



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:15 PM GMT

PDB ID : 3WIR
Title : Crystal structure of kojibiose phosphorylase complexed with glucose
Authors : Okada, S.; Yamamoto, T.; Watanabe, H.; Nishimoto, T.; Chaen, H.; Fukuda, S.; Wakagi, T.; Fushinobu, S.
Deposited on : 2013-09-24
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

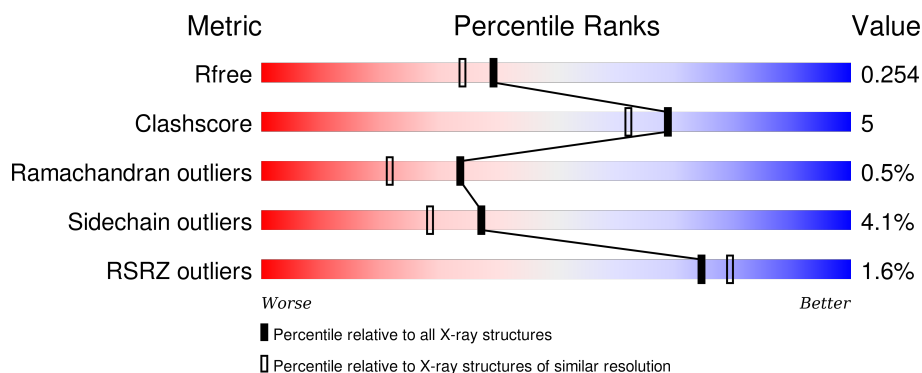
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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 ≥ 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	764	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	B	764	<div> <div>2%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	C	764	<div> <div>%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	D	764	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>

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	GOL	A	804	-	-	-	X
3	GOL	C	803	-	-	-	X
3	GOL	D	803	-	-	-	X
3	GOL	D	804	-	-	-	X
3	GOL	D	806	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26306 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 Kojibiose phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	756	Total	C	N	O	S	0	0	0
			6187	3985	1019	1162	21			
1	B	756	Total	C	N	O	S	0	0	0
			6187	3985	1019	1162	21			
1	C	756	Total	C	N	O	S	0	0	0
			6187	3985	1019	1162	21			
1	D	756	Total	C	N	O	S	0	0	0
			6187	3985	1019	1162	21			

There are 32 discrepancies between the modelled and reference sequences:

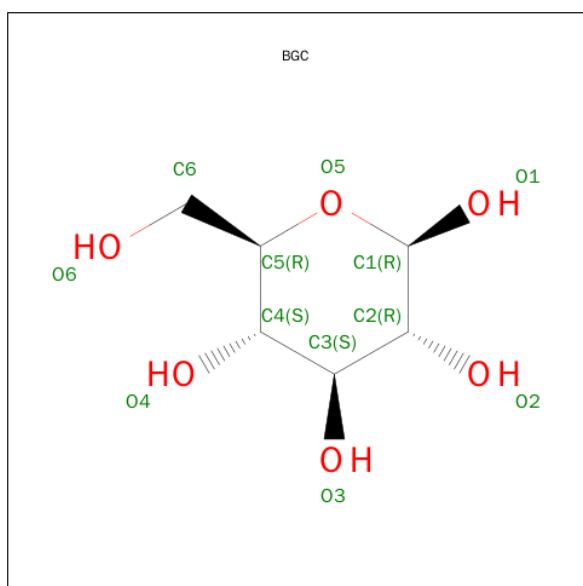
Chain	Residue	Modelled	Actual	Comment	Reference
A	757	GLY	-	EXPRESSION TAG	UNP A4XGP2
A	758	SER	-	EXPRESSION TAG	UNP A4XGP2
A	759	HIS	-	EXPRESSION TAG	UNP A4XGP2
A	760	HIS	-	EXPRESSION TAG	UNP A4XGP2
A	761	HIS	-	EXPRESSION TAG	UNP A4XGP2
A	762	HIS	-	EXPRESSION TAG	UNP A4XGP2
A	763	HIS	-	EXPRESSION TAG	UNP A4XGP2
A	764	HIS	-	EXPRESSION TAG	UNP A4XGP2
B	757	GLY	-	EXPRESSION TAG	UNP A4XGP2
B	758	SER	-	EXPRESSION TAG	UNP A4XGP2
B	759	HIS	-	EXPRESSION TAG	UNP A4XGP2
B	760	HIS	-	EXPRESSION TAG	UNP A4XGP2
B	761	HIS	-	EXPRESSION TAG	UNP A4XGP2
B	762	HIS	-	EXPRESSION TAG	UNP A4XGP2
B	763	HIS	-	EXPRESSION TAG	UNP A4XGP2
B	764	HIS	-	EXPRESSION TAG	UNP A4XGP2
C	757	GLY	-	EXPRESSION TAG	UNP A4XGP2
C	758	SER	-	EXPRESSION TAG	UNP A4XGP2
C	759	HIS	-	EXPRESSION TAG	UNP A4XGP2
C	760	HIS	-	EXPRESSION TAG	UNP A4XGP2
C	761	HIS	-	EXPRESSION TAG	UNP A4XGP2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	762	HIS	-	EXPRESSION TAG	UNP A4XGP2
C	763	HIS	-	EXPRESSION TAG	UNP A4XGP2
C	764	HIS	-	EXPRESSION TAG	UNP A4XGP2
D	757	GLY	-	EXPRESSION TAG	UNP A4XGP2
D	758	SER	-	EXPRESSION TAG	UNP A4XGP2
D	759	HIS	-	EXPRESSION TAG	UNP A4XGP2
D	760	HIS	-	EXPRESSION TAG	UNP A4XGP2
D	761	HIS	-	EXPRESSION TAG	UNP A4XGP2
D	762	HIS	-	EXPRESSION TAG	UNP A4XGP2
D	763	HIS	-	EXPRESSION TAG	UNP A4XGP2
D	764	HIS	-	EXPRESSION TAG	UNP A4XGP2

- Molecule 2 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



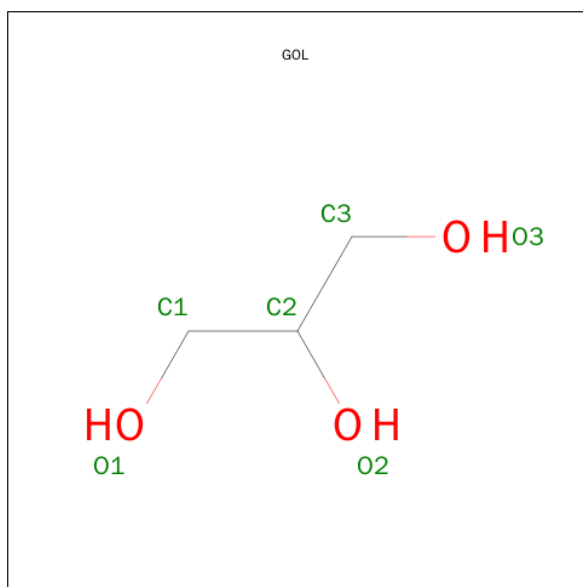
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0

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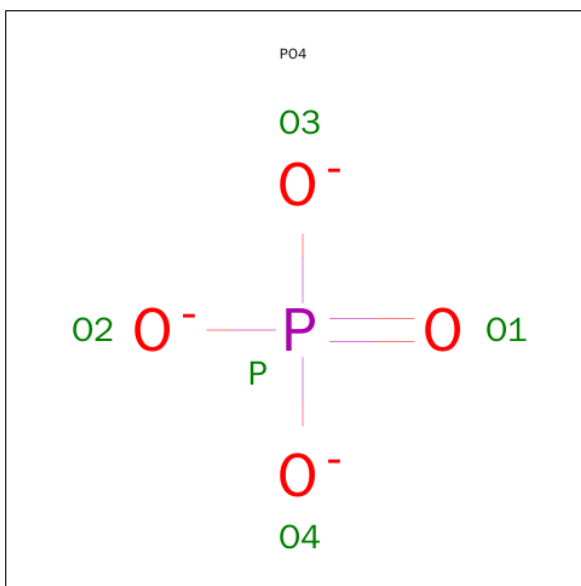
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

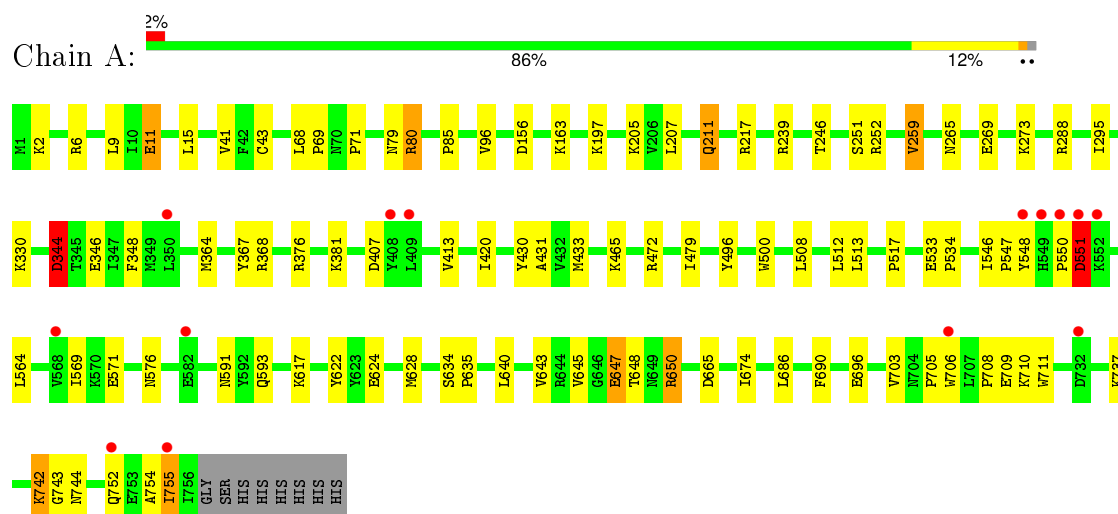
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	371	Total	O	0	0
			371	371		
5	B	387	Total	O	0	0
			387	387		
5	C	299	Total	O	0	0
			299	299		
5	D	321	Total	O	0	0
			321	321		

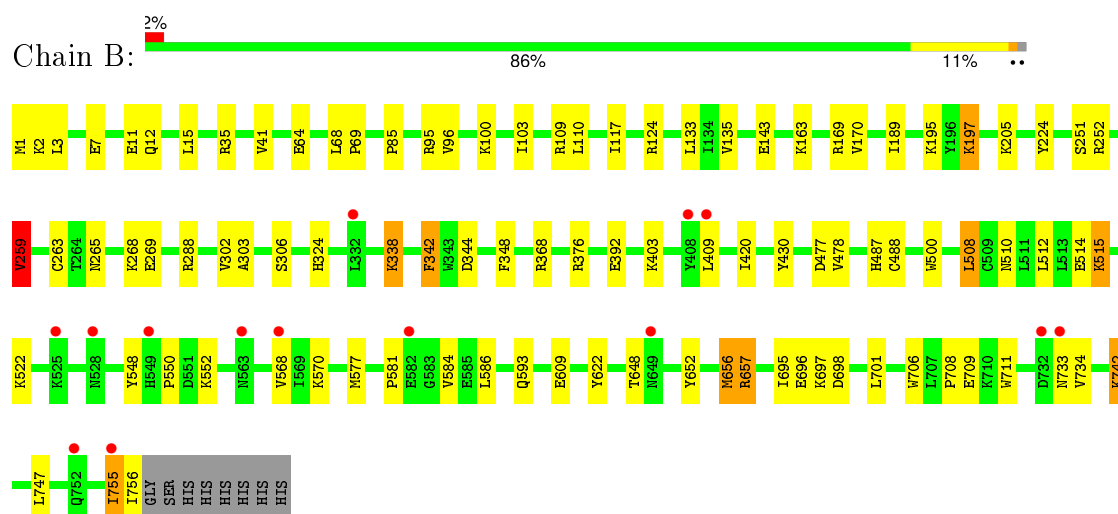
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

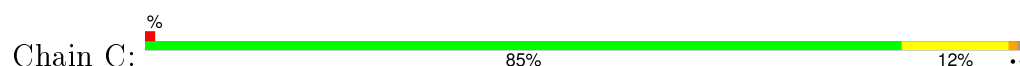
• Molecule 1: Kojibiose phosphorylase

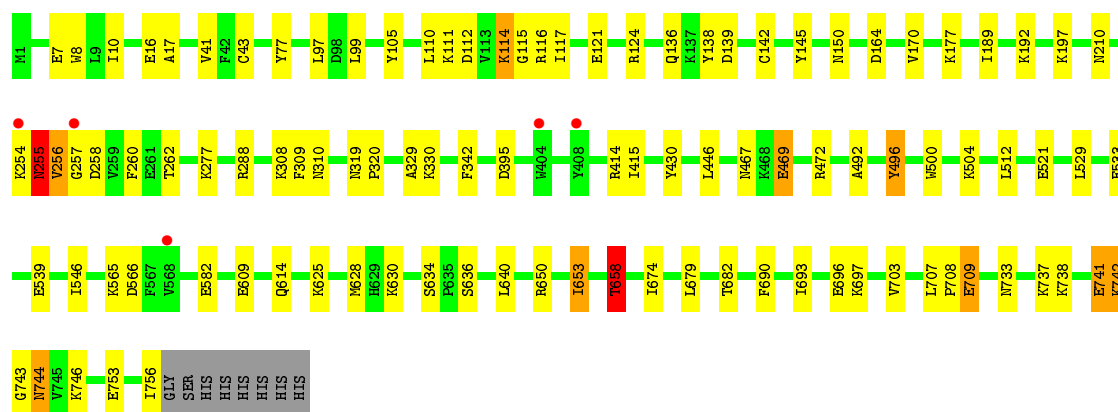


• Molecule 1: Kojibiose phosphorylase

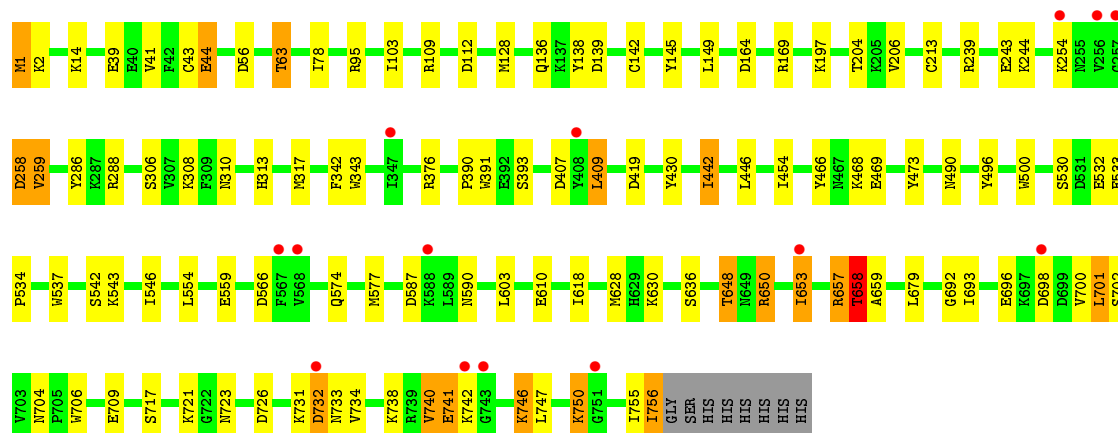
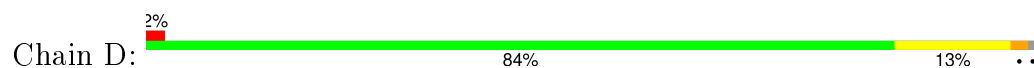


• Molecule 1: Kojibiose phosphorylase





● Molecule 1: Kojibiose phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.58Å 104.46Å 124.16Å 68.83° 86.02° 90.06°	Depositor
Resolution (Å)	46.26 – 2.05 46.26 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.26-2.05) 85.3 (46.26-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.191 , 0.251 0.196 , 0.254	Depositor DCC
R_{free} test set	10233 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 203950 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26306	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.80 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.0405e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, PO4, BGC

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	0.93	0/6328	0.94	12/8550 (0.1%)
1	B	0.91	1/6328 (0.0%)	0.95	12/8550 (0.1%)
1	C	0.81	0/6328	0.88	6/8550 (0.1%)
1	D	0.82	1/6328 (0.0%)	0.93	14/8550 (0.2%)
All	All	0.87	2/25312 (0.0%)	0.93	44/34200 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	658	THR	CB-CG2	-5.97	1.32	1.52
1	B	488	CYS	CB-SG	-5.47	1.72	1.81

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	657	ARG	NE-CZ-NH1	11.81	126.21	120.30
1	D	95	ARG	NE-CZ-NH1	-9.29	115.65	120.30
1	B	657	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	D	95	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	D	657	ARG	NE-CZ-NH1	8.03	124.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	C	124	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	B	376	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	D	419	ASP	CB-CG-OD1	-7.16	111.86	118.30
1	A	217	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	D	657	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	B	252	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	A	376	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	B	252	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	368	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	665	ASP	CB-CG-OD1	6.55	124.20	118.30
1	B	35	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	252	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	376	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	344	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	A	368	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	395	ASP	CB-CG-OD1	5.97	123.67	118.30
1	B	656	MET	CG-SD-CE	5.95	109.71	100.20
1	D	419	ASP	CB-CG-OD2	5.94	123.64	118.30
1	B	376	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	252	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	112	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	156	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	239	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	133	LEU	CB-CG-CD2	-5.58	101.51	111.00
1	D	112	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	C	658	THR	CB-CA-C	-5.55	96.62	111.60
1	D	139	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	368	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	D	376	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	433	MET	CG-SD-CE	5.39	108.83	100.20
1	C	164	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	D	407	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	C	139	ASP	CB-CG-OD2	5.12	122.90	118.30
1	B	263	CYS	CA-CB-SG	-5.10	104.83	114.00
1	D	164	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	B	259	VAL	CB-CA-C	-5.04	101.82	111.40
1	C	112	ASP	CB-CG-OD2	5.00	122.80	118.30
1	D	164	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	551	ASP	Peptide
1	C	255	ASN	Peptide

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	6187	0	6120	47	0
1	B	6187	0	6119	60	0
1	C	6187	0	6120	57	0
1	D	6187	0	6119	66	0
2	A	24	0	24	0	0
2	B	24	0	24	0	0
2	C	24	0	24	0	0
2	D	24	0	24	0	0
3	A	12	0	16	0	0
3	B	6	0	8	1	0
3	C	12	0	16	0	0
3	D	24	0	32	2	0
4	A	5	0	0	0	0
4	B	10	0	0	1	0
4	C	10	0	0	0	0
4	D	5	0	0	0	0
5	A	371	0	0	6	0
5	B	387	0	0	2	0
5	C	299	0	0	5	0
5	D	321	0	0	9	0
All	All	26306	0	24646	229	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 (229) 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:D:636:SER:HB3	1:D:658:THR:HG21	1.54	0.87
1:B:303:ALA:HB2	1:B:656:MET:HE1	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ALA:HB2	1:B:656:MET:CE	2.07	0.85
1:C:10:ILE:HD12	1:C:99:LEU:HD21	1.65	0.78
1:D:709:GLU:CD	1:D:709:GLU:H	1.88	0.76
1:C:105:TYR:OH	1:C:121:GLU:OE2	2.03	0.76
1:D:496:TYR:CD1	1:D:603:LEU:HD21	2.22	0.73
1:D:496:TYR:CE1	1:D:546:ILE:HG21	2.24	0.72
1:B:742:LYS:O	1:B:742:LYS:HG3	1.91	0.71
1:B:648:THR:HB	1:B:706:TRP:CH2	2.27	0.70
1:B:1:MET:CE	1:B:103:ILE:HD11	2.23	0.69
1:D:496:TYR:CZ	1:D:546:ILE:HG21	2.29	0.68
3:D:805:GOL:H11	5:D:989:HOH:O	1.95	0.67
1:C:529:LEU:HD12	1:C:533:GLU:OE1	1.95	0.67
1:C:738:LYS:NZ	1:C:743:GLY:O	2.29	0.66
1:B:11:GLU:HB3	1:B:96:VAL:HG12	1.76	0.66
1:A:617:LYS:HD3	1:A:645:VAL:HB	1.78	0.66
1:C:636:SER:HB3	1:C:658:THR:HG21	1.77	0.65
1:D:308:LYS:CE	5:D:1105:HOH:O	2.45	0.64
1:B:303:ALA:CB	1:B:656:MET:HE1	2.26	0.64
1:C:696:GLU:HA	1:C:696:GLU:OE2	1.98	0.62
1:D:723:ASN:OD1	1:D:742:LYS:N	2.25	0.62
1:B:755:ILE:N	1:B:755:ILE:HD13	2.15	0.62
1:B:197:LYS:HE3	1:B:259:VAL:CG2	2.29	0.62
1:C:10:ILE:HD13	1:C:309:PHE:CD1	2.33	0.62
1:D:288:ARG:NH2	5:D:1044:HOH:O	2.31	0.61
1:A:548:TYR:HB3	1:A:550:PRO:HD3	1.83	0.61
1:C:10:ILE:CD1	1:C:309:PHE:HD1	2.14	0.61
1:B:1:MET:HE1	1:B:3:LEU:HA	1.82	0.60
1:B:1:MET:HE3	1:B:3:LEU:HD23	1.83	0.60
1:D:442:ILE:HD13	1:D:446:LEU:HG	1.84	0.60
1:D:740:VAL:O	1:D:741:GLU:CB	2.50	0.60
1:D:496:TYR:CE1	1:D:546:ILE:CG2	2.85	0.60
1:A:211:GLN:HG2	1:B:195:LYS:HD2	1.85	0.59
1:B:303:ALA:HB2	1:B:656:MET:HE3	1.84	0.59
1:D:39:GLU:OE2	1:D:138:TYR:OH	2.21	0.58
1:D:308:LYS:HE2	5:D:1105:HOH:O	2.04	0.58
1:D:658:THR:CG2	5:D:1098:HOH:O	2.51	0.58
1:B:581:PRO:O	1:B:584:VAL:HG13	2.04	0.57
1:D:308:LYS:HE3	5:D:1105:HOH:O	2.03	0.57
1:A:407:ASP:HB3	1:A:413:VAL:HG11	1.86	0.57
1:D:78:ILE:HD13	1:D:149:LEU:HD22	1.86	0.57
1:D:693:ILE:HG23	1:D:701:LEU:HD22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:ILE:CD1	1:B:701:LEU:HD12	2.34	0.57
1:D:738:LYS:HE2	1:D:756:ILE:HD11	1.85	0.57
1:A:648:THR:HB	1:A:706:TRP:CH2	2.41	0.56
1:D:310:ASN:HA	1:D:679:LEU:HD22	1.86	0.56
1:D:258:ASP:O	1:D:259:VAL:HG13	2.05	0.56
1:C:741:GLU:O	1:C:742:LYS:HG2	2.06	0.56
1:D:740:VAL:HG22	1:D:741:GLU:N	2.21	0.56
1:C:467:ASN:OD1	1:C:469:GLU:HG3	2.06	0.56
1:C:746:LYS:NZ	1:C:753:GLU:OE2	2.39	0.55
1:C:10:ILE:CD1	1:C:309:PHE:CD1	2.89	0.55
1:B:302:VAL:O	1:B:306:SER:OG	2.22	0.55
1:A:11:GLU:HG3	1:A:96:VAL:HG12	1.89	0.55
1:A:703:VAL:HG12	1:A:705:PRO:HD3	1.87	0.55
1:C:446:LEU:HD23	1:C:512:LEU:CD2	2.38	0.54
1:A:43:CYS:HG	1:C:43:CYS:HG	0.55	0.54
1:B:747:LEU:HD22	1:B:756:ILE:HD11	1.90	0.54
1:C:446:LEU:HD23	1:C:512:LEU:HD21	1.88	0.53
1:B:197:LYS:HE3	1:B:259:VAL:HG22	1.90	0.53
1:C:430:TYR:HA	1:C:500:TRP:CH2	2.44	0.53
1:B:1:MET:HE3	1:B:103:ILE:HD11	1.88	0.53
1:C:744:ASN:N	1:C:744:ASN:OD1	2.42	0.52
1:A:273:LYS:NZ	5:A:1117:HOH:O	2.41	0.52
1:D:746:LYS:HG2	1:D:755:ILE:CD1	2.40	0.52
1:C:414:ARG:NH1	1:C:415:ILE:O	2.43	0.52
1:D:496:TYR:CE1	1:D:603:LEU:HD21	2.45	0.52
1:D:496:TYR:CD1	1:D:603:LEU:CD2	2.93	0.52
1:B:1:MET:HE1	1:B:2:LYS:C	2.31	0.52
1:C:136:GLN:HB3	1:C:138:TYR:CE2	2.45	0.52
1:B:510:ASN:O	1:B:514:GLU:HG3	2.09	0.51
1:A:259:VAL:HG23	5:A:1196:HOH:O	2.09	0.51
1:B:224:TYR:OH	4:B:805:PO4:O3	2.23	0.51
1:D:628:MET:HB3	1:D:630:LYS:HG2	1.93	0.51
1:C:741:GLU:O	1:C:742:LYS:CG	2.58	0.51
1:D:56:ASP:C	1:D:63:THR:HG22	2.31	0.51
1:A:742:LYS:HG3	1:A:743:GLY:N	2.26	0.51
1:D:454:ILE:HG23	1:D:537:TRP:CH2	2.46	0.51
1:D:740:VAL:O	1:D:741:GLU:HB3	2.10	0.51
1:C:255:ASN:N	1:C:255:ASN:OD1	2.42	0.50
1:C:640:LEU:C	1:C:640:LEU:HD23	2.30	0.50
1:C:310:ASN:HA	1:C:679:LEU:HD22	1.93	0.50
1:B:1:MET:HE2	1:B:103:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:GLU:CD	1:C:7:GLU:H	2.15	0.50
1:D:648:THR:HG21	1:D:706:TRP:CZ2	2.47	0.50
1:C:741:GLU:O	1:C:742:LYS:CB	2.59	0.50
1:D:756:ILE:C	1:D:756:ILE:HD12	2.31	0.50
1:A:6:ARG:HD2	1:A:9:LEU:HD12	1.92	0.50
1:D:128:MET:HG3	1:D:286:TYR:CE2	2.46	0.50
1:B:265:ASN:O	1:B:269:GLU:HG3	2.12	0.50
1:B:409:LEU:HD21	1:B:586:LEU:HB2	1.94	0.50
1:C:256:VAL:O	1:C:258:ASP:N	2.43	0.49
1:C:142:CYS:HB3	1:C:145:TYR:CE2	2.48	0.49
1:D:313:HIS:O	1:D:317:MET:HB2	2.12	0.49
1:A:79:ASN:O	1:A:80:ARG:HB2	2.11	0.49
1:C:258:ASP:OD2	1:C:260:PHE:HB3	2.12	0.49
1:D:43:CYS:HB3	1:D:44:GLU:HG3	1.95	0.49
1:D:533:GLU:N	1:D:534:PRO:HD2	2.28	0.49
1:B:197:LYS:HG2	1:B:251:SER:HB3	1.95	0.48
1:D:142:CYS:HB3	1:D:145:TYR:CE2	2.48	0.48
1:C:628:MET:HB3	1:C:630:LYS:HG2	1.95	0.48
1:C:472:ARG:NH1	5:C:1057:HOH:O	2.31	0.48
1:D:136:GLN:OE1	1:D:244:LYS:HD2	2.13	0.48
1:A:197:LYS:HG3	1:A:251:SER:HB3	1.95	0.48
1:C:658:THR:HB	1:C:682:THR:OG1	2.14	0.48
1:A:710:LYS:NZ	5:A:1162:HOH:O	2.46	0.48
1:C:16:GLU:HG3	1:C:17:ALA:O	2.14	0.47
1:A:546:ILE:O	1:A:548:TYR:N	2.45	0.47
1:C:256:VAL:HG12	1:C:262:THR:HG21	1.97	0.47
1:C:696:GLU:OE2	1:C:696:GLU:CA	2.63	0.47
1:D:741:GLU:N	5:D:912:HOH:O	2.46	0.47
1:D:653:ILE:O	1:D:657:ARG:HG3	2.14	0.47
1:B:420:ILE:HB	1:B:478:VAL:HA	1.96	0.47
1:D:78:ILE:CD1	1:D:149:LEU:HD22	2.43	0.47
1:D:692:GLY:HA2	5:D:1183:HOH:O	2.14	0.47
1:C:693:ILE:HD13	1:C:703:VAL:HG13	1.97	0.47
1:B:568:VAL:O	1:B:570:LYS:HE3	2.15	0.47
1:C:77:TYR:HB2	1:C:150:ASN:HB3	1.97	0.47
1:B:15:LEU:HD21	1:B:85:PRO:HB2	1.97	0.47
1:A:430:TYR:HA	1:A:500:TRP:CH2	2.50	0.47
1:B:755:ILE:H	1:B:755:ILE:HD13	1.77	0.47
1:C:446:LEU:CD2	1:C:512:LEU:CD2	2.93	0.47
1:D:306:SER:HB3	1:D:659:ALA:HB1	1.96	0.47
1:A:593:GLN:NE2	1:A:622:TYR:OH	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:TYR:CE1	1:B:656:MET:HE2	2.49	0.46
1:B:342:PHE:CE1	1:B:392:GLU:HG2	2.51	0.46
1:B:430:TYR:HA	1:B:500:TRP:CH2	2.50	0.46
1:B:477:ASP:OD1	1:B:487:HIS:HA	2.16	0.46
1:D:542:SER:OG	1:D:543:LYS:HG3	2.16	0.46
1:B:696:GLU:OE1	1:B:696:GLU:HA	2.15	0.46
1:A:68:LEU:HB3	1:A:69:PRO:HD2	1.96	0.46
1:D:391:TRP:HB2	5:D:1104:HOH:O	2.15	0.46
1:A:265:ASN:O	1:A:269:GLU:HG3	2.16	0.46
1:A:634:SER:HB3	1:A:635:PRO:HD3	1.98	0.46
1:D:704:ASN:OD1	1:D:750:LYS:HA	2.15	0.46
1:D:490:ASN:ND2	1:D:559:GLU:OE1	2.47	0.46
1:D:390:PRO:HG2	1:D:393:SER:HB2	1.98	0.46
1:D:650:ARG:HB2	1:D:653:ILE:HD11	1.98	0.45
1:D:577:MET:SD	1:D:657:ARG:HD2	2.56	0.45
1:B:124:ARG:HA	1:B:135:VAL:O	2.16	0.45
1:C:10:ILE:HD11	1:C:99:LEU:HD11	1.98	0.45
1:A:564:LEU:HD22	1:A:591:ASN:HA	1.99	0.45
1:A:755:ILE:HD13	1:A:755:ILE:N	2.31	0.45
1:D:746:LYS:O	1:D:747:LEU:HD23	2.16	0.45
1:B:344:ASP:O	1:B:348:PHE:HB2	2.16	0.45
1:A:344:ASP:O	1:A:348:PHE:HB2	2.16	0.45
1:D:409:LEU:HD23	1:D:587:ASP:OD1	2.17	0.45
1:B:68:LEU:HB3	1:B:69:PRO:HD2	1.98	0.45
1:B:609:GLU:HB3	1:B:697:LYS:HE2	1.99	0.45
1:C:10:ILE:CD1	1:C:99:LEU:HD11	2.47	0.45
1:B:755:ILE:O	1:B:756:ILE:HG13	2.17	0.45
1:C:8:TRP:CE3	1:C:308:LYS:HD3	2.51	0.45
1:B:64:GLU:HG2	1:B:338:LYS:HD2	1.99	0.44
1:A:550:PRO:HA	1:A:551:ASP:HA	1.72	0.44
1:C:142:CYS:HB3	1:C:145:TYR:CZ	2.52	0.44
1:C:492:ALA:O	1:C:496:TYR:HB2	2.17	0.44
1:D:648:THR:CG2	1:D:706:TRP:CZ2	3.00	0.44
1:C:653:ILE:O	1:C:653:ILE:HD13	2.18	0.44
1:B:189:ILE:C	1:B:189:ILE:HD12	2.38	0.44
1:C:111:LYS:HE2	1:C:115:GLY:HA2	2.00	0.44
1:A:11:GLU:CG	1:A:96:VAL:HG12	2.47	0.44
1:B:708:PRO:HD2	1:B:711:TRP:CD2	2.52	0.44
1:D:732:ASP:OD2	1:D:732:ASP:N	2.48	0.44
1:D:142:CYS:HB3	1:D:145:TYR:CZ	2.53	0.44
1:A:624:GLU:OE1	1:A:650:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:O	1:B:117:ILE:HA	2.18	0.43
1:B:324:HIS:CG	3:B:803:GOL:H11	2.53	0.43
1:B:109:ARG:NE	1:B:143:GLU:OE1	2.51	0.43
1:B:648:THR:HG21	1:B:706:TRP:CD2	2.53	0.43
1:B:695:ILE:HD13	1:B:701:LEU:HD12	2.01	0.43
1:C:565:LYS:NZ	5:C:1141:HOH:O	2.49	0.43
1:A:11:GLU:HB2	5:A:1119:HOH:O	2.18	0.43
1:B:548:TYR:O	1:B:550:PRO:HD3	2.19	0.43
1:D:1:MET:CE	1:D:103:ILE:HD13	2.49	0.43
1:C:330:LYS:HA	1:C:674:ILE:O	2.18	0.43
1:A:15:LEU:HD21	1:A:85:PRO:HB2	2.01	0.43
1:B:593:GLN:OE1	1:B:622:TYR:OH	2.25	0.43
1:A:508:LEU:O	1:A:512:LEU:HD23	2.18	0.43
1:D:717:SER:OG	1:D:726:ASP:OD1	2.33	0.43
1:D:693:ILE:CG2	1:D:701:LEU:HD22	2.49	0.43
1:C:97:LEU:HG	1:C:99:LEU:HD23	2.01	0.42
1:C:634:SER:HA	5:C:1145:HOH:O	2.18	0.42
1:A:645:VAL:HG23	1:A:647:GLU:HB2	2.01	0.42
1:A:513:LEU:O	1:A:517:PRO:HB3	2.18	0.42
1:B:163:LYS:HA	1:B:169:ARG:HG3	2.01	0.42
1:D:466:TYR:HB2	1:D:473:TYR:CE1	2.54	0.42
1:B:100:LYS:HE3	5:B:1058:HOH:O	2.18	0.42
1:A:533:GLU:HB2	1:A:534:PRO:HD3	2.01	0.42
1:D:204:THR:OG1	1:D:244:LYS:HG3	2.20	0.42
1:A:569:ILE:HG12	1:A:628:MET:CE	2.50	0.42
1:A:346:GLU:HB3	1:A:431:ALA:HB2	2.02	0.42
1:A:754:ALA:HA	1:A:755:ILE:HD13	2.02	0.42
1:B:695:ILE:CD1	1:B:701:LEU:CD1	2.98	0.42
1:C:319:ASN:HA	1:C:320:PRO:HD2	1.92	0.42
1:A:420:ILE:HG13	1:A:479:ILE:HD12	2.02	0.41
1:B:733:ASN:ND2	5:B:1177:HOH:O	2.53	0.41
1:A:708:PRO:HD2	1:A:711:TRP:CE3	2.55	0.41
1:C:690:PHE:CD1	1:C:708:PRO:HD3	2.55	0.41
1:C:329:ALA:HB2	1:C:342:PHE:CD2	2.55	0.41
1:D:756:ILE:O	1:D:756:ILE:HD12	2.19	0.41
1:D:698:ASP:OD1	1:D:700:VAL:HG23	2.20	0.41
1:A:2:LYS:NZ	5:A:938:HOH:O	2.53	0.41
1:A:330:LYS:HA	1:A:674:ILE:O	2.20	0.41
1:D:554:LEU:HD13	1:D:618:ILE:HG22	2.02	0.41
1:C:116:ARG:NH1	5:C:1113:HOH:O	2.53	0.41
1:A:68:LEU:HB3	1:A:69:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:MET:SD	1:B:657:ARG:HD2	2.60	0.41
1:C:110:LEU:O	1:C:117:ILE:HA	2.20	0.41
1:C:653:ILE:O	1:C:653:ILE:CD1	2.69	0.41
1:D:1:MET:CE	1:D:103:ILE:CD1	2.98	0.41
1:C:189:ILE:HD12	1:C:189:ILE:C	2.41	0.41
1:A:295:ILE:HG21	1:A:686:LEU:HD13	2.02	0.41
1:D:430:TYR:HA	1:D:500:TRP:CH2	2.56	0.41
1:D:78:ILE:CD1	1:D:149:LEU:CD2	2.98	0.41
1:C:496:TYR:CD1	1:C:546:ILE:HD12	2.56	0.41
1:A:650:ARG:HH11	1:A:650:ARG:HB3	1.86	0.41
1:A:643:VAL:HG21	1:A:690:PHE:CD1	2.56	0.41
1:D:206:VAL:HG12	1:D:213:CYS:SG	2.61	0.41
1:B:515:LYS:N	1:B:515:LYS:CD	2.83	0.41
1:C:114:LYS:HG3	5:C:1012:HOH:O	2.21	0.41
1:B:648:THR:HG21	1:B:706:TRP:CE2	2.57	0.40
1:A:364:MET:O	1:A:367:TYR:HB3	2.21	0.40
1:A:71:PRO:HB2	1:A:246:THR:HG21	2.04	0.40
1:D:169:ARG:NH2	3:D:805:GOL:H2	2.36	0.40
1:B:648:THR:HB	1:B:706:TRP:CZ2	2.56	0.40
1:A:288:ARG:NH2	5:A:1176:HOH:O	2.42	0.40
1:B:12:GLN:OE1	1:B:95:ARG:HD3	2.22	0.40
1:B:508:LEU:O	1:B:512:LEU:HG	2.22	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	754/764 (99%)	724 (96%)	27 (4%)	3 (0%)	39	28
1	B	754/764 (99%)	729 (97%)	23 (3%)	2 (0%)	46	36
1	C	754/764 (99%)	726 (96%)	23 (3%)	5 (1%)	26	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	754/764 (99%)	717 (95%)	33 (4%)	4 (0%)	34	22
All	All	3016/3056 (99%)	2896 (96%)	106 (4%)	14 (0%)	34	22

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	742	LYS
1	D	259	VAL
1	D	741	GLU
1	D	258	ASP
1	B	742	LYS
1	C	257	GLY
1	A	742	LYS
1	C	709	GLU
1	A	547	PRO
1	A	41	VAL
1	B	41	VAL
1	C	256	VAL
1	D	41	VAL
1	C	41	VAL

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	669/676 (99%)	645 (96%)	24 (4%)	42	34
1	B	669/676 (99%)	651 (97%)	18 (3%)	52	45
1	C	669/676 (99%)	638 (95%)	31 (5%)	33	24
1	D	669/676 (99%)	631 (94%)	38 (6%)	25	15
All	All	2676/2704 (99%)	2565 (96%)	111 (4%)	37	28

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	80	ARG
1	A	163	LYS
1	A	205	LYS
1	A	207	LEU
1	A	211	GLN
1	A	259	VAL
1	A	344	ASP
1	A	381	LYS
1	A	465	LYS
1	A	472	ARG
1	A	496	TYR
1	A	551	ASP
1	A	571	GLU
1	A	576	ASN
1	A	640	LEU
1	A	647	GLU
1	A	650	ARG
1	A	696	GLU
1	A	709	GLU
1	A	737	LYS
1	A	744	ASN
1	A	752	GLN
1	A	755	ILE
1	B	7	GLU
1	B	170	VAL
1	B	197	LYS
1	B	205	LYS
1	B	259	VAL
1	B	268	LYS
1	B	288	ARG
1	B	338	LYS
1	B	342	PHE
1	B	403	LYS
1	B	508	LEU
1	B	515	LYS
1	B	522	LYS
1	B	552	LYS
1	B	698	ASP
1	B	709	GLU
1	B	734	VAL
1	B	755	ILE
1	C	114	LYS

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Mol	Chain	Res	Type
1	C	170	VAL
1	C	177	LYS
1	C	192	LYS
1	C	197	LYS
1	C	210	ASN
1	C	254	LYS
1	C	255	ASN
1	C	277	LYS
1	C	288	ARG
1	C	469	GLU
1	C	496	TYR
1	C	504	LYS
1	C	521	GLU
1	C	539	GLU
1	C	566	ASP
1	C	582	GLU
1	C	609	GLU
1	C	614	GLN
1	C	625	LYS
1	C	650	ARG
1	C	653	ILE
1	C	658	THR
1	C	697	LYS
1	C	707	LEU
1	C	709	GLU
1	C	733	ASN
1	C	737	LYS
1	C	741	GLU
1	C	744	ASN
1	C	756	ILE
1	D	1	MET
1	D	2	LYS
1	D	14	LYS
1	D	44	GLU
1	D	63	THR
1	D	109	ARG
1	D	197	LYS
1	D	239	ARG
1	D	243	GLU
1	D	254	LYS
1	D	342	PHE
1	D	343	TRP

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Mol	Chain	Res	Type
1	D	409	LEU
1	D	442	ILE
1	D	468	LYS
1	D	469	GLU
1	D	530	SER
1	D	532	GLU
1	D	566	ASP
1	D	574	GLN
1	D	590	ASN
1	D	610	GLU
1	D	648	THR
1	D	650	ARG
1	D	653	ILE
1	D	658	THR
1	D	696	GLU
1	D	701	LEU
1	D	702	SER
1	D	721	LYS
1	D	731	LYS
1	D	732	ASP
1	D	733	ASN
1	D	734	VAL
1	D	740	VAL
1	D	746	LYS
1	D	750	LYS
1	D	756	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	593	GLN
1	A	752	GLN
1	B	101	GLN
1	B	575	ASN

5.3.3 RNA ⓘ

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](#)

23 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	$\# Z > 2$
2	BGC	A	801	-	12,12,12	0.75	0	17,17,17	1.63	5 (29%)
2	BGC	A	802	-	12,12,12	0.64	0	17,17,17	2.00	5 (29%)
3	GOL	A	803	-	5,5,5	0.72	0	5,5,5	0.57	0
3	GOL	A	804	-	5,5,5	0.82	0	5,5,5	1.15	1 (20%)
4	PO4	A	805	-	4,4,4	0.45	0	6,6,6	0.31	0
2	BGC	B	801	-	12,12,12	1.26	2 (16%)	17,17,17	1.23	2 (11%)
2	BGC	B	802	-	12,12,12	0.57	0	17,17,17	1.35	2 (11%)
3	GOL	B	803	-	5,5,5	0.42	0	5,5,5	0.97	0
4	PO4	B	804	-	4,4,4	0.92	0	6,6,6	0.33	0
4	PO4	B	805	-	4,4,4	0.63	0	6,6,6	0.28	0
2	BGC	C	801	-	12,12,12	0.55	0	17,17,17	1.33	2 (11%)
2	BGC	C	802	-	12,12,12	0.98	1 (8%)	17,17,17	1.14	2 (11%)
3	GOL	C	803	-	5,5,5	0.64	0	5,5,5	0.49	0
3	GOL	C	804	-	5,5,5	0.38	0	5,5,5	0.28	0
4	PO4	C	805	-	4,4,4	0.76	0	6,6,6	0.33	0
4	PO4	C	806	-	4,4,4	0.55	0	6,6,6	0.29	0
2	BGC	D	801	-	12,12,12	0.68	0	17,17,17	1.01	1 (5%)
2	BGC	D	802	-	12,12,12	1.26	2 (16%)	17,17,17	1.88	6 (35%)
3	GOL	D	803	-	5,5,5	0.68	0	5,5,5	0.45	0
3	GOL	D	804	-	5,5,5	0.74	0	5,5,5	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	805	-	5,5,5	1.09	1 (20%)	5,5,5	0.96	0
3	GOL	D	806	-	5,5,5	0.58	0	5,5,5	0.48	0
4	PO4	D	807	-	4,4,4	0.66	0	6,6,6	0.31	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
2	BGC	A	801	-	-	0/2/22/22	0/1/1/1
2	BGC	A	802	-	-	0/2/22/22	0/1/1/1
3	GOL	A	803	-	-	0/4/4/4	0/0/0/0
3	GOL	A	804	-	-	0/4/4/4	0/0/0/0
4	PO4	A	805	-	-	0/0/0/0	0/0/0/0
2	BGC	B	801	-	-	0/2/22/22	0/1/1/1
2	BGC	B	802	-	-	0/2/22/22	0/1/1/1
3	GOL	B	803	-	-	0/4/4/4	0/0/0/0
4	PO4	B	804	-	-	0/0/0/0	0/0/0/0
4	PO4	B	805	-	-	0/0/0/0	0/0/0/0
2	BGC	C	801	-	-	0/2/22/22	0/1/1/1
2	BGC	C	802	-	-	0/2/22/22	0/1/1/1
3	GOL	C	803	-	-	0/4/4/4	0/0/0/0
3	GOL	C	804	-	-	0/4/4/4	0/0/0/0
4	PO4	C	805	-	-	0/0/0/0	0/0/0/0
4	PO4	C	806	-	-	0/0/0/0	0/0/0/0
2	BGC	D	801	-	-	0/2/22/22	0/1/1/1
2	BGC	D	802	-	-	0/2/22/22	0/1/1/1
3	GOL	D	803	-	-	0/4/4/4	0/0/0/0
3	GOL	D	804	-	-	0/4/4/4	0/0/0/0
3	GOL	D	805	-	-	0/4/4/4	0/0/0/0
3	GOL	D	806	-	-	0/4/4/4	0/0/0/0
4	PO4	D	807	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	802	BGC	O5-C5	-3.03	1.36	1.44
2	D	802	BGC	O1-C1	2.05	1.46	1.39
2	C	802	BGC	O1-C1	2.20	1.47	1.39
2	B	801	BGC	O5-C1	2.21	1.47	1.43
3	D	805	GOL	O2-C2	2.34	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	BGC	O4-C4	2.54	1.49	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	BGC	O2-C2-C1	-3.97	101.07	109.82
2	B	802	BGC	O1-C1-O5	-3.45	100.82	110.25
2	D	802	BGC	O2-C2-C1	-3.44	102.24	109.82
2	C	801	BGC	C4-C3-C2	-2.93	105.33	110.79
2	A	801	BGC	C4-C3-C2	-2.76	105.63	110.79
2	D	801	BGC	C4-C3-C2	-2.71	105.74	110.79
2	C	802	BGC	O2-C2-C1	-2.61	104.07	109.82
2	C	801	BGC	O1-C1-O5	-2.57	103.22	110.25
2	A	801	BGC	O3-C3-C4	-2.53	104.64	110.34
2	D	802	BGC	O5-C5-C6	-2.41	100.26	106.36
2	A	801	BGC	O4-C4-C3	-2.05	105.72	110.34
3	A	804	GOL	O2-C2-C1	2.09	118.23	108.65
2	B	801	BGC	O2-C2-C3	2.16	115.20	110.34
2	D	802	BGC	C6-C5-C4	2.19	118.41	113.02
2	D	802	BGC	O5-C5-C4	2.20	113.81	109.68
2	A	801	BGC	O2-C2-C3	2.20	115.29	110.34
2	A	801	BGC	C3-C4-C5	2.46	114.48	110.20
2	A	802	BGC	O5-C5-C4	2.47	114.32	109.68
2	C	802	BGC	C1-O5-C5	2.48	118.06	113.47
2	D	802	BGC	C1-O5-C5	2.54	118.17	113.47
2	A	802	BGC	O3-C3-C4	2.62	116.25	110.34
2	A	802	BGC	C1-C2-C3	2.95	114.81	110.43
2	A	802	BGC	O4-C4-C3	3.03	117.17	110.34
2	B	801	BGC	C1-O5-C5	3.28	119.53	113.47
2	B	802	BGC	O5-C1-C2	3.31	115.07	109.80
2	D	802	BGC	C1-C2-C3	4.19	116.66	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	803	GOL	1	0
4	B	805	PO4	1	0
3	D	805	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	756/764 (98%)	-0.04	14 (1%) 70 75	13, 27, 53, 93	0
1	B	756/764 (98%)	-0.05	14 (1%) 70 75	13, 26, 51, 69	0
1	C	756/764 (98%)	-0.12	5 (0%) 89 91	17, 30, 54, 72	0
1	D	756/764 (98%)	-0.03	14 (1%) 70 75	16, 30, 55, 75	0
All	All	3024/3056 (98%)	-0.06	47 (1%) 74 79	13, 29, 53, 93	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	257	GLY	4.7
1	D	743	GLY	4.4
1	A	550	PRO	4.3
1	A	568	VAL	4.1
1	B	568	VAL	3.9
1	A	755	ILE	3.9
1	A	549	HIS	3.9
1	A	551	ASP	3.8
1	A	752	GLN	3.7
1	D	567	PHE	3.3
1	B	755	ILE	3.3
1	A	732	ASP	3.3
1	D	732	ASP	3.2
1	D	408	TYR	3.1
1	A	706	TRP	2.9
1	D	742	LYS	2.9
1	B	408	TYR	2.9
1	D	257	GLY	2.8
1	B	733	ASN	2.7
1	B	752	GLN	2.7
1	B	732	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	332	LEU	2.6
1	D	254	LYS	2.6
1	C	404	TRP	2.5
1	B	582	GLU	2.5
1	A	552	LYS	2.5
1	B	549	HIS	2.5
1	A	408	TYR	2.5
1	C	254	LYS	2.5
1	D	347	ILE	2.5
1	C	568	VAL	2.4
1	D	568	VAL	2.4
1	D	698	ASP	2.3
1	B	528	ASN	2.3
1	B	563	ASN	2.3
1	D	588	LYS	2.2
1	D	751	GLY	2.2
1	B	649	ASN	2.2
1	D	256	VAL	2.2
1	A	409	LEU	2.1
1	B	525	LYS	2.1
1	A	582	GLU	2.1
1	D	653	ILE	2.1
1	A	350	LEU	2.1
1	B	409	LEU	2.0
1	A	548	TYR	2.0
1	C	408	TYR	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, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	A	804	6/6	0.84	0.25	4.12	33,35,40,41	0
3	GOL	D	803	6/6	0.72	0.17	3.90	44,54,61,61	0
3	GOL	D	804	6/6	0.77	0.28	3.41	55,57,60,64	0
3	GOL	C	803	6/6	0.81	0.18	3.34	46,55,59,62	0
3	GOL	D	806	6/6	0.81	0.12	2.76	46,47,49,49	0
2	BGC	A	802	12/12	0.92	0.13	1.47	21,26,29,32	0
2	BGC	B	802	12/12	0.93	0.14	0.67	19,26,29,31	0
3	GOL	D	805	6/6	0.85	0.13	0.53	27,36,38,50	0
2	BGC	C	802	12/12	0.94	0.10	0.06	20,25,29,30	0
2	BGC	D	802	12/12	0.94	0.12	-0.04	21,26,27,27	0
2	BGC	D	801	12/12	0.97	0.14	-0.11	21,24,25,25	0
2	BGC	B	801	12/12	0.96	0.14	-0.13	20,22,24,26	0
4	PO4	B	805	5/5	0.96	0.10	-0.18	42,43,47,47	0
2	BGC	A	801	12/12	0.95	0.11	-0.32	19,21,23,24	0
2	BGC	C	801	12/12	0.96	0.11	-0.45	19,24,25,25	0
3	GOL	C	804	6/6	0.90	0.11	-0.75	47,49,50,55	0
4	PO4	A	805	5/5	0.99	0.09	-1.25	20,20,23,24	0
4	PO4	B	804	5/5	0.99	0.11	-1.51	18,21,23,26	0
4	PO4	C	806	5/5	0.96	0.09	-1.98	45,46,46,50	0
4	PO4	D	807	5/5	0.99	0.07	-2.37	22,25,27,28	0
4	PO4	C	805	5/5	0.99	0.07	-2.57	22,24,26,27	0
3	GOL	A	803	6/6	0.88	0.14	-	29,41,45,47	0
3	GOL	B	803	6/6	0.91	0.22	-	30,40,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.