



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:54 PM GMT

PDB ID : 4GJJ  
Title : Crystal structure of Pseudomonas stutzeri L-rhamnose isomerase mutant H101N in complex with D-allopyranose  
Authors : Yoshida, H.; Kamitori, S.  
Deposited on : 2012-08-09  
Resolution : 2.38 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

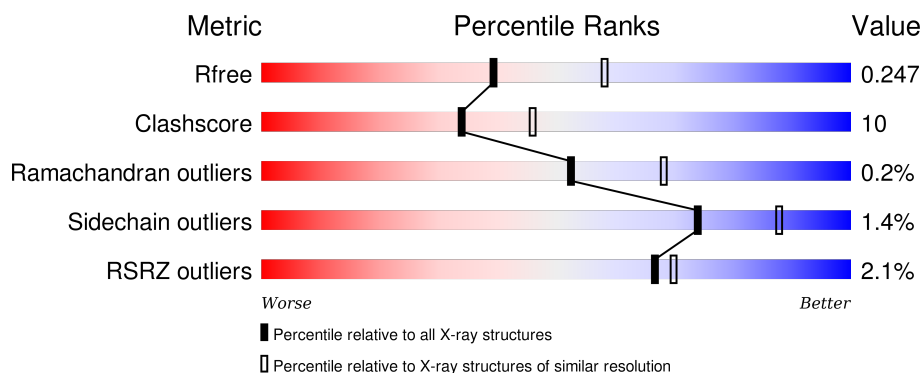
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 2.38 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))
$R_{free}$	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AOS	D	504	-	-	-	X
4	AFD	B	504	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13461 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
			3258	2046	583	620	9			
1	B	421	Total	C	N	O	S	0	0	0
			3258	2046	583	620	9			
1	C	429	Total	C	N	O	S	0	0	0
			3303	2073	591	630	9			
1	D	419	Total	C	N	O	S	0	0	0
			3249	2040	581	619	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	ASN	HIS	ENGINEERED MUTATION	UNP Q75WH8
A	150	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	101	ASN	HIS	ENGINEERED MUTATION	UNP Q75WH8
B	150	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	101	ASN	HIS	ENGINEERED MUTATION	UNP Q75WH8

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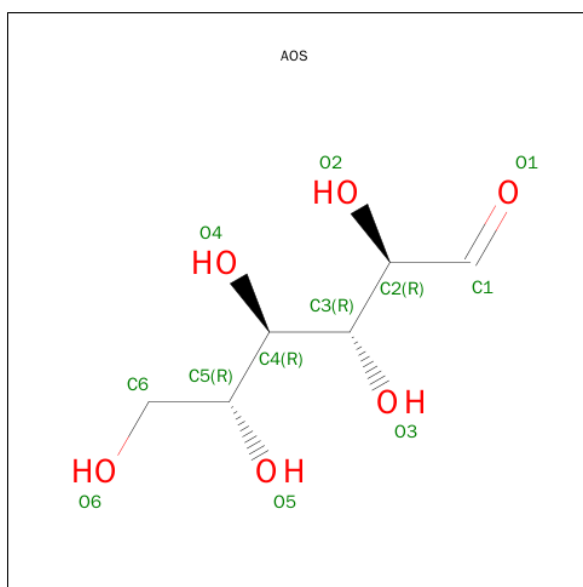
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Chain	Residue	Modelled	Actual	Comment	Reference
C	150	ASN	ASP	ENGINEERED MUTATION	UNP Q75WH8
C	431	GLY	-	EXPRESSION TAG	UNP Q75WH8
C	432	SER	-	EXPRESSION TAG	UNP Q75WH8
C	433	HIS	-	EXPRESSION TAG	UNP Q75WH8
C	434	HIS	-	EXPRESSION TAG	UNP Q75WH8
C	435	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	101	ASN	HIS	ENGINEERED MUTATION	UNP Q75WH8
D	150	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 (three-letter code: MN) (formula: Mn).

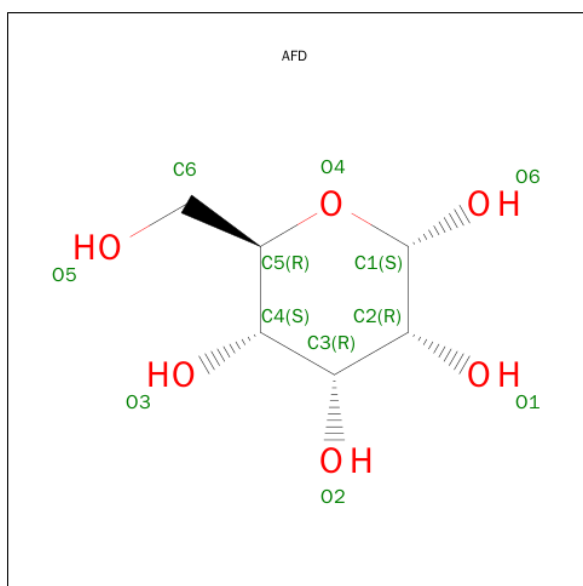
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mn 3 3	0	0
2	A	2	Total Mn 2 2	0	0
2	D	3	Total Mn 3 3	0	0
2	C	2	Total Mn 2 2	0	0

- Molecule 3 is SUGAR (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	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 SUGAR (ALPHA-D-ALLOPYRANOSE) (three-letter code: AFD) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	6	6		

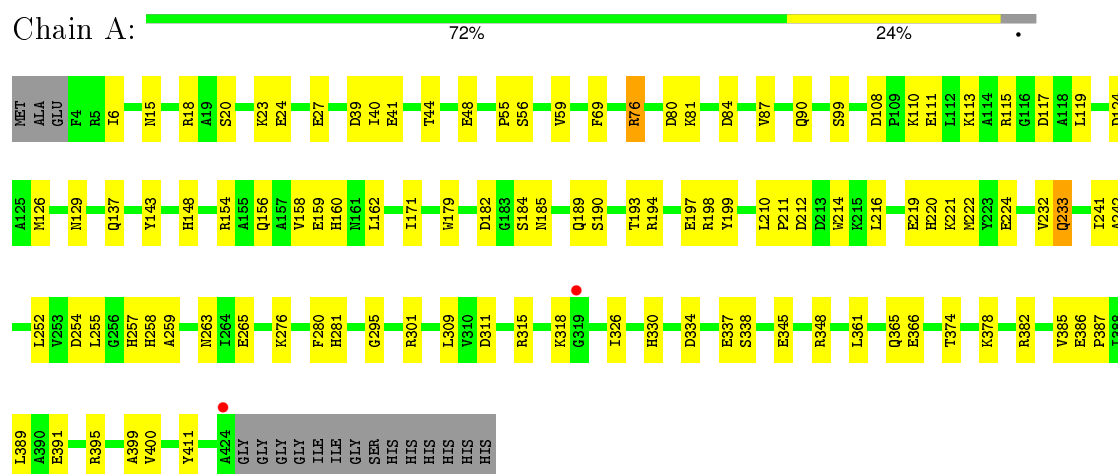
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	78	Total	O	0	0
			78	78		
5	C	55	Total	O	0	0
			55	55		
5	D	94	Total	O	0	0
			94	94		

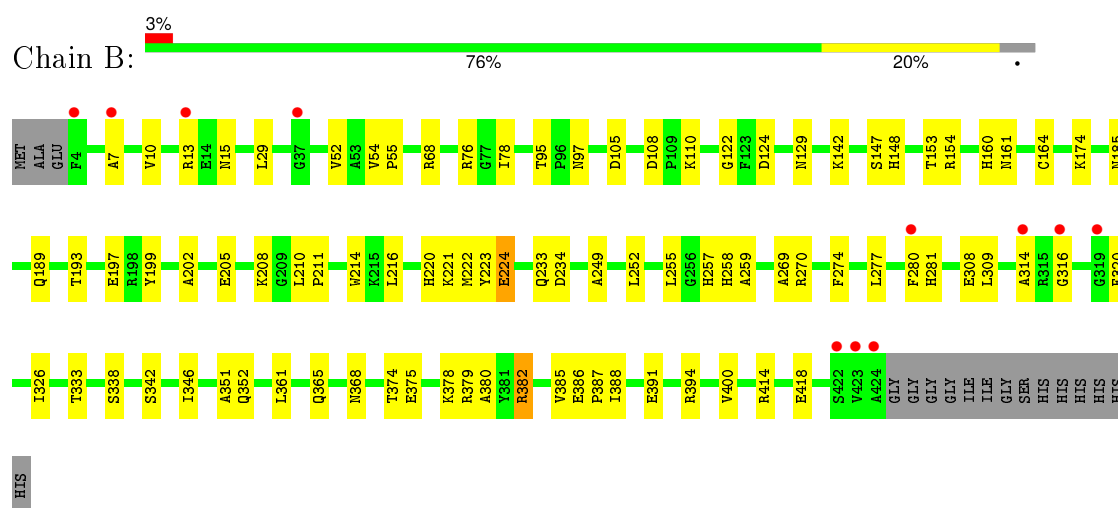
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

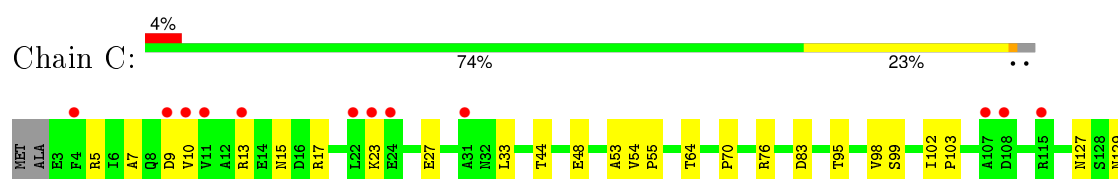
- Molecule 1: L-rhamnose isomerase



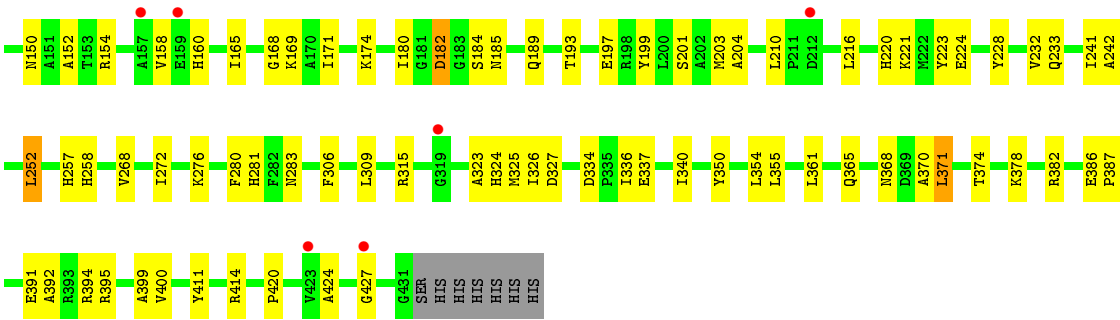
- Molecule 1: L-rhamnose isomerase



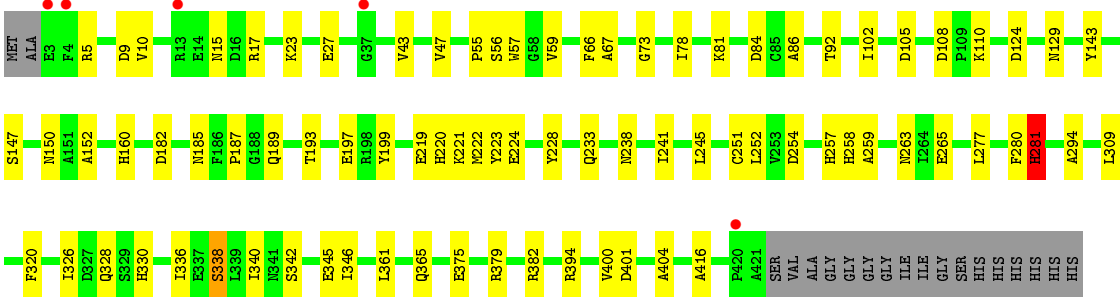
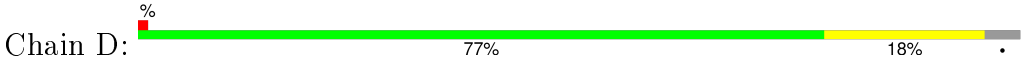
- Molecule 1: L-rhamnose isomerase







• 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, $\alpha$ , $\beta$ , $\gamma$	74.65Å 104.38Å 113.97Å 90.00° 107.91° 90.00°	Depositor
Resolution (Å)	37.60 – 2.38 37.60 – 2.37	Depositor EDS
% Data completeness (in resolution range)	82.1 (37.60-2.38) 81.5 (37.60-2.37)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.78 (at 2.37Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.196 , 0.249 0.195 , 0.247	Depositor DCC
$R_{free}$ test set	5535 reflections (10.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.7	EDS
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 62434 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13461	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: AFD, MN, AOS

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	0.38	0/3329	0.59	0/4514
1	B	0.37	0/3329	0.59	0/4514
1	C	0.36	0/3374	0.57	0/4573
1	D	0.36	0/3320	0.57	1/4501 (0.0%)
All	All	0.37	0/13352	0.58	1/18102 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	281	HIS	N-CA-C	-5.12	97.18	111.00

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	3258	0	3164	76	0
1	B	3258	0	3164	64	0
1	C	3303	0	3207	70	0
1	D	3249	0	3151	55	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	3	0	0	0	0
3	A	12	0	11	3	0
3	C	12	0	10	0	0
3	D	12	0	10	2	0
4	B	12	0	10	0	0
5	A	108	0	0	2	0
5	B	78	0	0	2	0
5	C	55	0	0	0	0
5	D	94	0	0	0	0
All	All	13461	0	12727	260	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 10.

All (260) 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:210:LEU:HD11	1:B:216:LEU:HB2	1.47	0.97
1:B:129:ASN:H	1:B:160:HIS:HE1	1.30	0.79
1:A:220:HIS:HE2	1:A:258:HIS:HE1	1.26	0.79
1:C:76:ARG:HD3	1:C:420:PRO:HD2	1.64	0.78
1:B:375:GLU:O	1:B:379:ARG:HG3	1.85	0.76
1:A:129:ASN:H	1:A:160:HIS:HE1	1.34	0.74
1:A:23:LYS:O	1:A:27:GLU:HG3	1.88	0.74
1:A:185:ASN:H	1:A:189:GLN:HE22	1.35	0.74
1:A:129:ASN:H	1:A:160:HIS:CE1	2.06	0.72
1:D:23:LYS:O	1:D:27:GLU:HG3	1.90	0.71
1:C:210:LEU:HD11	1:C:216:LEU:HB2	1.73	0.70
1:B:378:LYS:O	1:B:382:ARG:HB2	1.90	0.70
1:D:221:LYS:HA	1:D:257:HIS:HB3	1.73	0.70
1:B:394:ARG:HH21	1:B:394:ARG:HG2	1.56	0.69
1:C:221:LYS:HA	1:C:257:HIS:HB3	1.74	0.69
1:A:6:ILE:HB	1:A:90:GLN:HE22	1.57	0.69
1:A:220:HIS:HE2	1:A:258:HIS:CE1	2.09	0.68
1:C:129:ASN:H	1:C:160:HIS:CE1	2.12	0.68
1:A:6:ILE:HB	1:A:90:GLN:NE2	2.08	0.68
1:C:129:ASN:H	1:C:160:HIS:HE1	1.41	0.65
1:A:210:LEU:HD11	1:A:216:LEU:HB2	1.78	0.65
1:A:334:ASP:HB3	1:A:337:GLU:HG3	1.78	0.65
1:B:7:ALA:HB3	1:B:10:VAL:HG23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ASP:HB3	1:C:337:GLU:HG3	1.78	0.64
1:B:211:PRO:HD2	1:B:214:TRP:HB2	1.80	0.64
1:B:221:LYS:HA	1:B:257:HIS:HB3	1.79	0.63
1:B:220:HIS:HE2	1:B:258:HIS:CE1	2.16	0.63
1:A:113:LYS:HE2	1:A:117:ASP:OD2	1.99	0.63
1:A:257:HIS:HE1	3:A:503:AOS:H2	1.65	0.62
1:C:165:ILE:O	1:C:169:LYS:HG3	1.98	0.62
1:D:336:ILE:O	1:D:340:ILE:HG13	1.99	0.62
1:C:193:THR:O	1:C:197:GLU:HG3	1.99	0.62
1:C:220:HIS:HA	1:C:232:VAL:HG12	1.81	0.62
1:B:379:ARG:HD3	5:B:647:HOH:O	2.00	0.61
1:A:99:SER:HB3	5:A:652:HOH:O	1.99	0.61
1:C:185:ASN:H	1:C:189:GLN:HE22	1.48	0.61
1:A:301:ARG:HD3	5:A:685:HOH:O	2.00	0.61
1:C:220:HIS:HE2	1:C:258:HIS:HE1	1.47	0.61
1:C:154:ARG:O	1:C:158:VAL:HG23	2.00	0.61
1:D:193:THR:O	1:D:197:GLU:HG3	2.00	0.61
1:D:185:ASN:H	1:D:189:GLN:HE22	1.49	0.61
1:B:15:ASN:ND2	1:B:400:VAL:H	1.98	0.61
1:B:220:HIS:HE2	1:B:258:HIS:HE1	1.48	0.61
1:A:221:LYS:HA	1:A:257:HIS:HB3	1.82	0.60
1:A:185:ASN:H	1:A:189:GLN:NE2	1.99	0.60
1:B:129:ASN:H	1:B:160:HIS:CE1	2.16	0.60
1:D:222:MET:CE	1:D:259:ALA:HB2	2.32	0.59
1:C:55:PRO:HD3	1:C:326:ILE:O	2.02	0.59
1:C:76:ARG:HD3	1:C:420:PRO:CD	2.33	0.59
1:A:18:ARG:HG3	1:A:18:ARG:HH21	1.68	0.59
1:B:314:ALA:C	1:B:316:GLY:H	2.03	0.59
1:B:174:LYS:O	1:B:214:TRP:HA	2.03	0.58
1:C:99:SER:HB3	1:C:127:ASN:HD21	1.68	0.58
1:A:295:GLY:HA3	1:A:345:GLU:HG2	1.84	0.58
1:B:54:VAL:HG23	1:B:95:THR:HB	1.85	0.58
1:B:391:GLU:OE2	1:B:394:ARG:NH1	2.37	0.57
1:A:179:TRP:CG	3:A:503:AOS:H3	2.40	0.57
1:A:194:ARG:O	1:A:198:ARG:HG3	2.05	0.57
1:C:323:ALA:O	1:C:325:MET:HE2	2.05	0.56
1:B:394:ARG:NH2	1:B:394:ARG:HG2	2.20	0.56
1:B:211:PRO:HD2	1:B:214:TRP:CB	2.35	0.56
1:A:59:VAL:HG21	1:A:84:ASP:HB2	1.85	0.56
1:B:10:VAL:HA	1:B:13:ARG:NH1	2.21	0.56
1:D:17:ARG:HH11	1:D:17:ARG:HG3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:MET:SD	1:A:259:ALA:HA	2.46	0.56
1:D:150:ASN:HD21	1:D:152:ALA:HB3	1.71	0.56
1:A:15:ASN:ND2	1:A:400:VAL:H	2.04	0.56
1:D:257:HIS:HE1	3:D:504:AOS:H2	1.71	0.55
1:A:55:PRO:HD3	1:A:326:ILE:O	2.05	0.55
1:B:148:HIS:O	1:B:154:ARG:HD3	2.06	0.55
1:A:361:LEU:O	1:A:365:GLN:HG3	2.07	0.55
1:B:414:ARG:O	1:B:418:GLU:HG3	2.07	0.55
1:B:280:PHE:HE1	1:B:309:LEU:HD21	1.72	0.55
1:A:211:PRO:HD2	1:A:214:TRP:CG	2.41	0.55
1:A:59:VAL:CG1	1:A:81:LYS:HG2	2.37	0.55
1:C:23:LYS:O	1:C:27:GLU:HG3	2.07	0.55
1:C:7:ALA:HB1	1:C:9:ASP:OD1	2.07	0.55
1:D:394:ARG:HG2	1:D:394:ARG:HH11	1.72	0.54
1:A:115:ARG:HD2	1:A:119:LEU:HD11	1.90	0.54
1:D:129:ASN:H	1:D:160:HIS:CE1	2.25	0.54
1:A:56:SER:O	1:A:59:VAL:HG12	2.07	0.54
1:D:57:TRP:NE1	3:D:504:AOS:H62	2.22	0.54
1:A:345:GLU:O	1:A:348:ARG:HB3	2.08	0.54
1:B:211:PRO:HD2	1:B:214:TRP:CG	2.43	0.53
1:D:108:ASP:OD2	1:D:110:LYS:HB2	2.07	0.53
1:C:361:LEU:O	1:C:365:GLN:HG3	2.09	0.53
1:B:314:ALA:C	1:B:316:GLY:N	2.61	0.53
1:C:391:GLU:O	1:C:395:ARG:HG3	2.09	0.53
1:D:66:PHE:O	1:D:67:ALA:HB2	2.07	0.53
1:C:394:ARG:HH11	1:C:394:ARG:HG2	1.74	0.53
1:A:15:ASN:HD21	1:A:399:ALA:HA	1.74	0.53
1:C:44:THR:O	1:C:48:GLU:HG3	2.09	0.53
1:C:221:LYS:HE2	1:C:223:TYR:O	2.09	0.53
1:A:263:ASN:OD1	1:A:265:GLU:HG2	2.09	0.53
1:C:378:LYS:O	1:C:382:ARG:HG3	2.08	0.52
1:C:268:VAL:O	1:C:272:ILE:HG13	2.09	0.52
1:C:64:THR:O	1:C:427:GLY:HA3	2.10	0.52
1:C:242:ALA:HB1	1:C:276:LYS:HD2	1.90	0.52
1:D:221:LYS:O	1:D:233:GLN:HA	2.10	0.52
1:C:220:HIS:HE2	1:C:258:HIS:CE1	2.26	0.52
1:A:242:ALA:HB1	1:A:276:LYS:HD2	1.92	0.52
1:D:361:LEU:O	1:D:365:GLN:HG3	2.09	0.52
1:A:159:GLU:OE1	1:A:162:LEU:HD12	2.09	0.52
1:C:336:ILE:O	1:C:340:ILE:HG13	2.10	0.51
1:D:394:ARG:HG2	1:D:394:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ARG:HG3	1:C:13:ARG:HH11	1.76	0.51
1:C:252:LEU:HD11	1:C:281:HIS:CD2	2.45	0.51
1:C:15:ASN:HD21	1:C:399:ALA:HA	1.75	0.51
1:D:84:ASP:HB3	1:D:336:ILE:HD11	1.92	0.51
1:C:17:ARG:HG2	1:C:17:ARG:O	2.10	0.51
1:C:15:ASN:ND2	1:C:400:VAL:H	2.09	0.51
1:A:18:ARG:HG3	1:A:18:ARG:NH2	2.25	0.51
1:C:168:GLY:HA2	1:C:171:ILE:HG12	1.93	0.51
1:B:97:ASN:OD1	1:B:122:GLY:HA3	2.11	0.51
1:A:257:HIS:CE1	3:A:503:AOS:H2	2.46	0.50
1:D:185:ASN:H	1:D:189:GLN:NE2	2.10	0.50
1:A:154:ARG:O	1:A:158:VAL:HG23	2.11	0.50
1:A:348:ARG:HH21	1:A:348:ARG:HG3	1.75	0.50
1:B:378:LYS:HE3	5:B:644:HOH:O	2.12	0.50
1:A:184:SER:HB3	1:A:190:SER:OG	2.11	0.50
1:D:238:ASN:ND2	1:D:251:CYS:HB3	2.27	0.49
1:C:184:SER:O	1:C:228:TYR:HB3	2.12	0.49
1:D:222:MET:HE3	1:D:259:ALA:HB2	1.94	0.49
1:C:386:GLU:HB3	1:C:387:PRO:HD3	1.93	0.49
1:D:221:LYS:HE2	1:D:223:TYR:O	2.12	0.49
1:C:350:TYR:CE2	1:C:354:LEU:HD11	2.47	0.49
1:C:283:ASN:HB3	1:C:327:ASP:O	2.13	0.49
1:A:69:PHE:HB3	1:B:142:LYS:HD2	1.95	0.48
1:D:280:PHE:CZ	1:D:309:LEU:HD21	2.47	0.48
1:C:7:ALA:HB3	1:C:10:VAL:HG23	1.95	0.48
1:A:137:GLN:HG2	1:A:156:GLN:NE2	2.28	0.48
1:B:361:LEU:O	1:B:365:GLN:HG3	2.12	0.48
1:D:375:GLU:O	1:D:379:ARG:HG3	2.13	0.48
1:A:219:GLU:OE2	1:A:254:ASP:HB2	2.14	0.48
1:D:59:VAL:HG11	1:D:81:LYS:HA	1.94	0.48
1:B:233:GLN:HG2	1:B:234:ASP:N	2.28	0.48
1:B:368:ASN:ND2	1:D:143:TYR:HB3	2.29	0.48
1:B:185:ASN:H	1:B:189:GLN:NE2	2.11	0.48
1:C:411:TYR:O	1:C:414:ARG:HB3	2.13	0.47
1:B:342:SER:O	1:B:346:ILE:HG13	2.15	0.47
1:A:221:LYS:O	1:A:233:GLN:HA	2.14	0.47
1:A:280:PHE:CE1	1:A:309:LEU:HD21	2.49	0.47
1:D:102:ILE:O	1:D:129:ASN:HB3	2.15	0.47
1:A:148:HIS:O	1:A:154:ARG:HD3	2.13	0.47
1:A:137:GLN:HG2	1:A:156:GLN:HE22	1.80	0.47
1:A:126:MET:SD	1:A:171:ILE:HD11	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:VAL:O	1:A:389:LEU:HD13	2.15	0.47
1:B:78:ILE:HD13	1:B:105:ASP:HB3	1.96	0.47
1:C:180:ILE:HD12	1:C:182:ASP:HB2	1.96	0.47
1:B:314:ALA:O	1:B:316:GLY:N	2.48	0.46
1:D:220:HIS:NE2	1:D:258:HIS:CE1	2.83	0.46
1:B:185:ASN:H	1:B:189:GLN:HE22	1.63	0.46
1:A:386:GLU:HB3	1:A:387:PRO:HD3	1.97	0.46
1:D:147:SER:HB3	1:D:199:TYR:HB2	1.98	0.46
1:A:76:ARG:HG3	1:A:80:ASP:OD2	2.15	0.46
1:D:326:ILE:CG2	1:D:328:GLN:HG3	2.45	0.46
1:A:143:TYR:HB3	1:C:368:ASN:ND2	2.30	0.46
1:D:92:THR:CG2	1:D:340:ILE:HG23	2.46	0.46
1:D:252:LEU:HD21	1:D:281:HIS:CD2	2.51	0.46
1:C:371:LEU:O	1:C:374:THR:HG22	2.15	0.46
1:A:59:VAL:HG21	1:A:84:ASP:CB	2.45	0.46
1:D:43:VAL:O	1:D:47:VAL:HG23	2.16	0.46
1:C:70:PRO:HD2	1:C:424:ALA:HA	1.97	0.46
1:B:148:HIS:CD2	1:B:153:THR:HG21	2.51	0.45
1:C:150:ASN:HD21	1:C:152:ALA:HB3	1.81	0.45
1:B:55:PRO:HD3	1:B:326:ILE:O	2.17	0.45
1:A:220:HIS:HA	1:A:232:VAL:HG12	1.99	0.45
1:C:102:ILE:CG2	1:C:103:PRO:HA	2.47	0.45
1:C:394:ARG:NH1	1:C:394:ARG:HG2	2.32	0.45
1:D:294:ALA:O	1:D:345:GLU:HG2	2.16	0.45
1:A:15:ASN:HD21	1:A:400:VAL:H	1.62	0.45
1:C:391:GLU:OE2	1:C:395:ARG:HD3	2.16	0.45
1:D:78:ILE:HD13	1:D:105:ASP:HB3	1.99	0.45
1:C:53:ALA:HB3	1:C:325:MET:HG2	1.98	0.45
1:A:311:ASP:OD1	1:A:315:ARG:NH2	2.46	0.45
1:A:193:THR:O	1:A:197:GLU:HG3	2.17	0.45
1:D:219:GLU:OE2	1:D:254:ASP:HB2	2.17	0.44
1:A:345:GLU:OE2	1:D:382:ARG:NH1	2.50	0.44
1:B:252:LEU:HD21	1:B:281:HIS:CG	2.53	0.44
1:C:54:VAL:HG23	1:C:98:VAL:HG22	2.00	0.44
1:C:5:ARG:CZ	1:C:83:ASP:HB3	2.47	0.44
1:C:199:TYR:CZ	1:C:203:MET:HG3	2.52	0.44
1:D:401:ASP:HB3	1:D:404:ALA:HB3	1.99	0.44
1:D:277:LEU:HD23	1:D:320:PHE:CZ	2.53	0.44
1:C:102:ILE:O	1:C:129:ASN:HB3	2.18	0.44
1:D:280:PHE:HZ	1:D:309:LEU:HD21	1.83	0.44
1:D:55:PRO:HD3	1:D:326:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ASP:OD2	1:D:10:VAL:N	2.51	0.44
1:B:10:VAL:HA	1:B:13:ARG:HH12	1.83	0.44
1:A:366:GLU:HA	1:A:366:GLU:OE2	2.18	0.44
1:B:223:TYR:O	1:B:224:GLU:HB3	2.17	0.44
1:B:7:ALA:HB3	1:B:10:VAL:CG2	2.46	0.44
1:A:211:PRO:HD2	1:A:214:TRP:CB	2.48	0.43
1:D:129:ASN:H	1:D:160:HIS:HE1	1.64	0.43
1:C:54:VAL:HG13	1:C:95:THR:HB	2.00	0.43
1:B:269:ALA:HB2	1:B:308:GLU:OE1	2.18	0.43
1:A:252:LEU:HD21	1:A:281:HIS:CD2	2.53	0.43
1:A:39:ASP:OD1	1:A:41:GLU:HB3	2.18	0.43
1:A:391:GLU:O	1:A:395:ARG:HG3	2.18	0.43
1:B:386:GLU:N	1:B:387:PRO:CD	2.81	0.43
1:C:185:ASN:H	1:C:189:GLN:NE2	2.15	0.43
1:A:378:LYS:HB3	1:A:382:ARG:NH1	2.33	0.43
1:B:161:ASN:O	1:B:164:CYS:HB2	2.18	0.43
1:D:15:ASN:ND2	1:D:400:VAL:H	2.16	0.43
1:D:342:SER:O	1:D:346:ILE:HG13	2.19	0.43
1:B:255:LEU:O	1:B:258:HIS:HD2	2.01	0.43
1:B:108:ASP:OD2	1:B:110:LYS:HB2	2.18	0.43
1:A:194:ARG:HG2	1:A:194:ARG:NH2	2.33	0.43
1:D:330:HIS:CD2	1:D:338:SER:HB3	2.53	0.43
1:B:202:ALA:O	1:B:205:GLU:HB2	2.19	0.43
1:C:48:GLU:HG2	1:C:392:ALA:HB1	2.01	0.42
1:B:76:ARG:HG2	1:B:76:ARG:HH11	1.84	0.42
1:B:222:MET:SD	1:B:259:ALA:HA	2.59	0.42
1:B:352:GLN:O	1:B:380:ALA:HB1	2.19	0.42
1:C:280:PHE:CE1	1:C:309:LEU:HD21	2.54	0.42
1:D:15:ASN:HD21	1:D:400:VAL:H	1.67	0.42
1:C:174:LYS:HD3	1:C:174:LYS:HA	1.89	0.42
1:B:333:THR:HG22	1:C:370:ALA:HB3	2.00	0.42
1:B:147:SER:HB3	1:B:199:TYR:HB2	2.01	0.42
1:B:221:LYS:O	1:B:233:GLN:HA	2.19	0.42
1:D:241:ILE:O	1:D:245:LEU:HG	2.19	0.42
1:D:5:ARG:HG3	1:D:86:ALA:HB3	2.02	0.42
1:C:306:PHE:HA	1:C:309:LEU:HD12	2.01	0.42
1:A:211:PRO:HD2	1:A:214:TRP:HB2	2.01	0.42
1:A:44:THR:O	1:A:48:GLU:HG3	2.19	0.42
1:D:73:GLY:CA	1:D:416:ALA:HA	2.50	0.42
1:C:33:LEU:HD22	1:C:355:LEU:HD22	2.02	0.42
1:D:277:LEU:HD23	1:D:320:PHE:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:SER:O	1:A:24:GLU:HG2	2.19	0.41
1:B:270:ARG:O	1:B:274:PHE:HD2	2.02	0.41
1:B:15:ASN:HD21	1:B:400:VAL:H	1.64	0.41
1:B:351:ALA:HB3	1:B:385:VAL:HG21	2.02	0.41
1:A:87:VAL:HG21	1:A:411:TYR:CZ	2.55	0.41
1:C:201:SER:O	1:C:204:ALA:HB3	2.20	0.41
1:A:330:HIS:CD2	1:A:338:SER:CB	3.04	0.41
1:C:199:TYR:CE1	1:C:241:ILE:HD13	2.56	0.41
1:B:52:VAL:HG22	1:B:326:ILE:HG13	2.03	0.41
1:B:29:LEU:HD23	1:B:388:ILE:HG13	2.01	0.41
1:D:375:GLU:HG3	1:D:379:ARG:HE	1.86	0.41
1:A:108:ASP:HB3	1:A:111:GLU:HG3	2.03	0.41
1:B:216:LEU:O	1:B:249:ALA:HA	2.20	0.41
1:C:221:LYS:O	1:C:233:GLN:HA	2.21	0.41
1:A:59:VAL:O	1:A:59:VAL:HG22	2.20	0.41
1:C:150:ASN:ND2	1:C:152:ALA:HB3	2.36	0.41
1:A:40:ILE:HG23	1:A:41:GLU:N	2.36	0.41
1:D:187:PRO:HA	1:D:228:TYR:CE2	2.56	0.41
1:C:102:ILE:HG23	1:C:103:PRO:HA	2.03	0.41
1:B:205:GLU:HA	1:B:208:LYS:CE	2.51	0.41
1:B:76:ARG:HG2	1:B:76:ARG:NH1	2.35	0.41
1:D:56:SER:OG	1:D:105:ASP:OD2	2.30	0.40
1:B:193:THR:O	1:B:197:GLU:HG3	2.21	0.40
1:B:277:LEU:HD23	1:B:320:PHE:HE1	1.86	0.40
1:A:255:LEU:O	1:A:258:HIS:HD2	2.04	0.40
1:C:203:MET:HE1	1:C:216:LEU:HD21	2.03	0.40
1:A:318:LYS:HA	1:A:318:LYS:HD2	1.84	0.40
1:C:315:ARG:HH21	1:C:315:ARG:HG2	1.86	0.40
1:A:108:ASP:OD1	1:A:110:LYS:HB2	2.20	0.40
1:D:263:ASN:OD1	1:D:265:GLU:HG2	2.21	0.40
1:C:324:HIS:C	1:C:325:MET:HG3	2.42	0.40
1:A:199:TYR:CE1	1:A:241:ILE:HD13	2.57	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%)	406 (97%)	12 (3%)	1 (0%)	52	68
1	B	419/438 (96%)	398 (95%)	20 (5%)	1 (0%)	52	68
1	C	427/438 (98%)	400 (94%)	26 (6%)	1 (0%)	52	68
1	D	417/438 (95%)	401 (96%)	15 (4%)	1 (0%)	52	68
All	All	1682/1752 (96%)	1605 (95%)	73 (4%)	4 (0%)	52	68

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 ⓘ

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%)	324 (98%)	6 (2%)	66	83
1	B	330/341 (97%)	325 (98%)	5 (2%)	72	86
1	C	333/341 (98%)	330 (99%)	3 (1%)	84	93
1	D	329/341 (96%)	325 (99%)	4 (1%)	78	90
All	All	1322/1364 (97%)	1304 (99%)	18 (1%)	74	88

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	124	ASP

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Mol	Chain	Res	Type
1	A	182	ASP
1	A	212	ASP
1	A	233	GLN
1	A	374	THR
1	B	68	ARG
1	B	124	ASP
1	B	338	SER
1	B	374	THR
1	B	382	ARG
1	C	182	ASP
1	C	252	LEU
1	C	371	LEU
1	D	124	ASP
1	D	182	ASP
1	D	281	HIS
1	D	338	SER

Some 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	150	ASN
1	A	160	HIS
1	A	189	GLN
1	A	258	HIS
1	A	344	ASN
1	A	368	ASN
1	B	15	ASN
1	B	150	ASN
1	B	160	HIS
1	B	189	GLN
1	B	243	GLN
1	B	258	HIS
1	B	344	ASN
1	B	368	ASN
1	C	8	GLN
1	C	15	ASN
1	C	150	ASN
1	C	160	HIS
1	C	189	GLN
1	C	258	HIS

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Mol	Chain	Res	Type
1	C	344	ASN
1	C	368	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	344	ASN
1	D	368	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 10 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	503	2	11,11,11	0.63	0	14,14,14	0.75	0
4	AFD	B	504	2	12,12,12	0.56	0	17,17,17	0.42	0
3	AOS	C	503	2	11,11,11	0.65	0	14,14,14	0.71	1 (7%)
3	AOS	D	504	2	11,11,11	0.57	0	14,14,14	0.72	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	503	2	-	0/14/16/16	0/0/0/0
4	AFD	B	504	2	-	0/2/22/22	0/1/1/1
3	AOS	C	503	2	-	0/14/16/16	0/0/0/0
3	AOS	D	504	2	-	0/14/16/16	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	AOS	O1-C1-C2	-2.10	119.47	125.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	AOS	3	0
3	D	504	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	2 (0%) 91 92	15, 26, 39, 52	0
1	B	421/438 (96%)	0.17	11 (2%) 59 62	18, 30, 47, 68	0
1	C	429/438 (97%)	0.41	18 (4%) 40 45	17, 34, 55, 72	0
1	D	419/438 (95%)	0.11	5 (1%) 81 83	18, 28, 43, 65	0
All	All	1690/1752 (96%)	0.15	36 (2%) 67 70	15, 29, 48, 72	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	107	ALA	4.4
1	B	316	GLY	4.4
1	D	420	PRO	4.1
1	C	10	VAL	4.0
1	B	4	PHE	3.9
1	C	9	ASP	3.7
1	C	4	PHE	3.5
1	D	4	PHE	3.4
1	B	314	ALA	3.3
1	C	319	GLY	3.2
1	B	319	GLY	3.1
1	C	22	LEU	3.0
1	C	13	ARG	3.0
1	D	3	GLU	2.8
1	A	319	GLY	2.8
1	C	23	LYS	2.6
1	C	423	VAL	2.5
1	A	424	ALA	2.5
1	C	115	ARG	2.5
1	B	422	SER	2.4
1	B	7	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	13	ARG	2.4
1	B	280	PHE	2.4
1	C	427	GLY	2.2
1	B	424	ALA	2.2
1	D	37	GLY	2.2
1	B	37	GLY	2.2
1	C	24	GLU	2.2
1	C	212	ASP	2.1
1	B	423	VAL	2.1
1	C	159	GLU	2.1
1	C	108	ASP	2.1
1	D	13	ARG	2.0
1	C	11	VAL	2.0
1	C	31	ALA	2.0
1	C	157	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	AOS	D	504	12/12	0.92	0.19	2.75	35,43,50,51	0
4	AFD	B	504	12/12	0.92	0.18	2.29	38,42,46,46	0
3	AOS	C	503	12/12	0.90	0.17	1.33	34,40,46,46	0
3	AOS	A	503	12/12	0.90	0.15	1.03	31,38,45,47	0
2	MN	A	502	1/1	0.96	0.11	-0.28	45,45,45,45	0
2	MN	C	502	1/1	0.89	0.14	-0.79	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	B	502	1/1	0.97	0.13	-1.02	41,41,41,41	0
2	MN	D	502	1/1	0.98	0.10	-2.11	37,37,37,37	0
2	MN	A	501	1/1	1.00	0.05	-3.11	27,27,27,27	0
2	MN	B	501	1/1	0.99	0.07	-3.55	24,24,24,24	0
2	MN	D	501	1/1	0.99	0.06	-	22,22,22,22	0
2	MN	C	501	1/1	0.99	0.09	-	31,31,31,31	0
2	MN	D	503	1/1	0.95	0.22	-	62,62,62,62	0
2	MN	B	503	1/1	0.74	0.14	-	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.