



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:43 am BST

PDB ID : 6I60  
Title : Structure of alpha-L-rhamnosidase from Dictyoglumus thermophilum  
Authors : Lafite, P.; Daniellou, R.  
Deposited on : 2018-11-15  
Resolution : 2.74 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.

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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 : 2.11  
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) : 2.11

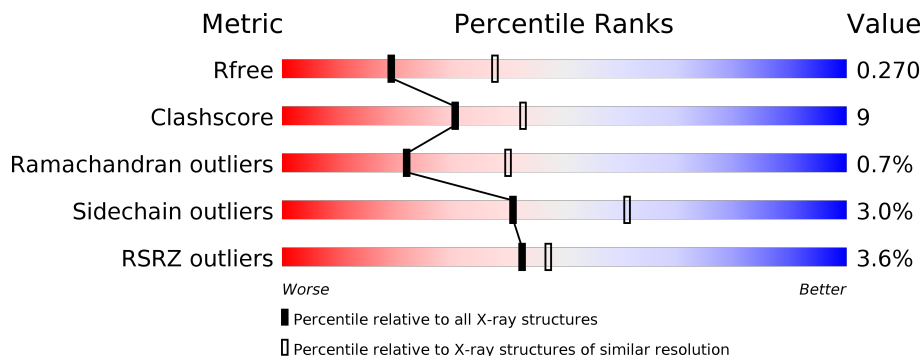
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 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	944	 3% 75% 18% • 6%
1	B	944	 3% 73% 20% • 6%

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
2	PGE	A	1001	-	-	X	-
2	PGE	A	1007	-	-	X	-
2	PGE	A	1010	-	-	X	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 14789 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 Alpha-rhamnosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	883	7237	4694	1169	1356	18	0	0	0
1	B	886	7251	4705	1174	1354	18	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

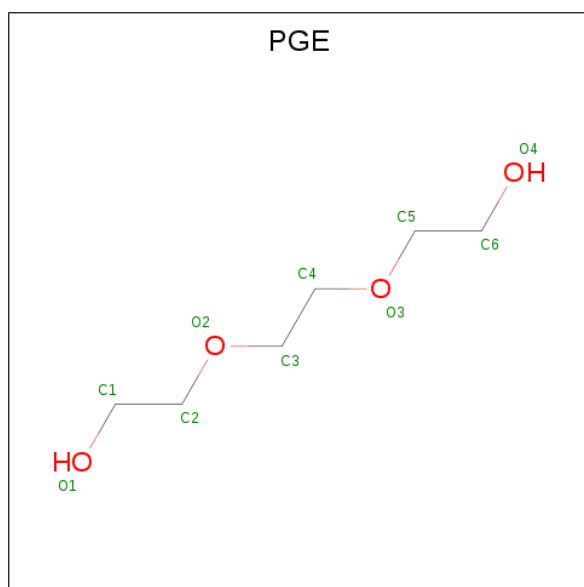
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B5YC64
A	2	GLY	-	expression tag	UNP B5YC64
A	3	SER	-	expression tag	UNP B5YC64
A	4	SER	-	expression tag	UNP B5YC64
A	5	HIS	-	expression tag	UNP B5YC64
A	6	HIS	-	expression tag	UNP B5YC64
A	7	HIS	-	expression tag	UNP B5YC64
A	8	HIS	-	expression tag	UNP B5YC64
A	9	HIS	-	expression tag	UNP B5YC64
A	10	HIS	-	expression tag	UNP B5YC64
A	11	SER	-	expression tag	UNP B5YC64
A	12	SER	-	expression tag	UNP B5YC64
A	13	GLY	-	expression tag	UNP B5YC64
A	14	LEU	-	expression tag	UNP B5YC64
A	15	VAL	-	expression tag	UNP B5YC64
A	16	PRO	-	expression tag	UNP B5YC64
A	17	ARG	-	expression tag	UNP B5YC64
A	18	GLY	-	expression tag	UNP B5YC64
A	19	SER	-	expression tag	UNP B5YC64
A	20	HIS	-	expression tag	UNP B5YC64
A	21	MET	-	expression tag	UNP B5YC64
A	22	ALA	-	expression tag	UNP B5YC64
A	23	SER	-	expression tag	UNP B5YC64
B	1	MET	-	initiating methionine	UNP B5YC64
B	2	GLY	-	expression tag	UNP B5YC64

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	SER	-	expression tag	UNP B5YC64
B	4	SER	-	expression tag	UNP B5YC64
B	5	HIS	-	expression tag	UNP B5YC64
B	6	HIS	-	expression tag	UNP B5YC64
B	7	HIS	-	expression tag	UNP B5YC64
B	8	HIS	-	expression tag	UNP B5YC64
B	9	HIS	-	expression tag	UNP B5YC64
B	10	HIS	-	expression tag	UNP B5YC64
B	11	SER	-	expression tag	UNP B5YC64
B	12	SER	-	expression tag	UNP B5YC64
B	13	GLY	-	expression tag	UNP B5YC64
B	14	LEU	-	expression tag	UNP B5YC64
B	15	VAL	-	expression tag	UNP B5YC64
B	16	PRO	-	expression tag	UNP B5YC64
B	17	ARG	-	expression tag	UNP B5YC64
B	18	GLY	-	expression tag	UNP B5YC64
B	19	SER	-	expression tag	UNP B5YC64
B	20	HIS	-	expression tag	UNP B5YC64
B	21	MET	-	expression tag	UNP B5YC64
B	22	ALA	-	expression tag	UNP B5YC64
B	23	SER	-	expression tag	UNP B5YC64

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



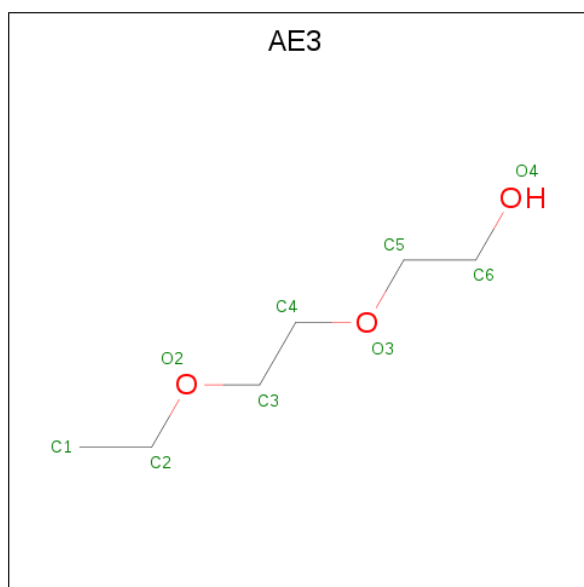
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is 2-(2-ETHOXYETHOXY)ETHANOL (three-letter code: AE3) (formula:  $C_6H_{14}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	6	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	5	3		
3	B	1	Total	C	O	0	0
			9	6	3		
3	B	1	Total	C	O	0	0
			8	5	3		
3	B	1	Total	C	O	0	0
			6	4	2		

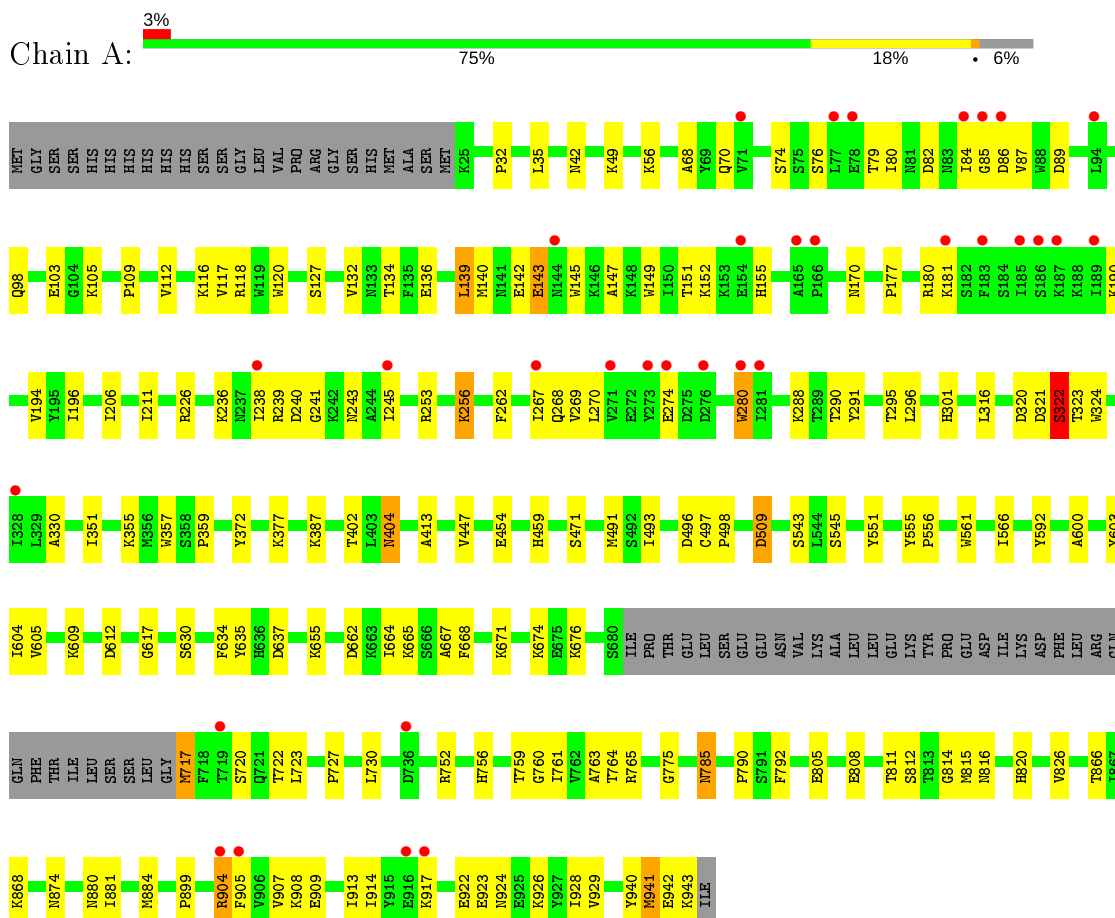
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	B	70	Total	O	0	0
			70	70		

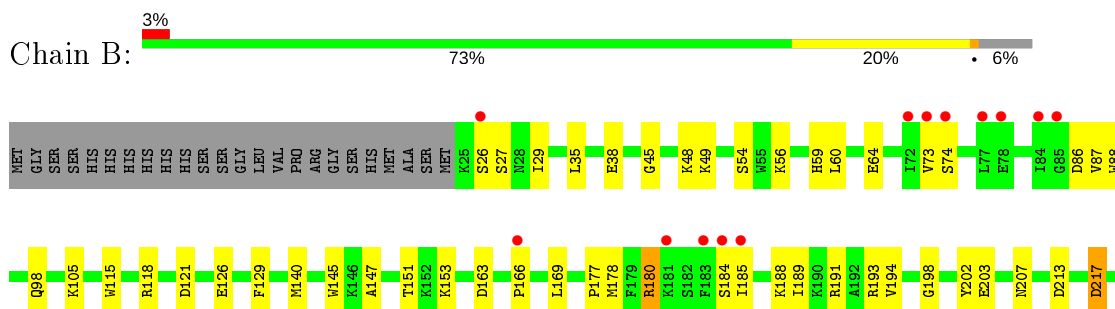
### 3 Residue-property plots

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

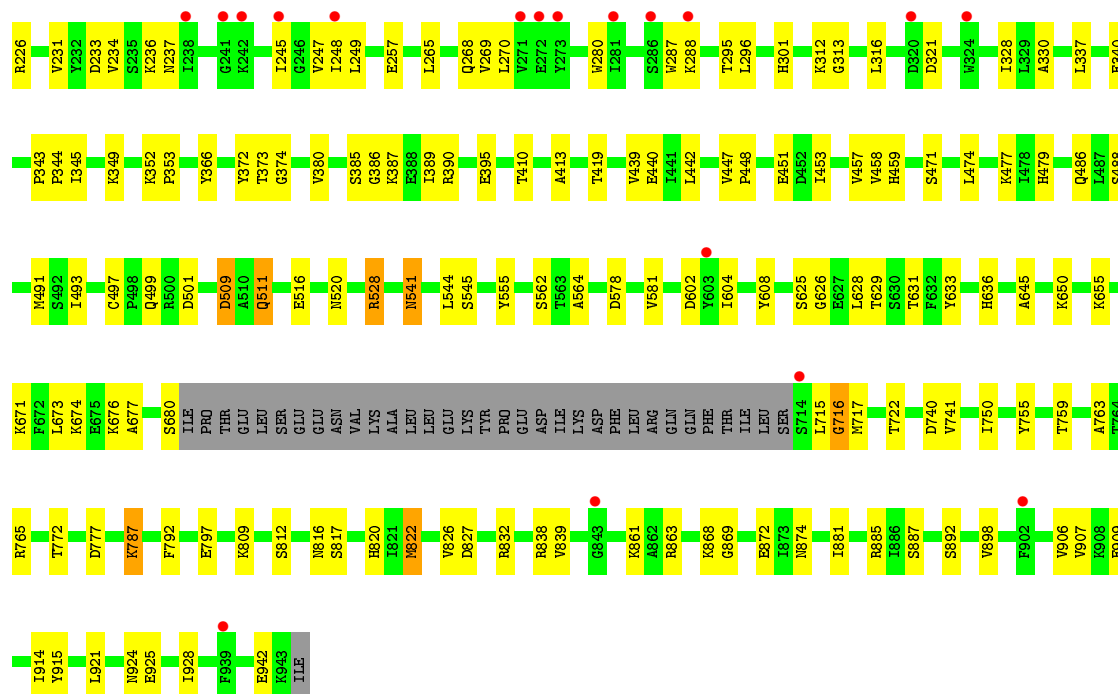
- Molecule 1: Alpha-rhamnosidase



- Molecule 1: Alpha-rhamnosidase







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.22Å 161.53Å 124.38Å 90.00° 132.14° 90.00°	Depositor
Resolution (Å)	43.28 – 2.74 49.21 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.9 (43.28-2.74) 97.1 (49.21-2.75)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.94 (at 2.73Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.226 , 0.270 0.227 , 0.270	Depositor DCC
$R_{free}$ test set	3203 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.8	Xtrriage
Anisotropy	0.149	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.042 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14789	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AE3, PGE

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	0.36	0/7442	0.44	0/10098
1	B	0.28	0/7456	0.42	0/10115
All	All	0.32	0/14898	0.43	0/20213

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

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	7237	0	7030	135	0
1	B	7251	0	7059	131	0
2	A	80	0	112	30	0
2	B	30	0	42	6	0
3	A	17	0	23	1	0
3	B	23	0	32	4	0
4	A	81	0	0	2	0
4	B	70	0	0	2	0
All	All	14789	0	14298	267	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 9.

All (267) 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:256:LYS:CE	2:A:1007:PGE:H42	1.79	1.11
1:A:355:LYS:HE2	2:A:1001:PGE:C6	1.81	1.10
1:A:256:LYS:HE3	2:A:1007:PGE:C4	1.83	1.08
1:B:787:LYS:HE3	3:B:1001:AE3:H1C2	1.40	1.04
1:B:27:SER:O	1:B:29:ILE:HD12	1.55	1.04
1:A:355:LYS:HE2	2:A:1001:PGE:H6	1.41	1.00
1:A:256:LYS:HE3	2:A:1007:PGE:H42	1.01	0.99
1:A:355:LYS:NZ	2:A:1001:PGE:H62	1.76	0.99
1:A:717:MET:HG2	1:A:752:ARG:NH2	1.77	0.98
1:A:355:LYS:CE	2:A:1001:PGE:H62	1.94	0.96
1:A:256:LYS:HE2	2:A:1007:PGE:H1	1.48	0.92
1:A:355:LYS:HE2	2:A:1001:PGE:H62	1.51	0.88
1:A:717:MET:HG2	1:A:752:ARG:HH22	1.39	0.87
1:A:355:LYS:CE	2:A:1001:PGE:C6	2.54	0.85
1:B:27:SER:O	1:B:29:ILE:CD1	2.29	0.80
1:A:206:ILE:HG12	1:A:245:ILE:HG22	1.67	0.77
1:A:268:GLN:NE2	1:A:280:TRP:CZ3	2.53	0.77
1:A:775:GLY:HA3	2:A:1010:PGE:H2	1.68	0.76
1:A:270:LEU:HD23	1:A:280:TRP:CE3	2.22	0.75
1:A:926:LYS:HE3	2:A:1010:PGE:H22	1.66	0.75
1:A:196:ILE:HB	1:A:267:ILE:HD13	1.69	0.75
1:B:906:VAL:HG12	1:B:942:GLU:HB2	1.67	0.74
1:B:29:ILE:HD13	1:B:60:LEU:HD13	1.69	0.74
1:A:85:GLY:HA3	1:A:89:ASP:HB2	1.70	0.74
1:B:477:LYS:HZ2	2:B:1004:PGE:H52	1.53	0.72
1:A:904:ARG:HH12	1:A:943:LYS:CB	2.02	0.71
1:B:180:ARG:NH1	1:B:321:ASP:OD1	2.23	0.71
1:B:194:VAL:HG22	1:B:269:VAL:HG22	1.71	0.70
1:A:181:LYS:HB3	1:A:245:ILE:HD11	1.74	0.69
1:A:355:LYS:HZ3	2:A:1001:PGE:H62	1.55	0.69
1:A:926:LYS:HD2	2:A:1010:PGE:H42	1.75	0.68
1:A:35:LEU:HD21	1:A:117:VAL:HG12	1.75	0.67
1:B:410:THR:HB	1:B:501:ASP:OD2	1.96	0.66
1:B:366:TYR:HB2	1:B:439:VAL:HG12	1.76	0.65
1:B:184:SER:O	1:B:185:ILE:HD12	1.97	0.65
1:A:256:LYS:HE2	2:A:1007:PGE:C1	2.28	0.64
1:A:70:GLN:OE1	1:A:118:ARG:NH2	2.31	0.63
1:B:907:VAL:HB	1:B:915:TYR:HB3	1.81	0.63
1:A:194:VAL:HG13	1:A:267:ILE:HD11	1.80	0.62
1:B:145:TRP:O	1:B:147:ALA:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:O	1:A:243:ASN:ND2	2.31	0.62
1:A:775:GLY:HA2	2:A:1010:PGE:H6	1.81	0.62
1:A:79:THR:HG23	1:A:84:ILE:HD11	1.82	0.62
1:A:256:LYS:CE	2:A:1007:PGE:C4	2.58	0.62
1:A:270:LEU:HA	1:A:280:TRP:HB3	1.81	0.62
1:A:604:ILE:N	1:A:604:ILE:HD12	2.15	0.62
1:B:295:THR:OG1	1:B:296:LEU:N	2.33	0.61
1:B:193:ARG:NH1	1:B:233:ASP:OD2	2.34	0.61
1:B:477:LYS:NZ	2:B:1004:PGE:H52	2.15	0.61
1:A:180:ARG:NH2	1:A:316:LEU:O	2.34	0.61
1:A:603:TYR:C	1:A:604:ILE:HD12	2.21	0.61
1:B:440:GLU:OE2	1:B:442:LEU:HD11	2.01	0.61
1:B:98:GLN:OE1	1:B:868:LYS:NZ	2.33	0.60
1:A:142:GLU:HA	1:A:145:TRP:CD1	2.36	0.60
1:A:322:SER:O	1:A:324:TRP:N	2.34	0.60
1:B:715:LEU:HD22	1:B:716:GLY:H	1.66	0.60
1:B:312:LYS:HD3	1:B:313:GLY:N	2.17	0.59
1:A:151:THR:OG1	1:A:330:ALA:HB2	2.02	0.59
1:B:226:ARG:NH1	1:B:340:GLU:OE1	2.37	0.58
1:A:909:GLU:HB2	1:A:914:ILE:HD13	1.84	0.58
1:A:556:PRO:O	1:A:609:LYS:NZ	2.35	0.58
1:B:477:LYS:NZ	2:B:1004:PGE:O1	2.34	0.58
1:B:184:SER:C	1:B:185:ILE:HD12	2.23	0.58
1:A:600:ALA:HB2	1:A:605:VAL:HG13	1.85	0.57
1:B:787:LYS:CE	3:B:1001:AE3:H1C2	2.25	0.57
1:B:528:ARG:NH1	1:B:578:ASP:OD2	2.37	0.57
1:A:256:LYS:HE3	2:A:1007:PGE:C3	2.33	0.57
1:A:497:CYS:HB3	1:A:820:HIS:CE1	2.39	0.57
1:B:604:ILE:HD13	1:B:631:THR:HG21	1.87	0.57
1:A:926:LYS:NZ	2:A:1010:PGE:O4	2.37	0.57
1:A:904:ARG:NH1	1:A:943:LYS:CB	2.68	0.57
1:B:188:LYS:HD3	1:B:189:ILE:H	1.71	0.56
1:B:499:GLN:NE2	1:B:817:SER:OG	2.35	0.56
1:B:915:TYR:HB2	1:B:921:LEU:HD12	1.88	0.56
1:A:617:GLY:N	1:A:808:GLU:OE2	2.37	0.56
1:A:604:ILE:HG12	1:A:671:LYS:HD2	1.87	0.56
1:B:151:THR:HB	1:B:330:ALA:HB2	1.87	0.56
1:A:98:GLN:OE1	1:A:868:LYS:NZ	2.35	0.56
1:B:64:GLU:OE1	1:B:121:ASP:HB2	2.05	0.56
1:B:73:VAL:HG12	1:B:88:TRP:HB3	1.89	0.55
1:A:496:ASP:OD2	2:A:1008:PGE:O4	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LYS:NZ	1:A:866:THR:O	2.40	0.55
1:A:145:TRP:O	1:A:147:ALA:N	2.33	0.54
1:B:352:LYS:HG3	1:B:353:PRO:HD2	1.89	0.54
1:B:245:ILE:HD11	1:B:287:TRP:CH2	2.43	0.54
1:A:139:LEU:HD12	1:A:145:TRP:CE2	2.43	0.54
1:A:664:ILE:O	1:A:665:LYS:C	2.46	0.54
1:A:922:GLU:HB2	1:A:929:VAL:HB	1.88	0.53
1:B:27:SER:C	1:B:29:ILE:HD12	2.26	0.53
1:A:256:LYS:NZ	2:A:1007:PGE:H42	2.23	0.53
1:A:268:GLN:NE2	1:A:280:TRP:CE3	2.69	0.53
1:B:345:ILE:HD13	1:B:491:MET:HE3	1.90	0.53
1:A:814:GLY:O	1:A:816:ASN:N	2.41	0.53
1:B:73:VAL:HG13	1:B:87:VAL:HB	1.91	0.53
1:A:239:ARG:NH1	4:A:1107:HOH:O	2.41	0.53
1:B:118:ARG:NH2	1:B:126:GLU:OE2	2.42	0.52
1:B:270:LEU:HB2	1:B:280:TRP:CZ3	2.43	0.52
1:B:390:ARG:HE	1:B:442:LEU:HD13	1.73	0.52
1:A:674:LYS:O	1:A:676:LYS:N	2.42	0.52
1:A:605:VAL:HG23	1:A:630:SER:HB3	1.92	0.52
1:A:103:GLU:OE2	2:A:1002:PGE:H42	2.10	0.52
1:B:145:TRP:O	1:B:268:GLN:NE2	2.43	0.52
1:B:86:ASP:OD1	1:B:86:ASP:N	2.43	0.52
1:A:206:ILE:HB	1:A:211:ILE:HD11	1.92	0.51
1:A:759:THR:HB	1:A:763:ALA:HB3	1.93	0.51
1:A:322:SER:C	1:A:324:TRP:H	2.14	0.51
1:A:180:ARG:HD3	1:A:321:ASP:OD1	2.11	0.51
1:A:404:ASN:OD1	1:A:811:THR:OG1	2.28	0.51
1:A:880:ASN:N	1:A:880:ASN:OD1	2.42	0.51
1:B:247:VAL:HG11	1:B:265:LEU:HD13	1.92	0.51
1:B:374:GLY:HA2	1:B:458:VAL:HB	1.93	0.51
1:A:566:ILE:HD11	1:A:637:ASP:OD2	2.10	0.51
1:A:280:TRP:N	1:A:280:TRP:CD1	2.77	0.51
1:B:633:TYR:HA	1:B:636:HIS:HB3	1.93	0.51
1:B:722:THR:HG23	1:B:763:ALA:HB2	1.93	0.50
1:A:74:SER:HA	1:A:86:ASP:HB3	1.93	0.50
1:B:153:LYS:HG2	1:B:328:ILE:HG23	1.94	0.50
1:B:486:GLN:NE2	1:B:516:GLU:OE1	2.44	0.50
1:B:832:ARG:HB3	1:B:838:ARG:HG2	1.92	0.50
1:B:715:LEU:O	1:B:717:MET:N	2.45	0.50
1:B:38:GLU:OE2	1:B:48:LYS:HD3	2.12	0.50
1:B:169:LEU:HD22	1:B:257:GLU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:LYS:HE2	1:B:451:GLU:HA	1.94	0.50
1:B:578:ASP:OD2	1:B:581:VAL:HB	2.12	0.50
1:B:797:GLU:OE2	3:B:1001:AE3:H2C1	2.12	0.49
1:B:198:GLY:HA3	1:B:202:TYR:HB3	1.93	0.49
1:B:313:GLY:HA2	1:B:316:LEU:HD12	1.94	0.49
1:B:497:CYS:HB2	1:B:499:GLN:OE1	2.11	0.49
1:A:604:ILE:HD11	1:A:667:ALA:HB1	1.95	0.49
1:B:45:GLY:HA3	1:B:231:VAL:HG11	1.93	0.49
1:B:544:LEU:HD12	1:B:562:SER:HB3	1.95	0.48
1:B:874:ASN:HB2	1:B:885:ARG:HB3	1.95	0.48
1:B:105:LYS:NZ	4:B:1107:HOH:O	2.45	0.48
1:B:861:LYS:NZ	1:B:863:ARG:HH21	2.11	0.48
1:A:491:MET:C	1:A:493:ILE:H	2.17	0.47
1:A:720:SER:H	1:A:723:LEU:HD12	1.78	0.47
1:B:477:LYS:HG2	2:B:1004:PGE:H22	1.96	0.47
1:A:112:VAL:HG22	1:A:136:GLU:HB2	1.96	0.47
1:A:149:TRP:HB3	1:A:330:ALA:HB3	1.96	0.47
1:B:202:TYR:CE1	1:B:217:ASP:HB3	2.49	0.47
1:B:541:ASN:HD22	1:B:541:ASN:C	2.14	0.47
1:B:759:THR:HB	1:B:763:ALA:HB3	1.96	0.47
1:B:74:SER:HA	1:B:86:ASP:OD1	2.14	0.47
1:A:509:ASP:N	1:A:509:ASP:OD1	2.48	0.47
1:B:545:SER:HB2	1:B:555:TYR:CZ	2.50	0.47
1:A:32:PRO:HG2	1:A:117:VAL:HG13	1.96	0.47
1:B:395:GLU:CD	1:B:499:GLN:HE21	2.18	0.47
1:B:491:MET:C	1:B:493:ILE:H	2.18	0.47
1:B:772:THR:HG23	1:B:777:ASP:HB3	1.97	0.47
1:B:511:GLN:HB2	1:B:564:ALA:HB2	1.96	0.46
1:A:295:THR:OG1	1:A:296:LEU:N	2.46	0.46
1:A:359:PRO:HB2	1:A:402:THR:HG22	1.97	0.46
1:B:385:SER:O	1:B:419:THR:OG1	2.26	0.46
1:B:188:LYS:CD	1:B:189:ILE:H	2.28	0.46
1:B:477:LYS:HD3	2:B:1004:PGE:H32	1.98	0.46
1:B:520:ASN:ND2	1:B:827:ASP:OD2	2.38	0.46
1:A:194:VAL:HG22	1:A:269:VAL:HG22	1.97	0.46
1:B:194:VAL:O	1:B:231:VAL:HA	2.16	0.46
1:A:351:ILE:HD11	1:A:372:TYR:CZ	2.51	0.46
1:A:68:ALA:HB3	1:A:120:TRP:HB2	1.98	0.46
1:B:236:LYS:HD3	1:B:236:LYS:HA	1.68	0.46
1:A:262:PHE:CZ	2:A:1007:PGE:H2	2.50	0.46
1:B:608:TYR:CD2	1:B:626:GLY:HA3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:881:ILE:HD13	1:B:942:GLU:HA	1.97	0.46
1:A:253:ARG:HD2	1:A:551:TYR:CE2	2.51	0.45
1:B:474:LEU:HB2	3:B:1001:AE3:H5C1	1.98	0.45
1:B:213:ASP:N	1:B:213:ASP:OD1	2.47	0.45
1:B:312:LYS:HD3	1:B:313:GLY:H	1.80	0.45
1:B:602:ASP:OD2	1:B:602:ASP:N	2.45	0.45
1:B:872:GLU:HB2	1:B:887:SER:HB2	1.98	0.45
1:A:109:PRO:HA	1:A:140:MET:HG3	1.99	0.45
1:B:509:ASP:OD1	1:B:509:ASP:N	2.50	0.45
1:A:874:ASN:HB3	1:B:447:VAL:HG23	1.99	0.45
1:A:634:PHE:CD2	1:A:664:ILE:HD13	2.52	0.45
1:B:645:ALA:HB1	1:B:650:LYS:HB2	1.98	0.45
1:A:236:LYS:HA	1:A:236:LYS:HD2	1.79	0.45
1:B:178:MET:HG2	1:B:248:ILE:HD13	1.98	0.45
1:A:612:ASP:OD2	1:A:722:THR:OG1	2.24	0.45
1:B:27:SER:OG	1:B:27:SER:O	2.32	0.45
2:A:1004:PGE:H22	2:A:1004:PGE:H4	1.76	0.44
1:B:343:PRO:HA	1:B:344:PRO:HD3	1.92	0.44
1:B:194:VAL:HG23	1:B:234:VAL:HG21	2.00	0.44
1:B:312:LYS:HE2	1:B:312:LYS:HA	2.00	0.44
1:A:717:MET:CG	1:A:752:ARG:HH22	2.20	0.44
1:A:357:TRP:CD2	2:A:1001:PGE:H3	2.53	0.44
1:A:756:HIS:HB3	1:A:790:PRO:HD2	1.99	0.44
1:A:74:SER:HB2	1:A:80:ILE:HB	1.99	0.44
1:B:625:SER:O	1:B:629:THR:HG23	2.18	0.44
1:B:59:HIS:CG	1:B:64:GLU:HG3	2.52	0.44
1:A:190:LYS:HD3	1:A:274:GLU:HA	1.99	0.44
1:A:592:TYR:HE2	1:A:637:ASP:OD1	2.01	0.44
1:A:923:GLU:HB3	1:A:928:ILE:HD13	1.99	0.43
1:A:152:LYS:HD3	1:A:177:PRO:HB3	2.00	0.43
1:A:924:ASN:ND2	4:A:1112:HOH:O	2.50	0.43
1:A:926:LYS:CD	2:A:1010:PGE:H42	2.44	0.43
1:A:49:LYS:HE2	1:A:140:MET:HE3	2.00	0.43
1:A:142:GLU:HA	1:A:145:TRP:HD1	1.83	0.43
1:A:908:LYS:HB2	1:A:908:LYS:HE3	1.65	0.43
1:A:908:LYS:HB2	1:A:940:TYR:HB2	2.01	0.43
1:A:262:PHE:CZ	2:A:1007:PGE:C2	3.02	0.43
1:A:87:VAL:HB	1:A:105:LYS:HB3	2.00	0.43
1:A:170:ASN:HD21	2:A:1007:PGE:H6	1.84	0.43
1:B:715:LEU:HD13	1:B:716:GLY:N	2.33	0.43
1:B:909:GLU:HB2	1:B:914:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:O	1:A:143:GLU:HB2	2.19	0.43
1:A:288:LYS:HG3	1:A:321:ASP:O	2.18	0.43
1:B:145:TRP:CE2	1:B:337:LEU:HD13	2.54	0.43
1:B:459:HIS:HA	1:B:491:MET:SD	2.59	0.43
1:A:604:ILE:N	1:A:604:ILE:CD1	2.82	0.43
1:A:635:TYR:HD2	1:A:730:LEU:HD13	1.83	0.43
1:B:177:PRO:HD2	1:B:249:LEU:HB2	2.01	0.43
1:B:604:ILE:HG21	1:B:671:LYS:HD2	2.00	0.42
1:B:822:MET:H	1:B:822:MET:HG3	1.59	0.42
1:B:56:LYS:HD3	1:B:869:GLY:HA2	2.02	0.42
1:A:805:GLU:OE2	2:A:1008:PGE:H62	2.20	0.42
1:A:377:LYS:NZ	1:A:454:GLU:OE1	2.52	0.42
1:B:288:LYS:HG3	1:B:321:ASP:OD2	2.19	0.42
1:A:760:GLY:O	1:A:764:THR:OG1	2.24	0.42
1:A:387:LYS:HD3	1:A:387:LYS:HA	1.97	0.42
1:A:545:SER:HB2	1:A:555:TYR:CZ	2.54	0.42
1:A:792:PHE:CE2	1:A:826:VAL:HG21	2.55	0.42
1:A:785:ASN:O	1:A:785:ASN:ND2	2.43	0.42
1:B:203:GLU:HB3	1:B:248:ILE:CG2	2.50	0.42
1:A:301:HIS:HA	1:A:413:ALA:H	1.84	0.42
1:B:366:TYR:OH	1:B:448:PRO:HB2	2.19	0.42
1:B:301:HIS:HA	1:B:413:ALA:H	1.85	0.42
1:A:42:ASN:HA	1:A:134:THR:O	2.19	0.42
1:B:479:HIS:ND1	1:B:827:ASP:OD1	2.32	0.42
1:A:561:TRP:CH2	1:A:761:ILE:HD11	2.55	0.42
1:A:668:PHE:HE1	1:A:727:PRO:HB3	1.84	0.41
1:B:59:HIS:CE1	1:B:64:GLU:OE2	2.73	0.41
1:B:861:LYS:HG3	1:B:874:ASN:OD1	2.19	0.41
1:B:924:ASN:O	1:B:925:GLU:HB3	2.20	0.41
1:B:674:LYS:O	1:B:676:LYS:N	2.51	0.41
1:B:898:VAL:HB	1:B:928:ILE:HB	2.02	0.41
1:A:881:ILE:HG12	1:A:942:GLU:HG2	2.03	0.41
1:B:207:ASN:ND2	1:B:237:ASN:O	2.50	0.41
1:B:373:THR:HG21	1:B:488:SER:HA	2.02	0.41
1:B:385:SER:O	1:B:387:LYS:N	2.46	0.41
1:B:372:TYR:CD2	1:B:457:VAL:HG12	2.56	0.41
1:A:447:VAL:HB	1:B:861:LYS:HB2	2.03	0.41
1:B:54:SER:HA	1:B:98:GLN:O	2.21	0.41
1:A:905:PHE:HA	1:A:942:GLU:O	2.19	0.41
1:A:109:PRO:HG3	1:A:140:MET:HB2	2.02	0.41
1:A:459:HIS:HA	1:A:491:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:ASN:O	1:A:884:MET:HA	2.21	0.41
2:B:1005:PGE:H12	2:B:1005:PGE:H32	1.89	0.41
1:B:35:LEU:HB3	1:B:115:TRP:CZ2	2.56	0.41
1:A:913:ILE:HD12	1:A:913:ILE:H	1.85	0.41
1:A:262:PHE:CE2	2:A:1007:PGE:C2	3.03	0.41
1:A:155:HIS:CE1	1:A:262:PHE:HB3	2.56	0.41
1:A:899:PRO:O	1:A:941:MET:HE3	2.20	0.41
1:B:380:VAL:HG21	1:B:389:ILE:HD13	2.02	0.41
1:B:677:ALA:HA	1:B:741:VAL:HG22	2.02	0.41
1:B:750:ILE:HG12	1:B:755:TYR:CZ	2.56	0.41
1:B:509:ASP:OD2	1:B:822:MET:HG2	2.20	0.41
1:B:366:TYR:CE1	1:B:453:ILE:HG13	2.56	0.40
1:B:792:PHE:CE2	1:B:826:VAL:HG21	2.56	0.40
3:A:1005:AE3:H5C1	3:A:1005:AE3:H3C1	1.68	0.40
1:A:49:LYS:CE	1:A:140:MET:HE3	2.51	0.40
1:A:239:ARG:HG2	1:A:240:ASP:H	1.86	0.40
1:B:145:TRP:HA	1:B:268:GLN:HE22	1.85	0.40
1:B:349:LYS:HE2	1:B:349:LYS:HB2	1.97	0.40
1:A:116:LYS:HG2	1:A:132:VAL:HG22	2.04	0.40
1:A:290:THR:OG1	1:A:291:TYR:N	2.55	0.40
1:B:180:ARG:HD3	1:B:321:ASP:HB3	2.02	0.40
1:B:839:VAL:HG12	4:B:1134:HOH:O	2.21	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	879/944 (93%)	818 (93%)	54 (6%)	7 (1%)	19	36
1	B	882/944 (93%)	814 (92%)	63 (7%)	5 (1%)	25	44
All	All	1761/1888 (93%)	1632 (93%)	117 (7%)	12 (1%)	22	40

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	THR
1	A	241	GLY
1	A	322	SER
1	A	815	MET
1	B	716	GLY
1	A	498	PRO
1	B	140	MET
1	B	673	LEU
1	A	320	ASP
1	A	907	VAL
1	B	386	GLY
1	B	166	PRO

### 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	777/840 (92%)	755 (97%)	22 (3%)	43 63
1	B	778/840 (93%)	754 (97%)	24 (3%)	40 60
All	All	1555/1680 (93%)	1509 (97%)	46 (3%)	41 61

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	SER
1	A	82	ASP
1	A	127	SER
1	A	139	LEU
1	A	143	GLU
1	A	226	ARG
1	A	256	LYS
1	A	280	TRP
1	A	322	SER
1	A	404	ASN
1	A	471	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	509	ASP
1	A	543	SER
1	A	655	LYS
1	A	662	ASP
1	A	717	MET
1	A	765	ARG
1	A	785	ASN
1	A	812	SER
1	A	904	ARG
1	A	917	LYS
1	A	941	MET
1	B	26	SER
1	B	49	LYS
1	B	129	PHE
1	B	163	ASP
1	B	180	ARG
1	B	191	ARG
1	B	217	ASP
1	B	471	SER
1	B	509	ASP
1	B	511	GLN
1	B	528	ARG
1	B	541	ASN
1	B	628	LEU
1	B	655	LYS
1	B	680	SER
1	B	740	ASP
1	B	765	ARG
1	B	787	LYS
1	B	809	LYS
1	B	812	SER
1	B	816	ASN
1	B	820	HIS
1	B	822	MET
1	B	892	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	404	ASN
1	A	499	GLN
1	A	731	ASN

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Mol	Chain	Res	Type
1	B	268	GLN
1	B	541	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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	AE3	A	1005	-	8,8,8	0.38	0	7,7,7	0.55	0
2	PGE	B	1004	-	9,9,9	0.31	0	8,8,8	0.30	0
2	PGE	B	1003	-	9,9,9	0.32	0	8,8,8	0.26	0
2	PGE	A	1003	-	9,9,9	0.32	0	8,8,8	0.29	0
2	PGE	A	1004	-	9,9,9	0.30	0	8,8,8	0.30	0
3	AE3	A	1006	-	7,7,8	0.30	0	6,6,7	0.27	0
2	PGE	B	1005	-	9,9,9	0.32	0	8,8,8	0.29	0
2	PGE	A	1007	-	9,9,9	0.27	0	8,8,8	0.64	0
2	PGE	A	1009	-	9,9,9	0.31	0	8,8,8	0.33	0
2	PGE	A	1002	-	9,9,9	0.31	0	8,8,8	0.28	0
2	PGE	A	1010	-	9,9,9	0.51	0	8,8,8	0.80	0
2	PGE	A	1001	-	9,9,9	0.32	0	8,8,8	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AE3	B	1002	-	7,7,8	0.32	0	6,6,7	0.24	0
3	AE3	B	1006	-	5,5,8	0.38	0	4,4,7	0.30	0
2	PGE	A	1008	-	9,9,9	0.31	0	8,8,8	0.26	0
3	AE3	B	1001	-	8,8,8	0.38	0	7,7,7	0.29	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	AE3	A	1005	-	-	4/6/6/6	-
2	PGE	B	1004	-	-	6/7/7/7	-
2	PGE	B	1003	-	-	1/7/7/7	-
2	PGE	A	1003	-	-	0/7/7/7	-
2	PGE	A	1004	-	-	3/7/7/7	-
3	AE3	A	1006	-	-	0/5/5/6	-
2	PGE	B	1005	-	-	5/7/7/7	-
2	PGE	A	1007	-	-	6/7/7/7	-
2	PGE	A	1009	-	-	0/7/7/7	-
2	PGE	A	1002	-	-	2/7/7/7	-
2	PGE	A	1010	-	-	4/7/7/7	-
2	PGE	A	1001	-	-	1/7/7/7	-
3	AE3	B	1002	-	-	2/5/5/6	-
3	AE3	B	1006	-	-	1/3/3/6	-
2	PGE	A	1008	-	-	2/7/7/7	-
3	AE3	B	1001	-	-	2/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1010	PGE	C4-C3-O2-C2
3	A	1005	AE3	C3-C4-O3-C5
3	A	1005	AE3	O2-C3-C4-O3
2	B	1005	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
2	A	1004	PGE	O2-C3-C4-O3
3	B	1002	AE3	O2-C3-C4-O3
2	A	1007	PGE	O2-C3-C4-O3
2	B	1004	PGE	O1-C1-C2-O2
2	A	1010	PGE	O3-C5-C6-O4
2	B	1004	PGE	O2-C3-C4-O3
2	B	1003	PGE	O3-C5-C6-O4
2	A	1010	PGE	O1-C1-C2-O2
2	A	1010	PGE	O2-C3-C4-O3
2	A	1008	PGE	O2-C3-C4-O3
2	A	1008	PGE	C6-C5-O3-C4
2	A	1007	PGE	C1-C2-O2-C3
2	A	1004	PGE	C6-C5-O3-C4
3	B	1001	AE3	C6-C5-O3-C4
2	A	1001	PGE	C3-C4-O3-C5
2	B	1004	PGE	O3-C5-C6-O4
2	A	1002	PGE	C3-C4-O3-C5
2	B	1004	PGE	C3-C4-O3-C5
3	A	1005	AE3	C6-C5-O3-C4
2	A	1007	PGE	C4-C3-O2-C2
2	B	1005	PGE	O1-C1-C2-O2
3	A	1005	AE3	C1-C2-O2-C3
2	B	1004	PGE	C1-C2-O2-C3
3	B	1001	AE3	C3-C4-O3-C5
2	A	1007	PGE	O3-C5-C6-O4
2	A	1004	PGE	C4-C3-O2-C2
2	B	1004	PGE	C4-C3-O2-C2
2	B	1005	PGE	C4-C3-O2-C2
2	A	1007	PGE	C6-C5-O3-C4
2	A	1002	PGE	O3-C5-C6-O4
2	A	1007	PGE	C3-C4-O3-C5
2	B	1005	PGE	C1-C2-O2-C3
2	B	1005	PGE	C3-C4-O3-C5
3	B	1006	AE3	C1-C2-O2-C3
3	B	1002	AE3	C3-C4-O3-C5

There are no ring outliers.

10 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1005	AE3	1	0
2	B	1004	PGE	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1004	PGE	1	0
2	B	1005	PGE	1	0
2	A	1007	PGE	12	0
2	A	1002	PGE	1	0
2	A	1010	PGE	6	0
2	A	1001	PGE	8	0
2	A	1008	PGE	2	0
3	B	1001	AE3	4	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	883/944 (93%)	0.36	33 (3%) 41 46	42, 58, 81, 102	0
1	B	886/944 (93%)	0.31	31 (3%) 44 49	42, 60, 83, 97	0
All	All	1769/1888 (93%)	0.34	64 (3%) 42 47	42, 59, 82, 102	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	VAL	4.5
1	A	281	ILE	4.3
1	A	189	ILE	4.1
1	A	238	ILE	4.0
1	B	184	SER	3.8
1	A	185	ILE	3.7
1	B	183	PHE	3.4
1	B	286	SER	3.4
1	B	84	ILE	3.3
1	A	154	GLU	3.3
1	B	714	SER	3.0
1	A	183	PHE	3.0
1	B	185	ILE	2.9
1	B	281	ILE	2.9
1	A	181	LYS	2.8
1	A	144	ASN	2.8
1	B	248	ILE	2.8
1	A	85	GLY	2.8
1	A	84	ILE	2.8
1	B	78	GLU	2.7
1	A	917	LYS	2.7
1	B	902	PHE	2.7
1	B	272	GLU	2.7
1	B	241	GLY	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	186	SER	2.7
1	B	238	ILE	2.6
1	A	904	ARG	2.6
1	B	939	PHE	2.5
1	B	181	LYS	2.5
1	A	78	GLU	2.5
1	B	242	LYS	2.4
1	A	271	VAL	2.4
1	A	276	ASP	2.4
1	B	324	TRP	2.4
1	B	273	TYR	2.4
1	A	736	ASP	2.4
1	B	26	SER	2.4
1	A	274	GLU	2.4
1	B	85	GLY	2.4
1	B	73	VAL	2.4
1	B	166	PRO	2.3
1	B	245	ILE	2.3
1	A	166	PRO	2.3
1	A	905	PHE	2.3
1	A	245	ILE	2.3
1	B	603	TYR	2.2
1	A	267	ILE	2.2
1	A	94	LEU	2.2
1	A	273	TYR	2.2
1	A	280	TRP	2.2
1	A	187	LYS	2.2
1	B	843	GLY	2.2
1	A	77	LEU	2.2
1	A	916	GLU	2.1
1	B	320	ASP	2.1
1	A	165	ALA	2.1
1	B	288	LYS	2.1
1	A	71	VAL	2.1
1	A	328	ILE	2.1
1	B	77	LEU	2.1
1	B	72	ILE	2.0
1	A	719	THR	2.0
1	A	86	ASP	2.0
1	B	74	SER	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. 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( $\text{\AA}^2$ )	Q<0.9
3	AE3	B	1001	9/9	0.55	0.33	60,78,100,105	0
2	PGE	A	1004	10/10	0.69	0.30	64,77,83,84	0
3	AE3	A	1005	9/9	0.70	0.26	76,108,124,125	0
2	PGE	A	1007	10/10	0.71	0.36	79,82,87,88	0
3	AE3	B	1006	6/9	0.73	0.22	65,68,82,86	0
2	PGE	B	1004	10/10	0.76	0.24	64,71,78,80	0
3	AE3	B	1002	8/9	0.81	0.26	59,65,67,69	0
2	PGE	A	1010	10/10	0.85	0.29	20,20,20,20	0
2	PGE	A	1003	10/10	0.87	0.30	53,62,85,92	0
2	PGE	A	1002	10/10	0.87	0.23	62,66,74,75	0
2	PGE	A	1008	10/10	0.87	0.27	55,62,67,69	0
2	PGE	B	1005	10/10	0.87	0.26	55,62,67,67	0
2	PGE	B	1003	10/10	0.88	0.21	66,73,86,87	0
2	PGE	A	1009	10/10	0.88	0.26	57,63,67,71	0
3	AE3	A	1006	8/9	0.89	0.23	67,75,77,80	0
2	PGE	A	1001	10/10	0.89	0.19	61,67,72,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.