



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2023 – 02:34 AM EDT

PDB ID : 3M0M  
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](mailto: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>.

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

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

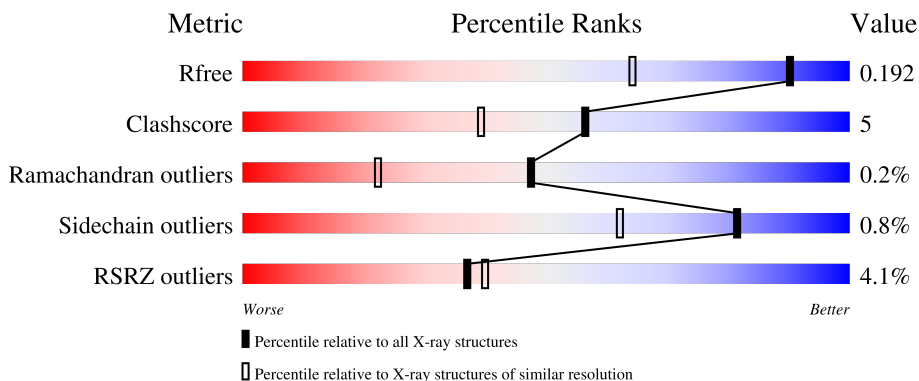
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (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  $\geq 3$ , 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% 85% 11% .
1	B	438	 2% 87% 8% .
1	C	438	 9% 86% 13% .
1	D	438	 % 85% 10% .

## 2 Entry composition i

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
			Total	C	N	O	S			
1	A	421	3265	2054	584	618	9	0	0	0
1	B	421	3265	2054	584	618	9	0	0	0
1	C	431	3326	2090	596	631	9	0	0	0
1	D	419	3256	2048	582	617	9	0	0	0

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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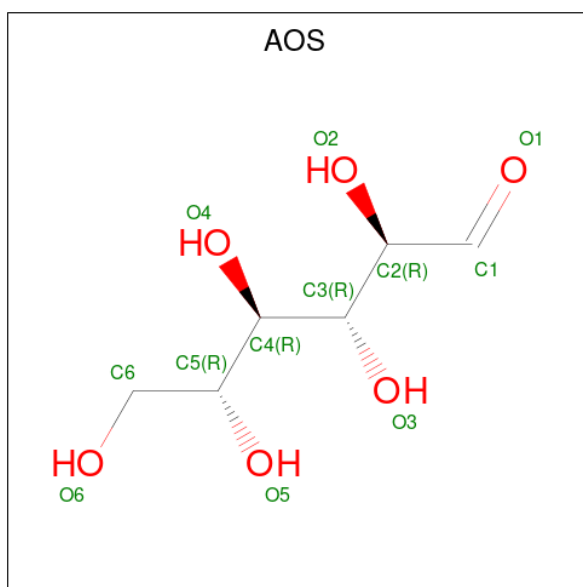
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Chain	Residue	Modelled	Actual	Comment	Reference
C	329	PHE	SER	engineered mutation	UNP Q75WH8
C	431	GLY	-	expression tag	UNP Q75WH8
C	432	SER	-	expression tag	UNP Q75WH8
C	433	HIS	-	expression tag	UNP Q75WH8
C	434	HIS	-	expression tag	UNP Q75WH8
C	435	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 (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is D-ALLOSE (three-letter code: AOS) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

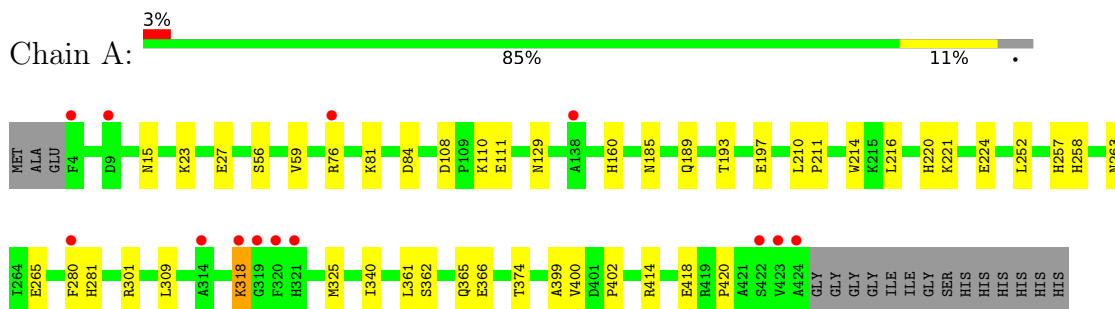
- Molecule 4 is water.

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

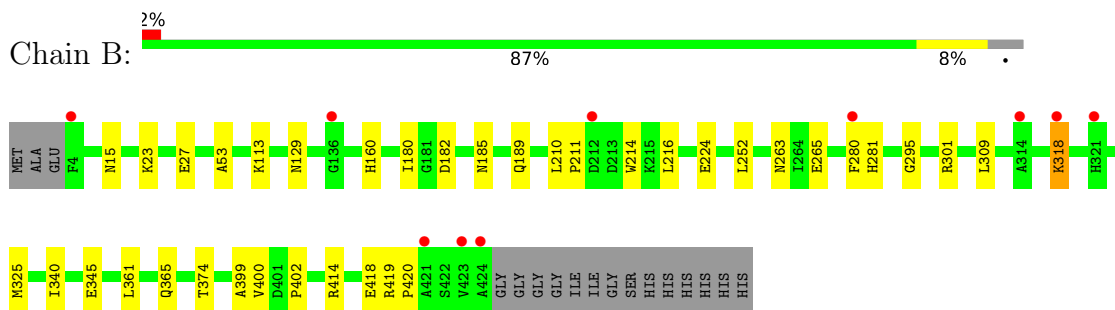
### 3 Residue-property plots i

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.

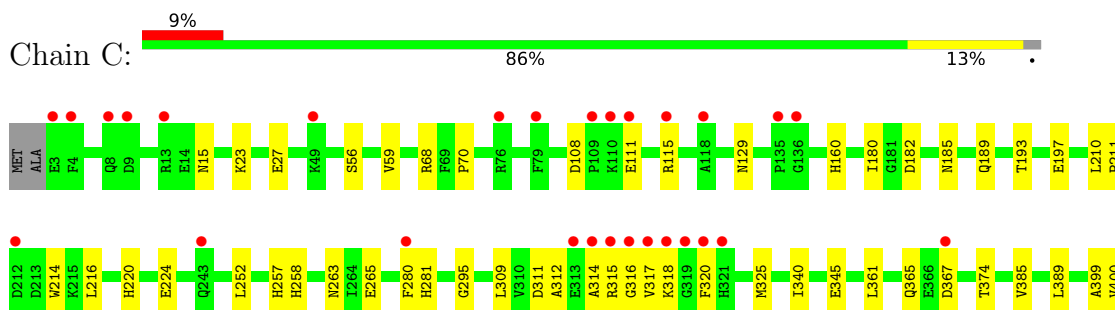
- Molecule 1: L-rhamnose isomerase



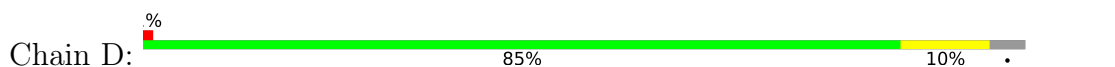
- Molecule 1: L-rhamnose isomerase



- Molecule 1: L-rhamnose isomerase



- 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, $\alpha$ , $\beta$ , $\gamma$	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) 95.4 (30.10-1.45)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 1.45Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.177 , 0.196 0.173 , 0.192	Depositor DCC
$R_{free}$ test set	27405 reflections (9.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.1	Xtrriage
Anisotropy	0.170	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.29	0/3338	0.56	0/4526
1	B	0.29	0/3338	0.54	0/4526
1	C	0.28	0/3400	0.53	0/4608
1	D	0.29	0/3329	0.54	0/4513
All	All	0.29	0/13405	0.54	0/18173

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	36	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	129	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 (129) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:318:LYS:C	1:C:320:PHE:H	2.16	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
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:D:180:ILE:HD12	1:D:182:ASP:CG	2.36	0.46
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:314:ALA:C	1:C:316:GLY:H	2.21	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
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
1:B:180:ILE:HD12	1:B:182:ASP:CG	2.41	0.41
1:C:180:ILE:HD12	1:C:182:ASP:CG	2.41	0.40
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%)	47 22
1	B	419/438 (96%)	409 (98%)	9 (2%)	1 (0%)	47 22
1	C	429/438 (98%)	415 (97%)	13 (3%)	1 (0%)	47 22
1	D	417/438 (95%)	408 (98%)	8 (2%)	1 (0%)	47 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1684/1752 (96%)	1642 (98%)	38 (2%)	4 (0%)	47 22

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%)	78 57
1	B	330/341 (97%)	328 (99%)	2 (1%)	86 69
1	C	335/341 (98%)	332 (99%)	3 (1%)	78 57
1	D	329/341 (96%)	326 (99%)	3 (1%)	78 57
All	All	1324/1364 (97%)	1313 (99%)	11 (1%)	81 62

All (11) 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	367	ASP
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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	150	ASN
1	A	160	HIS
1	A	189	GLN
1	A	258	HIS
1	A	344	ASN
1	B	15	ASN
1	B	160	HIS
1	B	189	GLN
1	B	243	GLN
1	B	321	HIS
1	B	344	ASN
1	C	15	ASN
1	C	160	HIS
1	C	189	GLN
1	C	258	HIS
1	C	344	ASN
1	D	15	ASN
1	D	160	HIS
1	D	189	GLN
1	D	258	HIS
1	D	324	HIS
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 monosaccharides 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	AOS	A	3001	2	10,11,11	0.56	0	13,14,14	0.64	0
3	AOS	B	3002	2	10,11,11	0.55	0	13,14,14	0.59	0
3	AOS	D	3004	2	10,11,11	0.58	0	13,14,14	0.80	0
3	AOS	C	3003	2	10,11,11	0.52	0	13,14,14	0.54	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	A	3001	2	-	5/14/16/16	-
3	AOS	B	3002	2	-	6/14/16/16	-
3	AOS	D	3004	2	-	6/14/16/16	-
3	AOS	C	3003	2	-	6/14/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

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

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

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	AOS	1	0
3	B	3002	AOS	1	0
3	D	3004	AOS	2	0
3	C	3003	AOS	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	421/438 (96%)	0.11	13 (3%) 49 52	8, 13, 23, 40	0
1	B	421/438 (96%)	0.11	10 (2%) 59 61	8, 13, 24, 36	0
1	C	431/438 (98%)	0.53	40 (9%) 8 10	8, 16, 31, 45	0
1	D	419/438 (95%)	0.10	6 (1%) 75 76	7, 13, 23, 43	0
All	All	1692/1752 (96%)	0.21	69 (4%) 37 40	7, 13, 26, 45	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	319	GLY	9.7
1	C	317	VAL	9.2
1	C	428	GLY	6.4
1	C	318	LYS	6.4
1	D	3	GLU	5.8
1	C	432	SER	5.7
1	C	433	HIS	5.7
1	C	316	GLY	5.3
1	D	421	ALA	5.2
1	C	3	GLU	5.2
1	C	136	GLY	4.9
1	B	423	VAL	4.9
1	D	4	PHE	4.8
1	C	4	PHE	4.6
1	C	427	GLY	4.6
1	A	318	LYS	4.6
1	C	320	PHE	4.5
1	C	424	ALA	4.4
1	C	321	HIS	4.2
1	B	4	PHE	4.1
1	C	426	GLY	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	430	ILE	4.1
1	A	424	ALA	4.0
1	B	424	ALA	3.8
1	C	423	VAL	3.8
1	A	423	VAL	3.7
1	C	110	LYS	3.5
1	C	315	ARG	3.5
1	C	135	PRO	3.5
1	A	320	PHE	3.5
1	A	422	SER	3.4
1	C	76	ARG	3.4
1	A	4	PHE	3.4
1	A	280	PHE	3.3
1	C	314	ALA	3.2
1	A	321	HIS	3.1
1	C	431	GLY	3.1
1	A	76	ARG	3.1
1	C	425	GLY	2.9
1	C	367	ASP	2.9
1	C	118	ALA	2.8
1	C	422	SER	2.8
1	B	318	LYS	2.8
1	B	136	GLY	2.8
1	D	136	GLY	2.7
1	A	319	GLY	2.6
1	B	280	PHE	2.6
1	C	79	PHE	2.5
1	C	280	PHE	2.5
1	C	109	PRO	2.4
1	B	314	ALA	2.4
1	B	421	ALA	2.4
1	C	111	GLU	2.4
1	D	420	PRO	2.4
1	C	9	ASP	2.4
1	C	212	ASP	2.3
1	C	115	ARG	2.3
1	C	243	GLN	2.3
1	A	138	ALA	2.3
1	B	321	HIS	2.3
1	C	429	ILE	2.2
1	A	9	ASP	2.2
1	C	8	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	313	GLU	2.2
1	B	212	ASP	2.1
1	D	118	ALA	2.1
1	C	13	ARG	2.1
1	C	49	LYS	2.1
1	A	314	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	AOS	B	3002	12/12	0.88	0.14	12,16,19,21	0
3	AOS	C	3003	12/12	0.89	0.13	16,20,22,23	0
3	AOS	D	3004	12/12	0.89	0.14	13,15,16,17	0
3	AOS	A	3001	12/12	0.94	0.12	12,15,19,20	0
2	MN	B	503	1/1	0.97	0.06	12,12,12,12	0
2	MN	D	507	1/1	0.97	0.06	11,11,11,11	0
2	MN	C	505	1/1	0.99	0.05	15,15,15,15	0
2	MN	A	501	1/1	0.99	0.05	12,12,12,12	0
2	MN	A	502	1/1	1.00	0.03	10,10,10,10	0
2	MN	C	506	1/1	1.00	0.02	12,12,12,12	0
2	MN	B	504	1/1	1.00	0.02	10,10,10,10	0
2	MN	D	508	1/1	1.00	0.03	9,9,9,9	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.