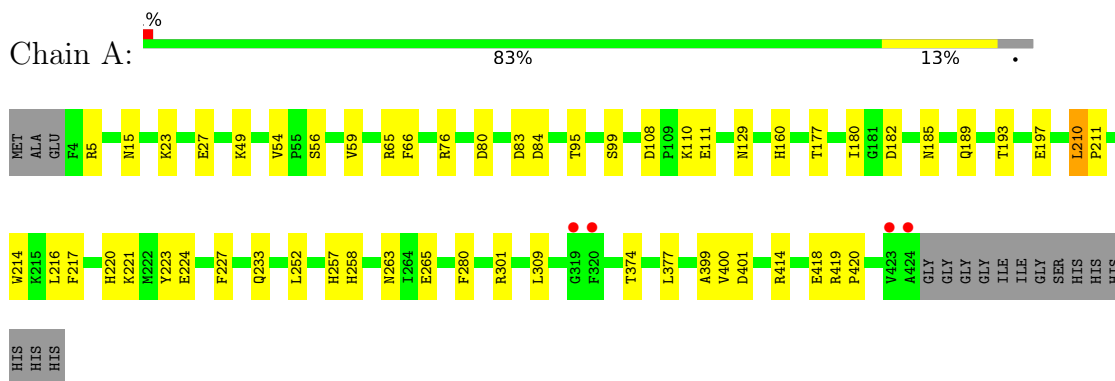
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	385	Total	O	0	0
			385	385		
4	B	345	Total	O	0	0
			345	345		
4	C	339	Total	O	0	0
			339	339		
4	D	367	Total	O	0	0
			367	367		

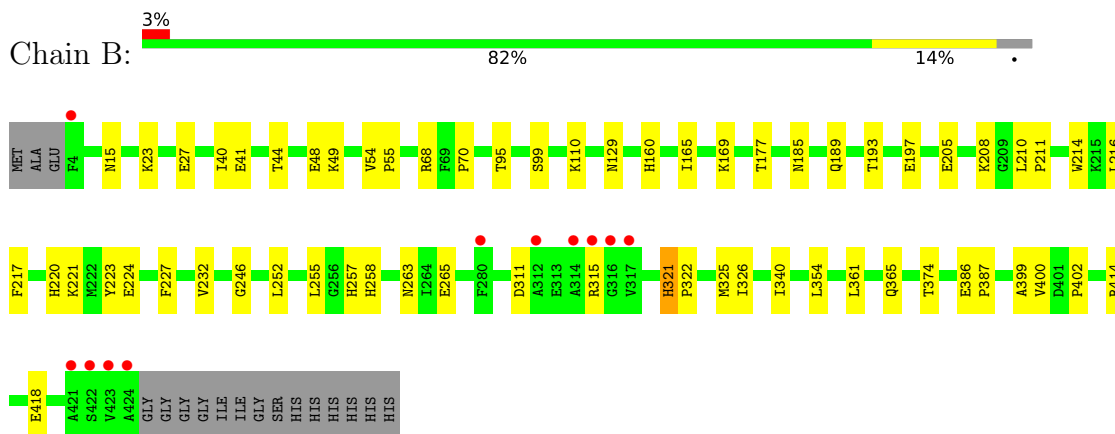
3 Residue-property plots

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.

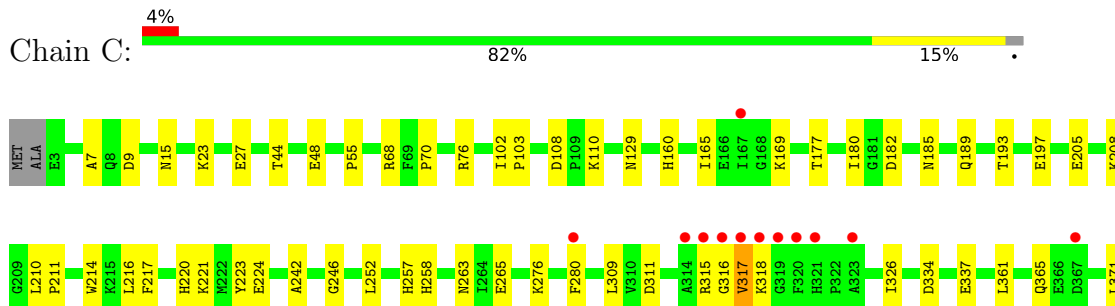
• Molecule 1: L-rhamnose isomerase

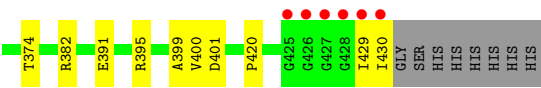


• Molecule 1: L-rhamnose isomerase

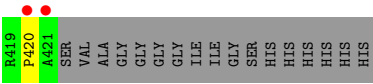
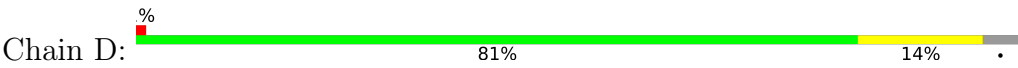


• Molecule 1: L-rhamnose isomerase





● 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	74.76Å 104.73Å 115.03Å 90.00° 108.24° 90.00°	Depositor
Resolution (Å)	42.15 – 1.90 42.15 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.3 (42.15-1.90) 92.3 (42.15-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.176 , 0.211 0.175 , 0.211	Depositor DCC
R_{free} test set	12186 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	12.3	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14564	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, PSV

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	0.35	0/3332	0.82	5/4518 (0.1%)
1	B	0.34	0/3332	0.83	5/4518 (0.1%)
1	C	0.34	0/3373	0.81	4/4572 (0.1%)
1	D	0.34	0/3323	0.83	6/4505 (0.1%)
All	All	0.34	0/13360	0.82	20/18113 (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	A	401	ASP	CA-C-N	6.40	125.90	119.24
1	A	401	ASP	C-N-CA	6.40	125.90	119.24
1	B	246	GLY	CA-C-N	5.81	126.21	119.47
1	B	246	GLY	C-N-CA	5.81	126.21	119.47
1	D	255	LEU	N-CA-C	5.78	118.32	111.33
1	C	401	ASP	CA-C-N	5.60	125.06	119.24
1	C	401	ASP	C-N-CA	5.60	125.06	119.24
1	D	227	PHE	N-CA-C	5.59	120.10	112.88
1	B	321	HIS	CA-C-N	5.59	125.60	119.90
1	B	321	HIS	C-N-CA	5.59	125.60	119.90
1	D	281	HIS	N-CA-C	-5.54	98.33	108.02
1	A	227	PHE	N-CA-C	5.46	119.64	112.92
1	A	233	GLN	N-CA-C	5.36	118.99	112.23
1	C	246	GLY	CA-C-N	5.32	125.64	119.47
1	C	246	GLY	C-N-CA	5.32	125.64	119.47
1	B	227	PHE	N-CA-C	5.30	119.44	112.92
1	D	246	GLY	CA-C-N	5.29	125.61	119.47
1	D	246	GLY	C-N-CA	5.29	125.61	119.47
1	A	210	LEU	N-CA-C	5.28	116.30	109.65
1	D	233	GLN	N-CA-C	5.22	118.81	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	3260	0	3167	41	0
1	B	3260	0	3167	39	0
1	C	3301	0	3207	42	0
1	D	3251	0	3154	42	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	12	0	10	0	0
3	B	12	0	10	1	0
3	C	12	0	10	0	0
3	D	12	0	9	0	0
4	A	385	0	0	5	0
4	B	345	0	0	1	0
4	C	339	0	0	1	0
4	D	367	0	0	1	0
All	All	14564	0	12734	164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (164) 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:129:ASN:H	1:B:160:HIS:HE1	1.16	0.93
1:A:129:ASN:H	1:A:160:HIS:HE1	1.14	0.90
1:C:217:PHE:HB3	1:C:252:LEU:HG	1.61	0.82
1:A:129:ASN:H	1:A:160:HIS:CE1	1.98	0.82
1:C:129:ASN:H	1:C:160:HIS:HE1	1.25	0.81
1:D:129:ASN:H	1:D:160:HIS:HE1	1.25	0.81
1:A:59:VAL:HG21	1:A:84:ASP:CB	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:PHE:HB3	1:A:252:LEU:HG	1.66	0.77
1:B:129:ASN:H	1:B:160:HIS:CE1	2.02	0.77
1:B:217:PHE:HB3	1:B:252:LEU:HG	1.65	0.77
1:D:220:HIS:HE2	1:D:258:HIS:CE1	2.04	0.75
1:D:129:ASN:H	1:D:160:HIS:CE1	2.05	0.74
1:A:220:HIS:HE2	1:A:258:HIS:CE1	2.06	0.74
1:C:220:HIS:HE2	1:C:258:HIS:CE1	2.06	0.73
1:A:59:VAL:HG21	1:A:84:ASP:HB2	1.69	0.72
1:C:220:HIS:HE2	1:C:258:HIS:HE1	1.37	0.72
1:C:129:ASN:H	1:C:160:HIS:CE1	2.09	0.71
1:C:280:PHE:HE2	1:C:309:LEU:HD21	1.55	0.70
1:D:108:ASP:OD2	1:D:111:GLU:HG3	1.91	0.69
1:A:177:THR:HG23	1:A:252:LEU:HD12	1.76	0.68
1:D:23:LYS:O	1:D:27:GLU:HG3	1.94	0.68
1:C:391:GLU:O	1:C:395:ARG:HG3	1.94	0.68
1:C:280:PHE:CE2	1:C:309:LEU:HD21	2.30	0.67
1:A:15:ASN:ND2	1:A:400:VAL:H	1.93	0.66
1:C:205:GLU:HA	1:C:208:LYS:HE2	1.78	0.66
1:B:220:HIS:HE2	1:B:258:HIS:CE1	2.15	0.65
1:B:23:LYS:O	1:B:27:GLU:HG3	1.97	0.64
1:A:23:LYS:O	1:A:27:GLU:HG3	1.98	0.63
1:B:54:VAL:HG23	1:B:95:THR:HB	1.79	0.63
1:D:320:PHE:CE1	1:D:322:PRO:HG3	2.33	0.63
1:D:220:HIS:HE2	1:D:258:HIS:HE1	1.46	0.62
1:A:15:ASN:HD21	1:A:400:VAL:H	1.47	0.62
1:C:177:THR:HG23	1:C:252:LEU:HD12	1.81	0.62
1:B:15:ASN:ND2	1:B:400:VAL:H	1.97	0.62
1:C:7:ALA:HB1	1:C:9:ASP:OD1	1.99	0.62
1:C:185:ASN:H	1:C:189:GLN:HE22	1.45	0.62
1:B:205:GLU:HA	1:B:208:LYS:HE2	1.81	0.61
1:A:59:VAL:HG21	1:A:84:ASP:HB3	1.83	0.61
1:A:193:THR:O	1:A:197:GLU:HG3	2.01	0.61
1:B:185:ASN:H	1:B:189:GLN:HE22	1.49	0.61
1:D:185:ASN:H	1:D:189:GLN:NE2	1.99	0.61
1:A:185:ASN:H	1:A:189:GLN:HE22	1.48	0.60
1:D:185:ASN:H	1:D:189:GLN:HE22	1.48	0.60
1:C:48:GLU:CD	1:C:395:ARG:HH21	2.09	0.60
1:B:165:ILE:O	1:B:169:LYS:HG3	2.01	0.59
1:B:210:LEU:HD11	1:B:216:LEU:HB2	1.83	0.59
1:C:165:ILE:O	1:C:169:LYS:HG3	2.03	0.58
1:B:177:THR:HG23	1:B:252:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ARG:HD3	1:D:420:PRO:CD	2.31	0.58
1:B:220:HIS:HE2	1:B:258:HIS:HE1	1.49	0.58
1:C:15:ASN:ND2	1:C:400:VAL:H	2.00	0.58
1:A:76:ARG:HD3	1:A:80:ASP:OD2	2.03	0.58
1:A:185:ASN:H	1:A:189:GLN:NE2	2.00	0.58
1:A:5:ARG:HD2	1:A:83:ASP:O	2.05	0.57
1:C:23:LYS:O	1:C:27:GLU:HG3	2.05	0.56
1:A:177:THR:HG23	1:A:252:LEU:CD1	2.35	0.56
1:B:193:THR:O	1:B:197:GLU:HG3	2.04	0.56
1:B:211:PRO:HD2	1:B:214:TRP:CG	2.40	0.56
1:A:210:LEU:HD11	1:A:216:LEU:HB2	1.88	0.56
1:B:263:ASN:OD1	1:B:265:GLU:HG2	2.06	0.56
1:A:76:ARG:HD2	1:A:420:PRO:HD2	1.88	0.55
1:B:185:ASN:H	1:B:189:GLN:NE2	2.05	0.55
1:A:108:ASP:OD2	1:A:111:GLU:HG3	2.07	0.55
1:C:361:LEU:O	1:C:365:GLN:HG3	2.07	0.55
1:C:185:ASN:H	1:C:189:GLN:NE2	2.05	0.55
1:C:15:ASN:HD21	1:C:400:VAL:H	1.53	0.55
1:C:44:THR:O	1:C:48:GLU:HG3	2.07	0.55
1:A:220:HIS:HE2	1:A:258:HIS:HE1	1.50	0.54
1:A:263:ASN:OD1	1:A:265:GLU:HG2	2.08	0.54
1:A:221:LYS:HA	1:A:257:HIS:HB3	1.88	0.54
1:D:414:ARG:O	1:D:418:GLU:HG3	2.07	0.54
1:D:76:ARG:HD3	1:D:420:PRO:HD3	1.90	0.54
1:D:15:ASN:ND2	1:D:400:VAL:H	2.06	0.54
1:A:15:ASN:HD21	1:A:399:ALA:HA	1.74	0.53
1:B:15:ASN:HD21	1:B:400:VAL:H	1.55	0.53
1:C:55:PRO:HD3	1:C:326:ILE:O	2.09	0.53
1:C:108:ASP:OD2	1:C:110:LYS:HB2	2.09	0.53
1:A:49:LYS:HE2	4:A:716:HOH:O	2.08	0.53
1:B:221:LYS:HA	1:B:257:HIS:HB3	1.92	0.52
1:D:108:ASP:OD2	1:D:110:LYS:HB2	2.09	0.52
1:A:211:PRO:HD2	1:A:214:TRP:CG	2.44	0.52
1:B:15:ASN:HD21	1:B:399:ALA:HA	1.74	0.52
1:C:221:LYS:HE2	1:C:223:TYR:O	2.10	0.52
1:C:221:LYS:HA	1:C:257:HIS:HB3	1.91	0.52
1:D:193:THR:O	1:D:197:GLU:HG3	2.09	0.52
1:B:255:LEU:C	1:B:255:LEU:HD23	2.35	0.51
1:B:311:ASP:OD1	1:B:315:ARG:NH1	2.43	0.51
4:A:554:HOH:O	1:D:382:ARG:HD3	2.11	0.51
1:B:55:PRO:HD3	1:B:326:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:LEU:HD11	1:C:216:LEU:HB2	1.92	0.51
1:A:280:PHE:CE2	1:A:309:LEU:HD21	2.47	0.50
1:D:263:ASN:OD1	1:D:265:GLU:HG2	2.11	0.50
1:C:211:PRO:HD2	1:C:214:TRP:CG	2.46	0.50
1:D:221:LYS:HA	1:D:257:HIS:HB3	1.93	0.50
1:D:13:ARG:HH21	1:D:13:ARG:HG3	1.77	0.49
1:B:361:LEU:O	1:B:365:GLN:HG3	2.11	0.49
1:B:340:ILE:HG21	1:B:402:PRO:HB2	1.93	0.49
1:C:429:ILE:HG23	1:C:430:ILE:HG23	1.95	0.49
1:B:414:ARG:O	1:B:418:GLU:HG3	2.12	0.49
1:D:324:HIS:C	1:D:325:MET:HG3	2.36	0.49
1:D:340:ILE:HG21	1:D:402:PRO:HB2	1.94	0.48
1:B:44:THR:O	1:B:48:GLU:HG2	2.13	0.48
1:D:15:ASN:HD21	1:D:399:ALA:HA	1.79	0.47
1:D:320:PHE:CZ	1:D:322:PRO:HG3	2.49	0.47
1:A:76:ARG:HH11	1:A:419:ARG:HG2	1.79	0.47
1:D:221:LYS:HE2	1:D:223:TYR:O	2.15	0.47
1:A:54:VAL:HG23	1:A:95:THR:HB	1.97	0.47
1:A:56:SER:O	1:A:59:VAL:HG12	2.15	0.47
1:C:382:ARG:HD3	4:C:458:HOH:O	2.13	0.46
1:C:15:ASN:HD21	1:C:399:ALA:HA	1.80	0.46
1:D:66:PHE:O	1:D:67:ALA:HB2	2.15	0.46
1:A:301:ARG:HD3	4:A:574:HOH:O	2.16	0.46
1:D:238:ASN:ND2	1:D:251:CYS:HB3	2.31	0.46
1:B:321:HIS:N	1:B:322:PRO:HD3	2.29	0.46
1:C:102:ILE:CG2	1:C:103:PRO:HA	2.46	0.46
1:A:221:LYS:HE2	1:A:223:TYR:O	2.16	0.45
1:D:361:LEU:O	1:D:365:GLN:HG3	2.16	0.45
1:A:59:VAL:HG22	1:A:59:VAL:O	2.16	0.45
1:D:15:ASN:HD21	1:D:400:VAL:H	1.62	0.45
1:A:65:ARG:HD3	4:A:1237:HOH:O	2.17	0.45
1:C:68:ARG:NH1	1:C:70:PRO:HB3	2.31	0.45
1:C:68:ARG:HH12	1:C:70:PRO:HB3	1.82	0.44
1:C:193:THR:O	1:C:197:GLU:HG3	2.16	0.44
1:C:311:ASP:O	1:C:315:ARG:HG3	2.17	0.44
1:A:108:ASP:OD2	1:A:110:LYS:HB2	2.17	0.44
1:C:102:ILE:HG23	1:C:103:PRO:HA	2.00	0.44
1:D:311:ASP:O	1:D:315:ARG:HG3	2.17	0.44
1:A:414:ARG:O	1:A:418:GLU:HG3	2.18	0.44
1:D:277:LEU:HD23	1:D:320:PHE:CZ	2.53	0.43
1:A:129:ASN:N	1:A:160:HIS:HE1	1.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ASP:HB3	1:C:337:GLU:HG3	1.99	0.43
1:D:8:GLN:HG3	4:D:623:HOH:O	2.18	0.43
1:B:177:THR:HG23	1:B:252:LEU:CD1	2.49	0.43
1:C:316:GLY:O	1:C:318:LYS:N	2.52	0.43
1:B:315:ARG:HH11	1:B:315:ARG:HG3	1.82	0.43
1:D:252:LEU:HD21	1:D:281:HIS:CG	2.53	0.43
1:D:208:LYS:HE3	1:D:208:LYS:HB2	1.88	0.43
1:D:165:ILE:O	1:D:169:LYS:HG3	2.19	0.43
1:A:180:ILE:HD12	1:A:182:ASP:CG	2.44	0.42
1:B:325:MET:HG2	1:B:326:ILE:N	2.34	0.42
1:D:129:ASN:OD1	1:D:129:ASN:C	2.62	0.42
1:B:386:GLU:N	1:B:387:PRO:CD	2.82	0.42
1:D:59:VAL:HG11	1:D:84:ASP:HB2	2.01	0.42
1:B:40:ILE:HG23	1:B:41:GLU:N	2.35	0.42
1:B:311:ASP:O	1:B:315:ARG:NH1	2.53	0.42
1:A:160:HIS:HD2	4:A:1247:HOH:O	2.03	0.42
1:C:76:ARG:HD3	1:C:420:PRO:CD	2.50	0.42
1:B:49:LYS:HE2	4:B:1177:HOH:O	2.20	0.41
1:A:66:PHE:HE1	3:B:602:PSV:H6	1.85	0.41
1:B:68:ARG:HH12	1:B:70:PRO:HB3	1.86	0.41
1:D:115:ARG:HA	1:D:115:ARG:HD2	1.85	0.41
1:D:336:ILE:O	1:D:340:ILE:HG13	2.20	0.41
1:D:59:VAL:HG21	1:D:85:CYS:SG	2.61	0.41
1:B:221:LYS:HE2	1:B:223:TYR:O	2.20	0.41
1:C:242:ALA:HB1	1:C:276:LYS:HD2	2.03	0.41
1:D:53:ALA:HB3	1:D:325:MET:HG2	2.02	0.41
1:D:56:SER:O	1:D:81:LYS:HD3	2.21	0.41
1:D:252:LEU:HD21	1:D:281:HIS:CD2	2.55	0.41
1:C:316:GLY:O	1:C:317:VAL:C	2.64	0.41
1:C:263:ASN:OD1	1:C:265:GLU:HG2	2.22	0.40
1:A:23:LYS:NZ	1:A:27:GLU:OE2	2.52	0.40
1:C:180:ILE:HD12	1:C:182:ASP:CG	2.46	0.40
1:B:220:HIS:HA	1:B:232:VAL:HG12	2.04	0.40
1:B:340:ILE:CG2	1:B:402:PRO:HB2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/438 (96%)	408 (97%)	10 (2%)	1 (0%)	43	36
1	B	419/438 (96%)	406 (97%)	12 (3%)	1 (0%)	43	36
1	C	426/438 (97%)	415 (97%)	9 (2%)	2 (0%)	24	16
1	D	417/438 (95%)	405 (97%)	11 (3%)	1 (0%)	43	36
All	All	1681/1752 (96%)	1634 (97%)	42 (2%)	5 (0%)	36	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	317	VAL
1	A	224	GLU
1	B	224	GLU
1	C	224	GLU
1	D	224	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/341 (97%)	327 (99%)	3 (1%)	70	73
1	B	330/341 (97%)	326 (99%)	4 (1%)	63	63
1	C	333/341 (98%)	331 (99%)	2 (1%)	78	81
1	D	329/341 (96%)	327 (99%)	2 (1%)	78	81
All	All	1322/1364 (97%)	1311 (99%)	11 (1%)	73	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	SER
1	A	374	THR
1	A	377	LEU
1	B	99	SER
1	B	110	LYS
1	B	354	LEU
1	B	374	THR
1	C	371	LEU
1	C	374	THR
1	D	371	LEU
1	D	374	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) 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	344	ASN
1	B	8	GLN
1	B	15	ASN
1	B	160	HIS
1	B	189	GLN
1	B	243	GLN
1	B	258	HIS
1	B	281	HIS
1	B	344	ASN
1	C	8	GLN
1	C	15	ASN
1	C	150	ASN
1	C	160	HIS
1	C	189	GLN
1	C	243	GLN
1	C	258	HIS
1	C	324	HIS
1	C	344	ASN
1	D	8	GLN
1	D	15	ASN
1	D	150	ASN

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Mol	Chain	Res	Type
1	D	160	HIS
1	D	189	GLN
1	D	258	HIS
1	D	328	GLN
1	D	344	ASN
1	D	365	GLN

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 oligosaccharides 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	PSV	B	602	2	11,12,12	0.41	0	10,18,18	0.63	0
3	PSV	D	604	2	11,12,12	0.38	0	10,18,18	0.56	0
3	PSV	A	601	2	11,12,12	0.31	0	10,18,18	0.51	0
3	PSV	C	603	2	11,12,12	0.38	0	10,18,18	0.61	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	PSV	B	602	2	-	3/5/24/24	0/1/1/1
3	PSV	D	604	2	-	3/5/24/24	0/1/1/1
3	PSV	A	601	2	-	3/5/24/24	0/1/1/1
3	PSV	C	603	2	-	3/5/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	603	PSV	O5-C5-C6-O6
3	B	602	PSV	C4-C5-C6-O6
3	C	603	PSV	C4-C5-C6-O6
3	B	602	PSV	O5-C5-C6-O6
3	D	604	PSV	C4-C5-C6-O6
3	D	604	PSV	O5-C5-C6-O6
3	A	601	PSV	C4-C5-C6-O6
3	A	601	PSV	O5-C5-C6-O6
3	A	601	PSV	O1-C1-C2-C3
3	B	602	PSV	O1-C1-C2-C3
3	D	604	PSV	O1-C1-C2-C3
3	C	603	PSV	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	PSV	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%)	-0.35	4 (0%) 79 82	5, 11, 23, 35	0
1	B	421/438 (96%)	-0.13	11 (2%) 57 61	6, 13, 27, 46	0
1	C	428/438 (97%)	0.05	18 (4%) 40 43	6, 15, 33, 57	0
1	D	419/438 (95%)	-0.25	5 (1%) 76 79	6, 12, 25, 48	0
All	All	1689/1752 (96%)	-0.17	38 (2%) 62 66	5, 13, 28, 57	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	427	GLY	6.8
1	C	319	GLY	5.5
1	B	316	GLY	4.9
1	C	317	VAL	4.6
1	C	316	GLY	4.6
1	B	317	VAL	4.2
1	C	428	GLY	4.2
1	D	421	ALA	4.0
1	B	280	PHE	4.0
1	B	423	VAL	3.8
1	B	315	ARG	3.6
1	C	430	ILE	3.6
1	C	318	LYS	3.6
1	B	421	ALA	3.5
1	B	424	ALA	3.5
1	D	420	PRO	3.4
1	D	3	GLU	3.3
1	A	423	VAL	3.3
1	C	426	GLY	3.3
1	C	315	ARG	3.2
1	C	314	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	424	ALA	3.0
1	C	280	PHE	2.9
1	A	319	GLY	2.8
1	C	321	HIS	2.7
1	C	429	ILE	2.7
1	C	323	ALA	2.6
1	A	320	PHE	2.5
1	C	425	GLY	2.4
1	B	4	PHE	2.3
1	B	422	SER	2.2
1	D	4	PHE	2.2
1	B	314	ALA	2.2
1	C	167	ILE	2.2
1	C	367	ASP	2.1
1	B	312	ALA	2.1
1	D	417	ALA	2.0
1	C	320	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(Å ²)	Q<0.9
3	PSV	B	602	12/12	0.80	0.16	26,30,33,37	0
3	PSV	C	603	12/12	0.83	0.15	26,31,34,38	0
3	PSV	D	604	12/12	0.90	0.10	15,21,27,30	0
3	PSV	A	601	12/12	0.91	0.10	12,19,25,29	0
2	MN	B	504	1/1	0.98	0.06	22,22,22,22	0
2	MN	B	503	1/1	0.99	0.06	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	A	501	1/1	0.99	0.05	13,13,13,13	0
2	MN	C	505	1/1	0.99	0.06	21,21,21,21	0
2	MN	D	508	1/1	0.99	0.04	14,14,14,14	0
2	MN	D	507	1/1	1.00	0.02	13,13,13,13	0
2	MN	A	502	1/1	1.00	0.02	13,13,13,13	0
2	MN	C	506	1/1	1.00	0.03	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.