



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:49 PM UTC

PDB ID : 3M0X / pdb_00003m0x
Title : Crystal structure of Pseudomonas stutzeri L-rhamnose isomerase mutant S329L in complex with D-psicose
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

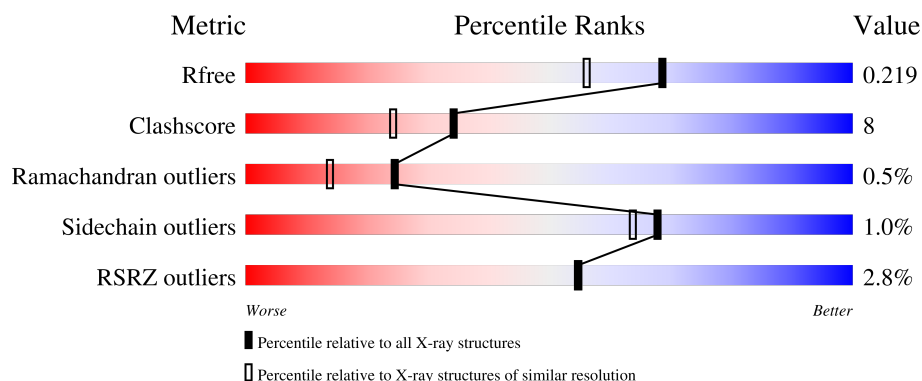
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

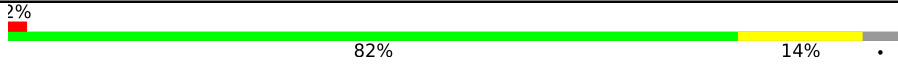
The reported resolution of this entry is 1.79 Å.

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 14571 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	430	Total	C	N	O	S	0	0	0
			3313	2081	593	630	9			
1	D	419	Total	C	N	O	S	0	0	0
			3253	2045	582	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	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...

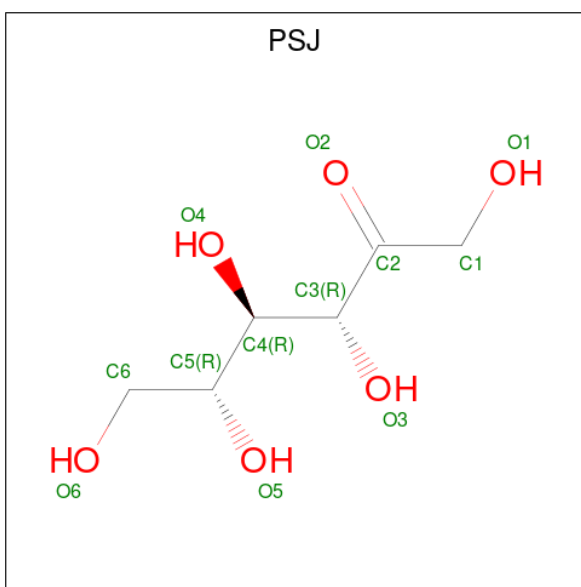
Continued from previous page...

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 D-psicose (CCD ID: PSJ) (formula: C₆H₁₂O₆).



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

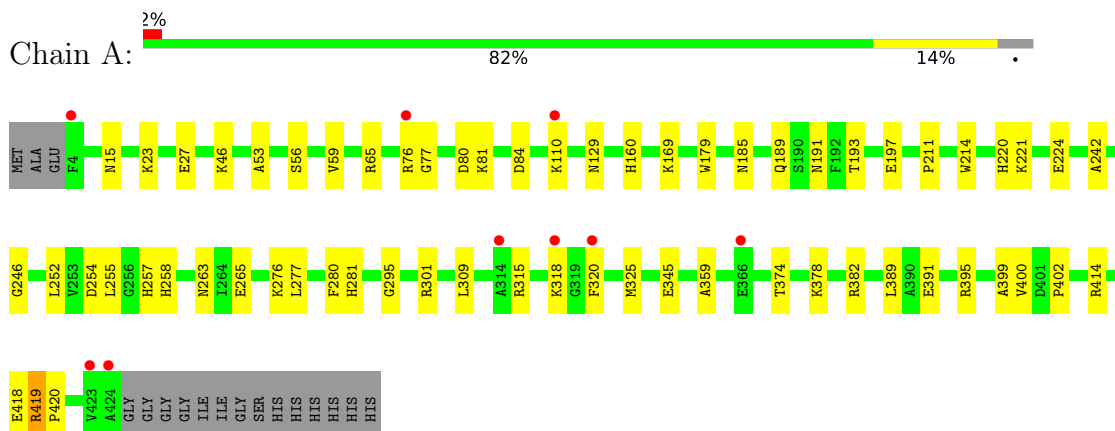
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	367	Total O 367 367	0	0
4	B	361	Total O 361 361	0	0
4	C	320	Total O 320 320	0	0
4	D	377	Total O 377 377	0	0

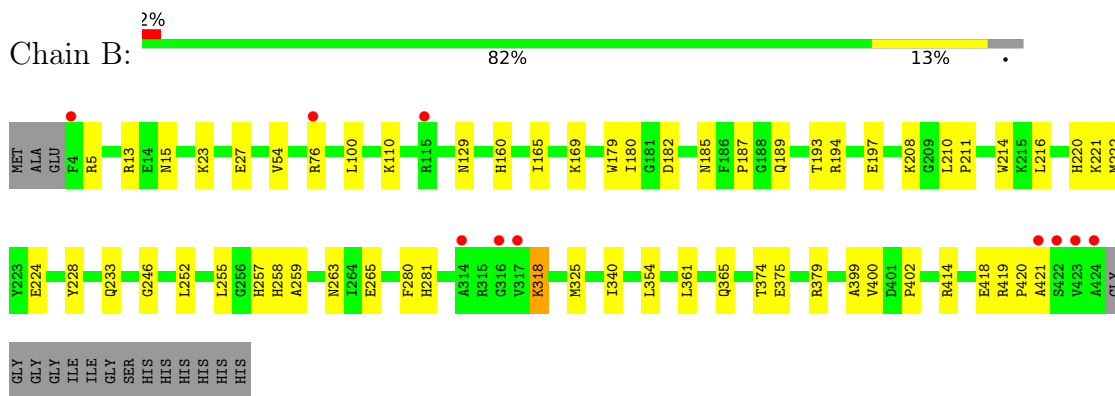
3 Residue-property plots [i](#)

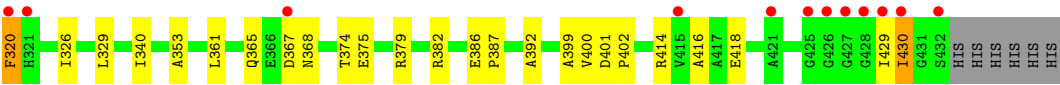
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

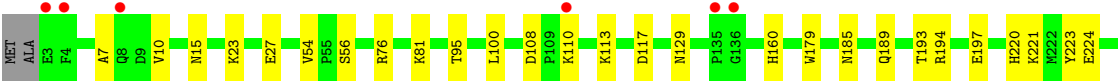
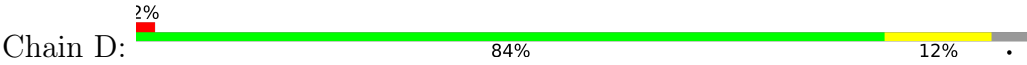


- Molecule 1: L-rhamnose isomerase





● 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	74.71Å 104.53Å 115.83Å 90.00° 112.03° 90.00°	Depositor
Resolution (Å)	47.76 – 1.79 47.76 – 1.79	Depositor EDS
% Data completeness (in resolution range)	91.8 (47.76-1.79) 91.9 (47.76-1.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.42 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.218 0.197 , 0.219	Depositor DCC
R_{free} test set	14123 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.2	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	0.93	EDS
Total number of atoms	14571	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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, PSJ

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	0.37	0/3334	0.85	6/4521 (0.1%)
1	B	0.36	0/3334	0.83	3/4521 (0.1%)
1	C	0.35	0/3385	0.84	7/4588 (0.2%)
1	D	0.35	0/3325	0.83	2/4508 (0.0%)
All	All	0.36	0/13378	0.84	18/18138 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	246	GLY	CA-C-N	7.12	127.73	119.47
1	C	246	GLY	C-N-CA	7.12	127.73	119.47
1	A	246	GLY	CA-C-N	6.44	126.20	119.05
1	A	246	GLY	C-N-CA	6.44	126.20	119.05
1	A	191	ASN	N-CA-C	-5.92	98.87	108.41
1	A	359	ALA	N-CA-C	-5.82	104.30	111.40
1	D	233	GLN	N-CA-C	5.81	119.55	112.23
1	C	227	PHE	N-CA-C	5.72	120.27	112.88
1	A	255	LEU	N-CA-C	5.67	118.18	111.33
1	B	246	GLY	CA-C-N	5.59	125.96	119.47
1	B	246	GLY	C-N-CA	5.59	125.96	119.47
1	C	401	ASP	CA-C-N	5.49	124.95	119.24
1	C	401	ASP	C-N-CA	5.49	124.95	119.24
1	A	419	ARG	N-CA-C	5.33	117.35	109.62
1	C	255	LEU	N-CA-C	5.32	117.76	111.33
1	B	233	GLN	N-CA-C	5.15	118.72	112.23
1	C	233	GLN	N-CA-C	5.13	118.70	112.23
1	D	255	LEU	N-CA-C	5.12	117.53	111.33

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	44	0
1	B	3262	0	3171	43	0
1	C	3313	0	3219	72	0
1	D	3253	0	3158	36	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	2	0
3	B	12	0	10	3	0
3	C	12	0	10	2	0
3	D	12	0	10	3	0
4	A	367	0	0	5	0
4	B	361	0	0	10	0
4	C	320	0	0	4	0
4	D	377	0	0	2	0
All	All	14571	0	12759	197	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (197) 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	1.05	0.98
1:A:56:SER:O	1:A:59:VAL:HG12	1.74	0.88
1:B:129:ASN:H	1:B:160:HIS:HE1	1.17	0.88
1:A:129:ASN:H	1:A:160:HIS:CE1	1.90	0.87
1:C:129:ASN:H	1:C:160:HIS:HE1	1.24	0.83
1:C:6:ILE:HD11	1:C:87:VAL:HG13	1.59	0.83
1:C:68:ARG:HH12	1:C:70:PRO:HB3	1.46	0.79
1:C:129:ASN:H	1:C:160:HIS:CE1	2.02	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HH11	1:A:419:ARG:HG2	1.50	0.76
1:B:129:ASN:H	1:B:160:HIS:CE1	2.04	0.75
1:D:129:ASN:H	1:D:160:HIS:HE1	1.32	0.75
1:C:220:HIS:HE2	1:C:258:HIS:CE1	2.05	0.74
1:B:220:HIS:HE2	1:B:258:HIS:CE1	2.05	0.73
1:D:185:ASN:H	1:D:189:GLN:HE22	1.37	0.72
1:B:23:LYS:O	1:B:27:GLU:HG3	1.91	0.71
1:A:129:ASN:N	1:A:160:HIS:HE1	1.85	0.70
1:D:129:ASN:H	1:D:160:HIS:CE1	2.09	0.70
1:D:220:HIS:HE2	1:D:258:HIS:CE1	2.10	0.69
1:B:220:HIS:HE2	1:B:258:HIS:HE1	1.39	0.69
1:C:220:HIS:HE2	1:C:258:HIS:HE1	1.41	0.69
1:C:68:ARG:NH1	1:C:70:PRO:HB3	2.09	0.68
1:C:185:ASN:H	1:C:189:GLN:HE22	1.40	0.68
1:A:15:ASN:ND2	1:A:400:VAL:H	1.91	0.68
1:D:185:ASN:H	1:D:189:GLN:NE2	1.93	0.66
1:B:414:ARG:O	1:B:418:GLU:HG3	1.96	0.65
1:A:110:LYS:HD2	1:A:110:LYS:H	1.62	0.65
1:B:110:LYS:HG3	4:B:1084:HOH:O	1.97	0.65
1:C:185:ASN:H	1:C:189:GLN:NE2	1.95	0.64
1:B:15:ASN:ND2	1:B:400:VAL:H	1.97	0.63
1:C:6:ILE:HD11	1:C:87:VAL:HG22	1.80	0.63
1:B:361:LEU:O	1:B:365:GLN:HG3	1.99	0.62
1:C:210:LEU:HD11	1:C:216:LEU:HB2	1.81	0.62
1:C:44:THR:O	1:C:48:GLU:HG3	1.99	0.62
1:D:23:LYS:O	1:D:27:GLU:HG3	1.99	0.62
1:C:6:ILE:HD12	1:C:6:ILE:N	2.15	0.62
1:D:220:HIS:HE2	1:D:258:HIS:HE1	1.48	0.62
1:A:15:ASN:HD21	1:A:400:VAL:H	1.46	0.61
1:B:185:ASN:H	1:B:189:GLN:HE22	1.49	0.61
1:C:165:ILE:O	1:C:169:LYS:HG3	2.00	0.61
1:A:185:ASN:H	1:A:189:GLN:HE22	1.46	0.61
4:A:1210:HOH:O	1:C:243:GLN:HG2	2.02	0.60
1:C:429:ILE:HG23	1:C:430:ILE:HD12	1.83	0.60
1:C:15:ASN:ND2	1:C:400:VAL:H	2.00	0.60
1:A:220:HIS:HE2	1:A:258:HIS:CE1	2.20	0.59
1:B:15:ASN:HD21	1:B:400:VAL:H	1.52	0.57
1:B:13:ARG:HD2	4:B:1038:HOH:O	2.04	0.57
1:B:185:ASN:H	1:B:189:GLN:NE2	2.02	0.57
1:C:15:ASN:HD21	1:C:399:ALA:HA	1.69	0.57
1:D:402:PRO:HG2	4:D:563:HOH:O	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:ILE:HG21	1:C:402:PRO:HB2	1.87	0.56
1:D:378:LYS:HB3	1:D:382:ARG:NH2	2.21	0.56
1:C:179:TRP:CE2	3:C:603:PSJ:H1A	2.41	0.56
1:B:15:ASN:HD21	1:B:399:ALA:HA	1.71	0.56
1:B:165:ILE:O	1:B:169:LYS:HG3	2.06	0.55
1:B:375:GLU:O	1:B:379:ARG:HG3	2.06	0.55
1:C:18:ARG:HB3	4:C:544:HOH:O	2.06	0.55
1:C:311:ASP:O	1:C:315:ARG:HG2	2.07	0.55
1:B:402:PRO:HG2	4:B:454:HOH:O	2.06	0.54
1:B:179:TRP:CE2	3:B:602:PSJ:H1A	2.42	0.54
3:C:603:PSJ:O5	3:C:603:PSJ:C2	2.56	0.54
1:C:7:ALA:HB3	1:C:10:VAL:HG23	1.88	0.54
1:C:318:LYS:O	1:C:318:LYS:HG3	2.09	0.53
1:C:180:ILE:HD12	1:C:182:ASP:CG	2.33	0.53
1:D:179:TRP:CE2	3:D:604:PSJ:H1A	2.43	0.53
1:C:430:ILE:H	1:C:430:ILE:HD13	1.73	0.53
1:B:54:VAL:HG11	4:B:966:HOH:O	2.08	0.53
1:C:318:LYS:C	1:C:320:PHE:N	2.65	0.53
1:D:15:ASN:ND2	1:D:400:VAL:H	2.07	0.53
1:A:185:ASN:H	1:A:189:GLN:NE2	2.06	0.53
1:C:108:ASP:OD2	1:C:110:LYS:HB2	2.10	0.52
1:D:221:LYS:HA	1:D:257:HIS:HB3	1.90	0.52
1:A:263:ASN:OD1	1:A:265:GLU:HG2	2.10	0.52
1:C:315:ARG:O	1:C:316:GLY:C	2.53	0.52
1:C:5:ARG:HB2	1:C:6:ILE:HD12	1.91	0.52
1:A:76:ARG:HD3	1:A:80:ASP:OD2	2.10	0.51
1:C:6:ILE:CD1	1:C:87:VAL:HG22	2.41	0.51
1:C:429:ILE:HG23	1:C:430:ILE:CD1	2.40	0.51
1:C:15:ASN:HD21	1:C:400:VAL:H	1.58	0.51
1:A:301:ARG:HD3	4:A:473:HOH:O	2.10	0.51
1:A:242:ALA:HB1	1:A:276:LYS:HD2	1.93	0.51
1:B:263:ASN:OD1	1:B:265:GLU:HG2	2.11	0.51
1:C:211:PRO:HD2	1:C:214:TRP:CG	2.46	0.50
1:B:210:LEU:HD11	1:B:216:LEU:HB2	1.92	0.50
1:A:59:VAL:HG21	1:A:84:ASP:HB2	1.94	0.50
1:A:277:LEU:HD23	1:A:320:PHE:CE1	2.47	0.50
1:A:402:PRO:HG2	4:A:485:HOH:O	2.11	0.50
1:D:263:ASN:OD1	1:D:265:GLU:HG2	2.12	0.50
1:C:318:LYS:O	1:C:320:PHE:N	2.45	0.49
1:A:221:LYS:HA	1:A:257:HIS:HB3	1.94	0.49
1:D:15:ASN:HD21	1:D:399:ALA:HA	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ILE:HD11	1:C:87:VAL:CG1	2.36	0.49
1:C:318:LYS:O	1:C:319:GLY:C	2.54	0.49
1:B:76:ARG:HH11	1:B:76:ARG:HG2	1.78	0.48
1:C:367:ASP:HB3	4:C:1097:HOH:O	2.12	0.48
1:A:23:LYS:O	1:A:27:GLU:HG3	2.13	0.48
1:C:73:GLY:CA	1:C:416:ALA:HA	2.44	0.48
3:A:601:PSJ:O5	3:A:601:PSJ:C2	2.62	0.48
1:C:48:GLU:HG2	1:C:392:ALA:HB1	1.96	0.48
1:D:193:THR:O	1:D:197:GLU:HG3	2.13	0.48
1:A:15:ASN:HD21	1:A:399:ALA:HA	1.79	0.47
1:A:169:LYS:HD3	1:A:211:PRO:CG	2.44	0.47
1:A:277:LEU:HD23	1:A:320:PHE:HE1	1.79	0.47
1:C:263:ASN:OD1	1:C:265:GLU:HG2	2.13	0.47
1:A:220:HIS:HE2	1:A:258:HIS:HE1	1.59	0.47
1:B:318:LYS:O	1:B:318:LYS:HD3	2.13	0.47
1:C:361:LEU:O	1:C:365:GLN:HG3	2.15	0.47
1:D:194:ARG:HG2	1:D:194:ARG:HH11	1.79	0.47
3:D:604:PSJ:O5	3:D:604:PSJ:C2	2.63	0.47
1:D:108:ASP:OD2	1:D:110:LYS:HB2	2.15	0.47
1:D:242:ALA:HB1	1:D:276:LYS:HD2	1.96	0.46
1:B:76:ARG:HH22	1:B:421:ALA:HA	1.81	0.46
1:A:77:GLY:O	1:A:81:LYS:HG3	2.15	0.46
1:A:211:PRO:HD2	1:A:214:TRP:CG	2.50	0.46
1:C:315:ARG:O	1:C:315:ARG:HG3	2.16	0.46
1:D:56:SER:O	1:D:81:LYS:HD3	2.16	0.46
1:C:221:LYS:HA	1:C:257:HIS:HB3	1.98	0.46
1:B:211:PRO:HD2	1:B:214:TRP:CG	2.51	0.46
1:C:430:ILE:HD13	1:C:430:ILE:N	2.30	0.46
1:B:340:ILE:HG21	1:B:402:PRO:HB2	1.97	0.45
1:A:76:ARG:HD2	1:A:420:PRO:HD2	1.97	0.45
1:B:169:LYS:HD3	1:B:211:PRO:HG2	1.99	0.45
1:D:252:LEU:HD21	1:D:281:HIS:CG	2.52	0.45
1:C:310:VAL:HG21	1:C:353:ALA:CB	2.46	0.45
1:C:340:ILE:CG2	1:C:402:PRO:HB2	2.47	0.45
3:B:602:PSJ:O5	3:B:602:PSJ:C2	2.65	0.45
4:B:590:HOH:O	1:C:382:ARG:HD3	2.16	0.45
1:D:113:LYS:NZ	1:D:117:ASP:OD2	2.49	0.45
1:B:208:LYS:HG2	4:B:835:HOH:O	2.16	0.45
1:C:367:ASP:O	1:C:368:ASN:HB2	2.17	0.44
1:D:15:ASN:HD21	1:D:400:VAL:H	1.64	0.44
1:C:78:ILE:HD13	1:C:105:ASP:CG	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:VAL:CG1	1:C:318:LYS:N	2.79	0.44
1:A:391:GLU:O	1:A:395:ARG:HG3	2.17	0.44
1:B:221:LYS:HG3	1:B:257:HIS:CG	2.52	0.44
1:B:180:ILE:HD12	1:B:182:ASP:CG	2.41	0.44
1:A:59:VAL:HG11	1:A:81:LYS:HB3	1.98	0.44
1:C:310:VAL:HG21	1:C:353:ALA:HB3	2.00	0.44
1:C:375:GLU:O	1:C:379:ARG:HG3	2.17	0.44
1:A:280:PHE:CE2	1:A:309:LEU:HD21	2.53	0.44
1:B:221:LYS:HA	1:B:257:HIS:HB3	1.99	0.43
1:C:193:THR:O	1:C:197:GLU:HG3	2.18	0.43
1:B:194:ARG:NH2	4:B:707:HOH:O	2.50	0.43
1:C:13:ARG:HD2	4:C:915:HOH:O	2.16	0.43
1:A:193:THR:O	1:A:197:GLU:HG3	2.17	0.43
1:D:221:LYS:HE2	1:D:223:TYR:O	2.18	0.43
1:D:378:LYS:HB3	1:D:382:ARG:CZ	2.48	0.43
1:D:386:GLU:N	1:D:387:PRO:CD	2.82	0.43
1:A:414:ARG:O	1:A:418:GLU:HG3	2.19	0.43
1:C:252:LEU:HD21	1:C:281:HIS:CG	2.54	0.43
1:D:295:GLY:HA3	1:D:345:GLU:HG2	2.01	0.43
1:B:280:PHE:O	1:B:325:MET:HE3	2.17	0.43
1:C:55:PRO:HD3	1:C:326:ILE:O	2.19	0.43
1:B:169:LYS:HA	4:B:720:HOH:O	2.19	0.43
1:D:76:ARG:HD3	1:D:420:PRO:HD2	2.00	0.43
1:A:179:TRP:CE2	3:A:601:PSJ:H1A	2.54	0.43
1:A:295:GLY:HA3	1:A:345:GLU:HG2	2.01	0.43
1:A:254:ASP:HA	1:A:281:HIS:HB2	2.01	0.42
1:A:65:ARG:HG2	4:A:615:HOH:O	2.18	0.42
1:C:65:ARG:HG2	4:D:441:HOH:O	2.19	0.42
1:D:108:ASP:OD2	1:D:110:LYS:HE2	2.20	0.42
1:C:56:SER:O	1:C:59:VAL:HG22	2.19	0.42
1:D:179:TRP:CD2	3:D:604:PSJ:H1A	2.55	0.42
1:A:252:LEU:HD21	1:A:281:HIS:CG	2.55	0.42
1:B:193:THR:O	1:B:197:GLU:HG3	2.20	0.42
1:C:194:ARG:O	1:C:198:ARG:HG3	2.20	0.41
1:A:280:PHE:CZ	1:A:309:LEU:HD21	2.55	0.41
1:D:129:ASN:OD1	1:D:129:ASN:C	2.63	0.41
1:B:76:ARG:HH11	1:B:76:ARG:CG	2.32	0.41
1:A:59:VAL:HG11	1:A:81:LYS:CB	2.51	0.41
1:B:252:LEU:HD21	1:B:281:HIS:CG	2.55	0.41
1:B:419:ARG:HA	1:B:420:PRO:HD3	1.81	0.41
1:C:386:GLU:N	1:C:387:PRO:CD	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LYS:HD3	1:A:211:PRO:HG2	2.02	0.41
1:B:222:MET:CE	1:B:259:ALA:HB2	2.51	0.41
1:C:221:LYS:HE2	1:C:223:TYR:O	2.20	0.41
1:A:53:ALA:HB3	1:A:325:MET:HG2	2.02	0.41
1:C:6:ILE:HD11	1:C:87:VAL:CG2	2.50	0.41
1:C:54:VAL:HG13	1:C:55:PRO:HD2	2.01	0.41
1:C:102:ILE:CG2	1:C:103:PRO:HA	2.51	0.41
1:D:54:VAL:HG13	1:D:95:THR:HB	2.02	0.41
4:B:533:HOH:O	1:D:194:ARG:HD2	2.20	0.41
1:C:154:ARG:O	1:C:158:VAL:HG23	2.20	0.41
1:D:7:ALA:HB3	1:D:10:VAL:HG23	2.03	0.41
1:A:378:LYS:O	1:A:382:ARG:HG3	2.21	0.40
1:B:187:PRO:HG3	1:B:228:TYR:CE1	2.55	0.40
1:C:317:VAL:CG1	1:C:318:LYS:HG2	2.51	0.40
1:C:429:ILE:HG13	1:D:329:LEU:HD11	2.03	0.40
1:B:179:TRP:CD2	3:B:602:PSJ:H1A	2.55	0.40
1:A:46:LYS:HB3	1:A:46:LYS:HE2	1.88	0.40
1:C:414:ARG:O	1:C:418:GLU:HG3	2.21	0.40
1:A:315:ARG:NH2	4:A:531:HOH:O	2.54	0.40
1:B:5:ARG:HG2	4:B:1235:HOH:O	2.20	0.40
1:B:169:LYS:HD3	1:B:211:PRO:CG	2.51	0.40
1:C:329:LEU:HG	4:C:1301:HOH:O	2.21	0.40
1:C:429:ILE:HG13	1:D:329:LEU:CD1	2.51	0.40
1:C:7:ALA:HB3	1:C:10:VAL:CG2	2.52	0.40
1:D:411:TYR:O	1:D:414:ARG:HB3	2.22	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%)	410 (98%)	8 (2%)	1 (0%)	43 31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	419/438 (96%)	409 (98%)	9 (2%)	1 (0%)	43	31
1	C	428/438 (98%)	412 (96%)	11 (3%)	5 (1%)	10	3
1	D	417/438 (95%)	407 (98%)	9 (2%)	1 (0%)	43	31
All	All	1683/1752 (96%)	1638 (97%)	37 (2%)	8 (0%)	24	14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	316	GLY
1	C	318	LYS
1	C	320	PHE
1	A	224	GLU
1	B	224	GLU
1	C	224	GLU
1	D	224	GLU
1	C	319	GLY

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	67
1	B	330/341 (97%)	325 (98%)	5 (2%)	57	49
1	C	334/341 (98%)	332 (99%)	2 (1%)	78	77
1	D	329/341 (96%)	326 (99%)	3 (1%)	70	67
All	All	1323/1364 (97%)	1310 (99%)	13 (1%)	68	64

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	LYS
1	A	374	THR
1	A	389	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	100	LEU
1	B	255	LEU
1	B	318	LYS
1	B	354	LEU
1	B	374	THR
1	C	374	THR
1	C	430	ILE
1	D	100	LEU
1	D	374	THR
1	D	389	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) 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	331	ASN
1	B	15	ASN
1	B	160	HIS
1	B	189	GLN
1	B	250	GLN
1	B	258	HIS
1	B	328	GLN
1	B	344	ASN
1	C	15	ASN
1	C	127	ASN
1	C	160	HIS
1	C	189	GLN
1	C	258	HIS
1	C	344	ASN
1	D	15	ASN
1	D	127	ASN
1	D	160	HIS
1	D	189	GLN
1	D	258	HIS

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	PSJ	C	603	2	11,11,11	0.42	0	10,14,14	0.69	0
3	PSJ	D	604	2	11,11,11	0.51	0	10,14,14	0.63	0
3	PSJ	B	602	2	11,11,11	0.57	0	10,14,14	0.63	0
3	PSJ	A	601	2	11,11,11	0.50	0	10,14,14	0.56	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	PSJ	C	603	2	-	1/16/16/16	-
3	PSJ	D	604	2	-	0/16/16/16	-
3	PSJ	B	602	2	-	0/16/16/16	-
3	PSJ	A	601	2	-	0/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	603	PSJ	O2-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	PSJ	2	0
3	D	604	PSJ	3	0
3	B	602	PSJ	3	0
3	A	601	PSJ	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, 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%)	0.13	9 (2%) 63 64	8, 14, 25, 39	0
1	B	421/438 (96%)	0.23	10 (2%) 59 60	8, 15, 26, 47	0
1	C	430/438 (98%)	0.48	22 (5%) 33 32	8, 17, 33, 53	0
1	D	419/438 (95%)	0.16	7 (1%) 69 69	8, 14, 25, 46	0
All	All	1691/1752 (96%)	0.25	48 (2%) 55 55	8, 15, 28, 53	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	317	VAL	7.0
1	B	424	ALA	6.2
1	B	423	VAL	5.9
1	B	421	ALA	4.9
1	C	314	ALA	4.8
1	B	422	SER	4.7
1	C	319	GLY	4.7
1	D	421	ALA	4.5
1	C	320	PHE	4.4
1	C	318	LYS	4.3
1	C	315	ARG	3.9
1	C	316	GLY	3.8
1	D	4	PHE	3.8
1	C	3	GLU	3.8
1	A	320	PHE	3.6
1	A	424	ALA	3.5
1	A	4	PHE	3.2
1	C	428	GLY	3.2
1	C	432	SER	3.1
1	C	321	HIS	3.1
1	C	430	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	4	PHE	3.0
1	A	318	LYS	2.9
1	B	317	VAL	2.7
1	C	429	ILE	2.7
1	A	423	VAL	2.7
1	A	314	ALA	2.7
1	C	426	GLY	2.6
1	C	427	GLY	2.6
1	D	135	PRO	2.6
1	D	3	GLU	2.6
1	D	8	GLN	2.5
1	A	110	LYS	2.5
1	D	110	LYS	2.5
1	C	421	ALA	2.5
1	C	425	GLY	2.5
1	B	316	GLY	2.4
1	A	76	ARG	2.4
1	B	4	PHE	2.3
1	C	312	ALA	2.3
1	D	136	GLY	2.2
1	C	415	VAL	2.1
1	B	115	ARG	2.1
1	C	367	ASP	2.1
1	A	366	GLU	2.1
1	B	76	ARG	2.1
1	B	314	ALA	2.0
1	C	76	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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	PSJ	D	604	12/12	0.92	0.09	10,14,18,20	0
3	PSJ	B	602	12/12	0.93	0.08	10,14,19,21	0
3	PSJ	C	603	12/12	0.95	0.06	10,16,19,19	0
3	PSJ	A	601	12/12	0.95	0.07	13,17,21,21	0
2	MN	D	508	1/1	0.99	0.03	11,11,11,11	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	15,15,15,15	0
2	MN	C	506	1/1	0.99	0.02	12,12,12,12	0
2	MN	D	507	1/1	0.99	0.01	11,11,11,11	0
2	MN	A	501	1/1	1.00	0.03	13,13,13,13	0
2	MN	A	502	1/1	1.00	0.03	10,10,10,10	0
2	MN	B	503	1/1	1.00	0.01	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.