



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:04 PM UTC

PDB ID : 3M0M / pdb_00003m0m
Title : Crystal structure of Pseudomonas stutzeri L-rhamnose isomerase mutant S329F in complex with D-allose
Authors : Yoshida, H.; Takeda, K.; Izumori, K.; Kamitori, S.
Deposited on : 2010-03-03
Resolution : 1.45 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

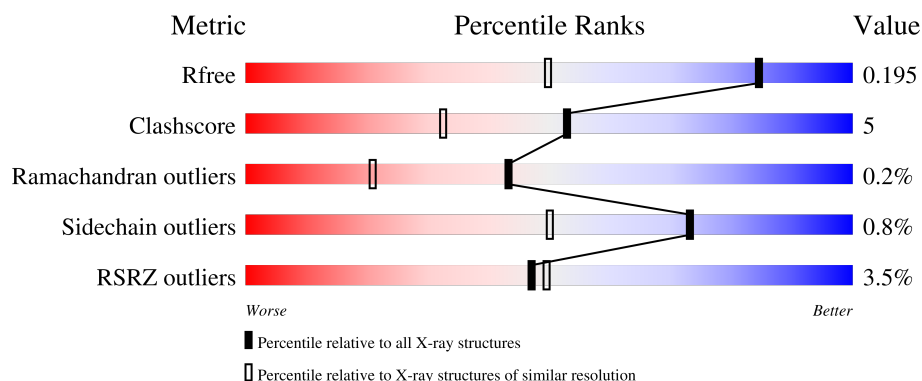
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	3% 83% 12% .
1	B	438	2% 87% 9% .
1	C	438	8% 85% 13% .
1	D	438	% 84% 11% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14910 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
			3265	2054	584	618	9			
1	B	421	Total	C	N	O	S	0	0	0
			3265	2054	584	618	9			
1	C	431	Total	C	N	O	S	0	0	0
			3326	2090	596	631	9			
1	D	419	Total	C	N	O	S	0	0	0
			3256	2048	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	PHE	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	PHE	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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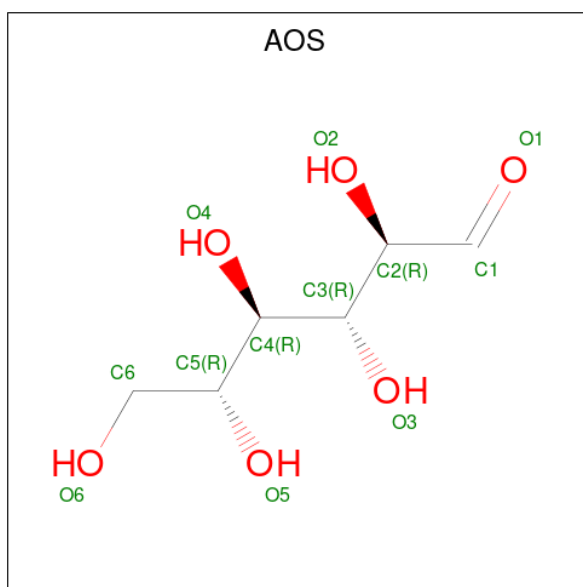
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Chain	Residue	Modelled	Actual	Comment	Reference
C	329	PHE	SER	engineered mutation	UNP Q75WH8
C	431	GLY	-	expression tag	UNP Q75WH8
C	432	SER	-	expression tag	UNP Q75WH8
C	433	HIS	-	expression tag	UNP Q75WH8
C	434	HIS	-	expression tag	UNP Q75WH8
C	435	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	PHE	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-ALLOSE (CCD ID: AOS) (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		

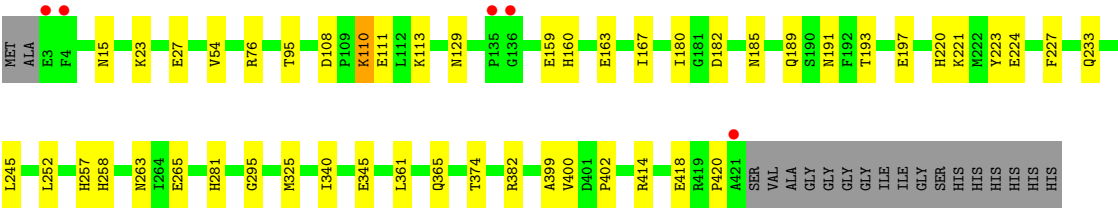
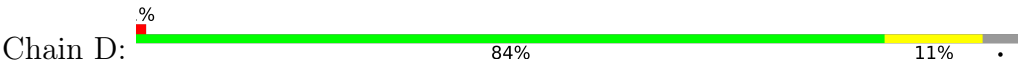
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	452	Total	O	0	0
			452	452		
4	B	448	Total	O	0	0
			448	448		
4	C	397	Total	O	0	0
			397	397		
4	D	445	Total	O	0	0
			445	445		

- 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	74.62Å 104.26Å 111.45Å 90.00° 106.20° 90.00°	Depositor
Resolution (Å)	30.10 – 1.45 30.10 – 1.45	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.10-1.45) 95.3 (30.10-1.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.177 , 0.196 0.177 , 0.195	Depositor DCC
R_{free} test set	27405 reflections (9.55%)	wwPDB-VP
Wilson B-factor (Å ²)	12.1	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14910	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 4.51% 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: AOS, 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	0.33	0/3338	0.82	10/4526 (0.2%)
1	B	0.33	0/3338	0.81	4/4526 (0.1%)
1	C	0.32	0/3400	0.81	6/4608 (0.1%)
1	D	0.32	0/3329	0.81	4/4513 (0.1%)
All	All	0.33	0/13405	0.81	24/18173 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ILE	N-CA-C	6.25	117.00	110.62
1	C	401	ASP	CA-C-N	6.12	125.60	119.24
1	C	401	ASP	C-N-CA	6.12	125.60	119.24
1	D	233	GLN	N-CA-C	5.95	119.73	112.23
1	A	191	ASN	N-CA-C	-5.86	98.98	108.41
1	C	233	GLN	N-CA-C	5.59	119.27	112.23
1	D	245	LEU	N-CA-C	5.38	117.23	111.36
1	C	334	ASP	N-CA-C	-5.38	101.47	109.42
1	B	233	GLN	N-CA-C	5.37	119.00	112.23
1	A	227	PHE	N-CA-C	5.36	119.80	112.88
1	B	227	PHE	N-CA-C	5.34	119.49	112.92
1	B	401	ASP	CA-C-N	5.32	124.78	119.24
1	B	401	ASP	C-N-CA	5.32	124.78	119.24
1	D	191	ASN	N-CA-C	-5.22	99.27	108.20
1	A	233	GLN	N-CA-C	5.13	118.70	112.23
1	C	191	ASN	N-CA-C	-5.12	99.44	108.20
1	C	227	PHE	N-CA-C	5.08	119.44	112.88
1	A	76	ARG	CA-C-N	-5.05	115.42	122.85
1	A	76	ARG	C-N-CA	-5.05	115.42	122.85
1	A	255	LEU	N-CA-C	5.03	117.42	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	401	ASP	CA-C-N	5.01	124.45	119.24
1	A	401	ASP	C-N-CA	5.01	124.45	119.24
1	D	227	PHE	N-CA-C	5.01	119.34	112.88
1	A	359	ALA	N-CA-C	-5.00	105.73	111.14

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	3265	0	3169	37	0
1	B	3265	0	3169	24	0
1	C	3326	0	3224	37	0
1	D	3256	0	3156	29	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	1	0
3	B	12	0	10	1	0
3	C	12	0	10	2	0
3	D	12	0	10	2	0
4	A	452	0	0	3	0
4	B	448	0	0	2	0
4	C	397	0	0	0	0
4	D	445	0	0	1	0
All	All	14910	0	12758	130	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (130) 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:76:ARG:HD3	1:A:420:PRO:HD2	1.39	1.03
1:C:68:ARG:HH12	1:C:70:PRO:HB3	1.36	0.88
1:B:129:ASN:H	1:B:160:HIS:HE1	1.22	0.87
1:A:129:ASN:H	1:A:160:HIS:HE1	1.17	0.87
1:C:129:ASN:H	1:C:160:HIS:HE1	1.21	0.85
1:C:317:VAL:O	1:C:320:PHE:HB3	1.79	0.82
1:A:129:ASN:H	1:A:160:HIS:CE1	2.00	0.80
1:D:129:ASN:H	1:D:160:HIS:HE1	1.26	0.80
1:A:56:SER:O	1:A:59:VAL:HG12	1.85	0.76
1:C:129:ASN:H	1:C:160:HIS:CE1	2.04	0.75
1:B:129:ASN:H	1:B:160:HIS:CE1	2.06	0.73
1:D:129:ASN:H	1:D:160:HIS:CE1	2.07	0.72
1:D:163:GLU:O	1:D:167:ILE:HD13	1.90	0.72
1:A:362:SER:O	1:A:366:GLU:HG3	1.91	0.71
1:D:220:HIS:HE2	1:D:258:HIS:CE1	2.10	0.69
1:C:220:HIS:HE2	1:C:258:HIS:CE1	2.11	0.69
1:A:220:HIS:HE2	1:A:258:HIS:CE1	2.12	0.67
1:C:210:LEU:HD11	1:C:216:LEU:HB2	1.78	0.64
1:A:59:VAL:HG21	1:A:84:ASP:HB2	1.80	0.64
1:B:185:ASN:H	1:B:189:GLN:HE22	1.45	0.64
1:A:15:ASN:ND2	1:A:400:VAL:H	1.95	0.64
1:A:76:ARG:CD	1:A:420:PRO:HD2	2.24	0.63
1:C:23:LYS:O	1:C:27:GLU:HG3	1.98	0.62
1:C:429:ILE:HG23	1:C:430:ILE:HG23	1.80	0.62
1:C:185:ASN:H	1:C:189:GLN:HE22	1.45	0.62
1:B:185:ASN:H	1:B:189:GLN:NE2	1.98	0.62
1:D:220:HIS:HE2	1:D:258:HIS:HE1	1.46	0.61
1:A:15:ASN:HD21	1:A:400:VAL:H	1.47	0.61
1:C:68:ARG:NH1	1:C:70:PRO:HB3	2.10	0.60
1:A:185:ASN:H	1:A:189:GLN:HE22	1.47	0.60
1:B:23:LYS:O	1:B:27:GLU:HG3	2.02	0.60
1:A:220:HIS:HE2	1:A:258:HIS:HE1	1.51	0.59
1:B:15:ASN:ND2	1:B:400:VAL:H	2.01	0.58
1:D:23:LYS:O	1:D:27:GLU:HG3	2.03	0.58
1:D:15:ASN:ND2	1:D:400:VAL:H	2.02	0.58
1:B:414:ARG:O	1:B:418:GLU:HG3	2.04	0.57
1:C:185:ASN:H	1:C:189:GLN:NE2	2.03	0.57
1:C:312:ALA:HB1	1:C:317:VAL:HG21	1.86	0.57
1:D:108:ASP:OD2	1:D:111:GLU:HG3	2.04	0.57
1:A:318:LYS:O	1:A:318:LYS:HD3	2.05	0.57
1:A:185:ASN:H	1:A:189:GLN:NE2	2.02	0.57
1:B:295:GLY:HA3	1:B:345:GLU:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:HIS:HE2	1:C:258:HIS:HE1	1.53	0.56
1:D:185:ASN:H	1:D:189:GLN:NE2	2.04	0.56
1:D:185:ASN:H	1:D:189:GLN:HE22	1.52	0.56
1:B:361:LEU:O	1:B:365:GLN:HG3	2.06	0.55
1:A:280:PHE:CE2	1:A:309:LEU:HD21	2.41	0.55
1:B:15:ASN:HD21	1:B:399:ALA:HA	1.72	0.55
1:C:312:ALA:O	1:C:317:VAL:HG22	2.06	0.55
1:A:210:LEU:HD11	1:A:216:LEU:HB2	1.89	0.55
1:D:110:LYS:N	1:D:110:LYS:HD2	2.21	0.54
1:C:15:ASN:ND2	1:C:400:VAL:H	2.06	0.54
1:D:15:ASN:HD21	1:D:399:ALA:HA	1.73	0.54
1:C:15:ASN:HD21	1:C:399:ALA:HA	1.74	0.53
1:D:54:VAL:HG13	1:D:95:THR:HB	1.90	0.53
1:D:361:LEU:O	1:D:365:GLN:HG3	2.09	0.53
1:B:340:ILE:HG21	1:B:402:PRO:HB2	1.91	0.52
1:B:211:PRO:HD2	1:B:214:TRP:CG	2.44	0.52
1:C:318:LYS:C	1:C:320:PHE:H	2.16	0.52
1:C:340:ILE:HG21	1:C:402:PRO:HB2	1.92	0.51
1:B:15:ASN:HD21	1:B:400:VAL:H	1.57	0.51
1:D:193:THR:O	1:D:197:GLU:HG3	2.10	0.51
1:D:180:ILE:HD12	1:D:182:ASP:CG	2.36	0.51
1:C:56:SER:O	1:C:59:VAL:HG22	2.11	0.51
1:A:108:ASP:HB3	1:A:111:GLU:HG3	1.91	0.50
1:D:295:GLY:HA3	1:D:345:GLU:HG2	1.94	0.50
4:A:577:HOH:O	1:D:382:ARG:HD3	2.12	0.50
1:C:295:GLY:HA3	1:C:345:GLU:HG2	1.93	0.50
1:D:15:ASN:HD21	1:D:400:VAL:H	1.59	0.49
1:B:113:LYS:HE2	4:B:1288:HOH:O	2.12	0.49
1:D:257:HIS:HE1	3:D:3004:AOS:H2	1.78	0.49
1:D:414:ARG:O	1:D:418:GLU:HG3	2.13	0.49
1:C:317:VAL:O	1:C:317:VAL:HG23	2.13	0.48
1:A:263:ASN:OD1	1:A:265:GLU:HG2	2.14	0.48
1:C:311:ASP:O	1:C:315:ARG:HG2	2.13	0.48
1:C:314:ALA:C	1:C:316:GLY:H	2.21	0.48
1:A:361:LEU:O	1:A:365:GLN:HG3	2.14	0.48
1:C:108:ASP:OD2	1:C:111:GLU:HG3	2.14	0.48
1:D:221:LYS:HA	1:D:257:HIS:HB3	1.96	0.48
1:A:211:PRO:HD2	1:A:214:TRP:CG	2.49	0.47
1:C:193:THR:O	1:C:197:GLU:HG3	2.14	0.47
1:B:53:ALA:HB3	1:B:325:MET:HG2	1.96	0.47
1:C:211:PRO:HD2	1:C:214:TRP:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:HD21	1:A:281:HIS:CG	2.50	0.47
1:A:108:ASP:OD2	1:A:110:LYS:HB2	2.14	0.47
1:A:340:ILE:HG21	1:A:402:PRO:HB2	1.97	0.46
1:A:257:HIS:HE1	3:A:3001:AOS:H2	1.81	0.46
1:B:180:ILE:HD12	1:B:182:ASP:CG	2.41	0.46
1:D:159:GLU:O	1:D:163:GLU:HG3	2.16	0.46
1:A:280:PHE:CZ	1:A:309:LEU:HD21	2.52	0.45
1:A:15:ASN:HD21	1:A:399:ALA:HA	1.82	0.45
1:A:108:ASP:OD2	1:A:111:GLU:HG3	2.16	0.45
1:C:252:LEU:HD21	1:C:281:HIS:CG	2.52	0.45
1:C:180:ILE:HD12	1:C:182:ASP:CG	2.41	0.45
1:C:15:ASN:HD21	1:C:400:VAL:H	1.63	0.45
1:A:110:LYS:HE2	4:A:1706:HOH:O	2.17	0.45
1:B:340:ILE:CG2	1:B:402:PRO:HB2	2.47	0.45
1:D:340:ILE:HG21	1:D:402:PRO:HB2	1.98	0.45
3:B:3002:AOS:H1	3:B:3002:AOS:H4	1.79	0.45
1:A:414:ARG:O	1:A:418:GLU:HG3	2.17	0.45
3:C:3003:AOS:H1	3:C:3003:AOS:H4	1.75	0.45
1:C:361:LEU:O	1:C:365:GLN:HG3	2.17	0.44
1:D:263:ASN:OD1	1:D:265:GLU:HG2	2.18	0.44
1:A:23:LYS:O	1:A:27:GLU:HG3	2.18	0.44
1:A:221:LYS:HA	1:A:257:HIS:HB3	1.99	0.44
1:C:340:ILE:CG2	1:C:402:PRO:HB2	2.48	0.44
1:B:280:PHE:CE2	1:B:309:LEU:HD21	2.54	0.43
1:B:252:LEU:HD21	1:B:281:HIS:CG	2.54	0.43
1:C:257:HIS:HE1	3:C:3003:AOS:H2	1.84	0.43
1:C:385:VAL:O	1:C:389:LEU:HD13	2.18	0.43
1:B:419:ARG:HA	1:B:420:PRO:HD3	1.87	0.43
1:C:263:ASN:OD1	1:C:265:GLU:HG2	2.19	0.42
1:C:317:VAL:O	1:C:320:PHE:CB	2.59	0.42
1:D:221:LYS:HE2	1:D:223:TYR:O	2.19	0.42
1:D:252:LEU:HD21	1:D:281:HIS:CG	2.53	0.42
1:A:193:THR:O	1:A:197:GLU:HG3	2.19	0.42
1:A:180:ILE:HD12	1:A:182:ASP:CG	2.45	0.42
1:B:210:LEU:HD11	1:B:216:LEU:HB2	2.00	0.42
1:A:59:VAL:HG21	1:A:84:ASP:CB	2.47	0.42
1:B:263:ASN:OD1	1:B:265:GLU:HG2	2.20	0.42
1:C:280:PHE:CE2	1:C:309:LEU:HD21	2.55	0.42
1:C:115:ARG:HA	1:C:115:ARG:HD2	1.90	0.41
1:A:59:VAL:CG1	1:A:81:LYS:HG2	2.50	0.41
1:B:301:ARG:HD3	4:B:518:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LYS:O	1:B:318:LYS:HD3	2.21	0.41
1:D:76:ARG:HD3	1:D:420:PRO:CD	2.51	0.41
1:D:113:LYS:HE2	4:D:970:HOH:O	2.20	0.41
1:A:129:ASN:N	1:A:160:HIS:HE1	1.99	0.41
1:A:301:ARG:HD3	4:A:685:HOH:O	2.20	0.41
3:D:3004:AOS:H4	3:D:3004:AOS:H1	1.84	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	21
1	B	419/438 (96%)	409 (98%)	9 (2%)	1 (0%)	43	21
1	C	429/438 (98%)	415 (97%)	13 (3%)	1 (0%)	43	21
1	D	417/438 (95%)	408 (98%)	8 (2%)	1 (0%)	43	21
All	All	1684/1752 (96%)	1642 (98%)	38 (2%)	4 (0%)	43	21

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/341 (97%)	327 (99%)	3 (1%)	70	46
1	B	330/341 (97%)	328 (99%)	2 (1%)	78	58
1	C	335/341 (98%)	333 (99%)	2 (1%)	78	58
1	D	329/341 (96%)	326 (99%)	3 (1%)	70	46
All	All	1324/1364 (97%)	1314 (99%)	10 (1%)	73	50

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	LYS
1	A	325	MET
1	A	374	THR
1	B	318	LYS
1	B	374	THR
1	C	325	MET
1	C	374	THR
1	D	110	LYS
1	D	325	MET
1	D	374	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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	321	HIS
1	A	331	ASN
1	A	344	ASN
1	B	15	ASN
1	B	160	HIS
1	B	189	GLN
1	B	243	GLN

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Mol	Chain	Res	Type
1	B	250	GLN
1	B	344	ASN
1	B	368	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	150	ASN
1	D	160	HIS
1	D	189	GLN
1	D	258	HIS
1	D	324	HIS
1	D	328	GLN
1	D	331	ASN
1	D	344	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	AOS	D	3004	2	10,11,11	0.61	0	13,14,14	0.81	0
3	AOS	A	3001	2	10,11,11	0.59	0	13,14,14	0.65	0
3	AOS	C	3003	2	10,11,11	0.54	0	13,14,14	0.55	0
3	AOS	B	3002	2	10,11,11	0.57	0	13,14,14	0.59	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	AOS	D	3004	2	-	7/15/16/16	-
3	AOS	A	3001	2	-	6/15/16/16	-
3	AOS	C	3003	2	-	7/15/16/16	-
3	AOS	B	3002	2	-	7/15/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3001	AOS	O1-C1-C2-C3
3	B	3002	AOS	O1-C1-C2-C3
3	B	3002	AOS	C1-C2-C3-O3
3	B	3002	AOS	O2-C2-C3-O3
3	B	3002	AOS	O2-C2-C3-C4
3	C	3003	AOS	O1-C1-C2-C3
3	C	3003	AOS	C1-C2-C3-O3
3	C	3003	AOS	O2-C2-C3-O3
3	C	3003	AOS	O2-C2-C3-C4
3	D	3004	AOS	O1-C1-C2-C3
3	D	3004	AOS	O2-C2-C3-O3
3	D	3004	AOS	O2-C2-C3-C4
3	C	3003	AOS	C2-C3-C4-O4
3	A	3001	AOS	C2-C3-C4-C5
3	C	3003	AOS	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	B	3002	AOS	C2-C3-C4-O4
3	A	3001	AOS	C2-C3-C4-O4
3	B	3002	AOS	C2-C3-C4-C5
3	D	3004	AOS	C2-C3-C4-C5
3	A	3001	AOS	O2-C2-C3-O3
3	D	3004	AOS	C2-C3-C4-O4
3	A	3001	AOS	O2-C2-C3-C4
3	B	3002	AOS	C1-C2-C3-C4
3	C	3003	AOS	C1-C2-C3-C4
3	D	3004	AOS	C1-C2-C3-C4
3	A	3001	AOS	C1-C2-C3-C4
3	D	3004	AOS	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3004	AOS	2	0
3	A	3001	AOS	1	0
3	C	3003	AOS	2	0
3	B	3002	AOS	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%)	0.02	13 (3%) 51 54	8, 13, 23, 40	0
1	B	421/438 (96%)	0.03	7 (1%) 69 72	8, 13, 24, 36	0
1	C	431/438 (98%)	0.41	34 (7%) 18 18	8, 16, 31, 45	0
1	D	419/438 (95%)	-0.03	5 (1%) 76 80	7, 13, 23, 43	0
All	All	1692/1752 (96%)	0.11	59 (3%) 47 49	7, 13, 26, 45	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	317	VAL	7.8
1	C	319	GLY	6.2
1	A	423	VAL	5.0
1	A	320	PHE	4.6
1	C	320	PHE	4.5
1	A	424	ALA	4.2
1	C	432	SER	4.1
1	B	424	ALA	4.1
1	B	423	VAL	4.1
1	B	421	ALA	4.1
1	C	318	LYS	4.0
1	C	428	GLY	4.0
1	C	433	HIS	4.0
1	A	422	SER	3.9
1	C	314	ALA	3.9
1	C	316	GLY	3.8
1	D	136	GLY	3.7
1	B	280	PHE	3.6
1	A	280	PHE	3.6
1	A	76	ARG	3.4
1	C	424	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	430	ILE	3.3
1	C	280	PHE	3.2
1	C	427	GLY	3.1
1	C	367	ASP	3.1
1	A	318	LYS	3.1
1	C	426	GLY	3.0
1	C	425	GLY	2.9
1	C	4	PHE	2.9
1	D	421	ALA	2.8
1	C	3	GLU	2.8
1	A	4	PHE	2.7
1	C	77	GLY	2.6
1	A	314	ALA	2.6
1	D	3	GLU	2.6
1	C	136	GLY	2.6
1	C	321	HIS	2.6
1	A	321	HIS	2.5
1	C	210	LEU	2.5
1	D	4	PHE	2.5
1	C	423	VAL	2.5
1	C	76	ARG	2.4
1	C	429	ILE	2.4
1	C	313	GLU	2.4
1	A	9	ASP	2.4
1	C	431	GLY	2.4
1	B	4	PHE	2.4
1	C	59	VAL	2.2
1	C	110	LYS	2.2
1	C	315	ARG	2.2
1	A	136	GLY	2.2
1	B	136	GLY	2.2
1	D	135	PRO	2.1
1	C	422	SER	2.1
1	C	415	VAL	2.1
1	B	422	SER	2.1
1	C	135	PRO	2.1
1	C	417	ALA	2.0
1	A	317	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	AOS	B	3002	12/12	0.90	0.10	12,16,19,21	0
3	AOS	C	3003	12/12	0.90	0.11	16,20,22,23	0
3	AOS	D	3004	12/12	0.90	0.10	13,15,16,17	0
3	AOS	A	3001	12/12	0.93	0.08	12,15,19,20	0
2	MN	A	501	1/1	0.97	0.05	12,12,12,12	0
2	MN	D	507	1/1	0.97	0.04	11,11,11,11	0
2	MN	C	505	1/1	0.98	0.05	15,15,15,15	0
2	MN	B	503	1/1	0.98	0.04	12,12,12,12	0
2	MN	A	502	1/1	1.00	0.05	10,10,10,10	0
2	MN	C	506	1/1	1.00	0.06	12,12,12,12	0
2	MN	B	504	1/1	1.00	0.04	10,10,10,10	0
2	MN	D	508	1/1	1.00	0.05	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.