



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:07 PM UTC

PDB ID : 3WIR / pdb_00003wir
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

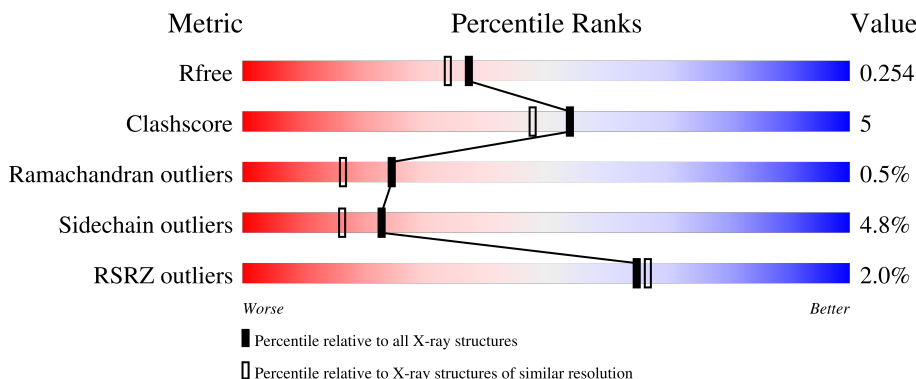
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

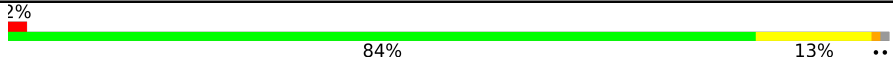
The reported resolution of this entry is 2.05 Å.

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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	764	 2% 84% 13% ..
1	B	764	 2% 84% 13% ..
1	C	764	 2% 84% 13% ..
1	D	764	 2% 82% 13% ...

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:

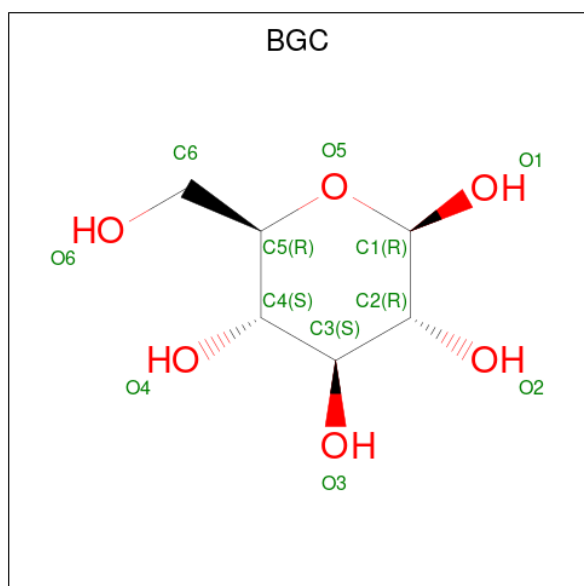
Chain	Residue	Modelled	Actual	Comment	Reference
A	757	GLY	-	expression tag	UNP A4XGP2
A	758	SER	-	expression tag	UNP A4XGP2
A	759	HIS	-	expression tag	UNP A4XGP2
A	760	HIS	-	expression tag	UNP A4XGP2
A	761	HIS	-	expression tag	UNP A4XGP2
A	762	HIS	-	expression tag	UNP A4XGP2
A	763	HIS	-	expression tag	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

Continued on next page...

Continued from previous page...

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 beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



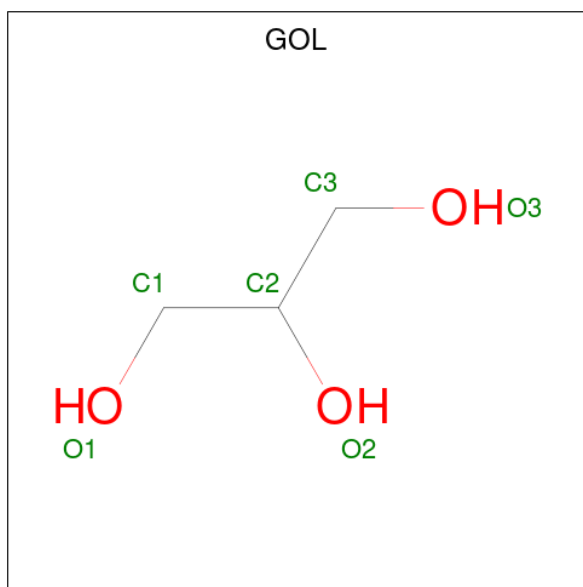
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0

Continued on next page...

Continued from previous page...

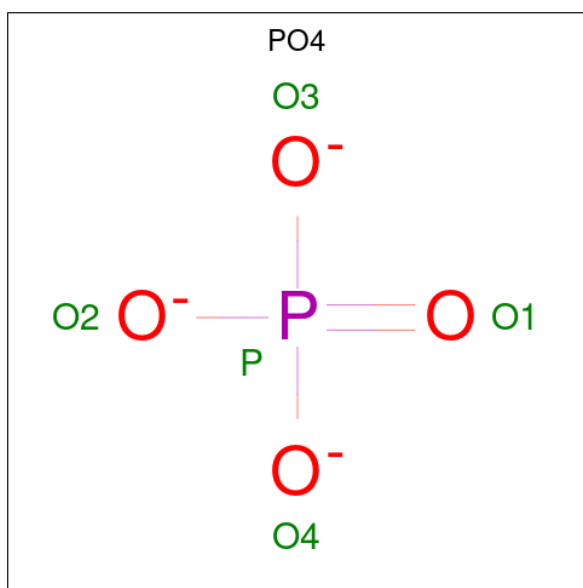
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is GLYCEROL (CCD ID: 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 (CCD ID: PO4) (formula: O_4P).

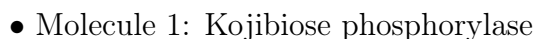
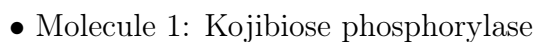


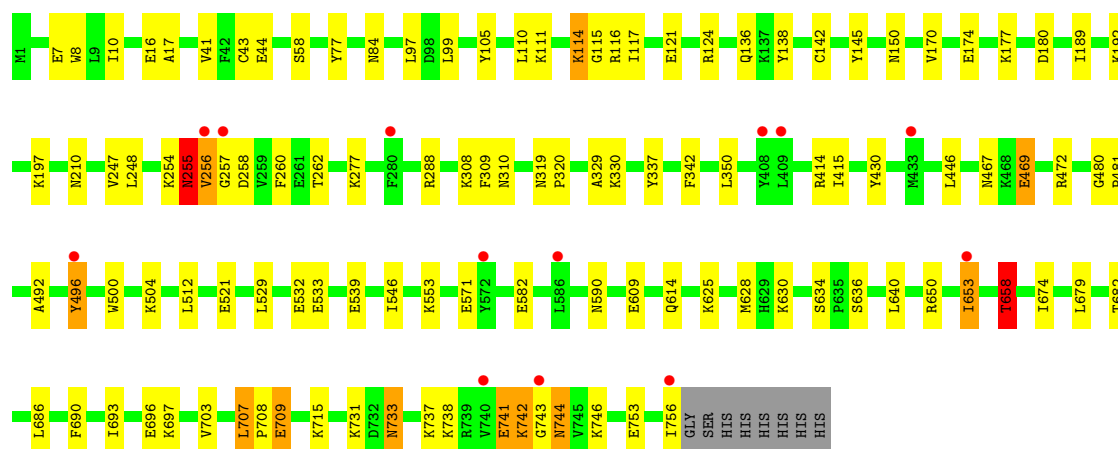
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

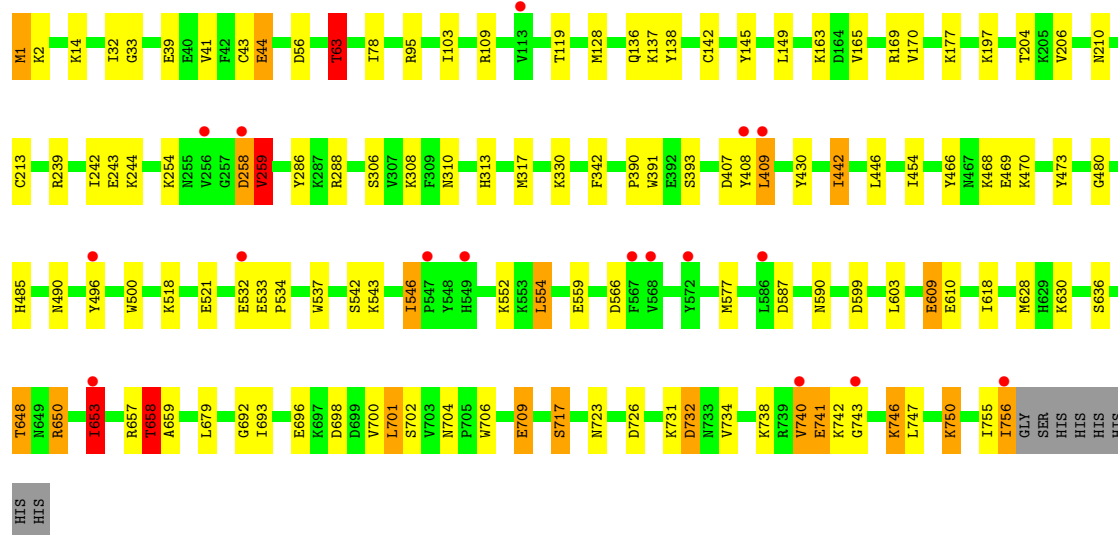
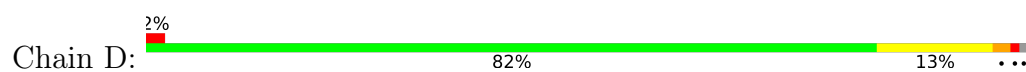
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	371	Total	O	0	0
			371	371		
5	B	387	Total	O	0	0
			387	387		
5	C	299	Total	O	0	0
			299	299		
5	D	321	Total	O	0	0
			321	321		

- 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) 97.1 (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	10235 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, PO4, GOL

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	1.22	14/6328 (0.2%)	1.12	7/8550 (0.1%)
1	B	1.19	15/6328 (0.2%)	1.14	10/8550 (0.1%)
1	C	1.08	0/6328	1.08	14/8550 (0.2%)
1	D	1.10	8/6328 (0.1%)	1.10	18/8550 (0.2%)
All	All	1.15	37/25312 (0.1%)	1.11	49/34200 (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 (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	679	LEU	C-O	6.97	1.32	1.24
1	B	252	ARG	CA-C	6.95	1.62	1.52
1	B	68	LEU	CA-C	-6.93	1.44	1.52
1	B	251	SER	N-CA	-6.92	1.36	1.46
1	A	95	ARG	CA-C	-6.45	1.45	1.52
1	B	96	VAL	C-O	6.12	1.30	1.24
1	D	599	ASP	CA-C	-6.04	1.44	1.52
1	D	658	THR	CB-CG2	-6.03	1.32	1.52
1	B	354	ILE	N-CA	-5.94	1.39	1.46
1	A	375	ALA	C-O	-5.87	1.17	1.24
1	B	314	LEU	CA-C	5.86	1.60	1.52
1	A	77	TYR	N-CA	-5.79	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	VAL	C-O	5.73	1.29	1.23
1	B	69	PRO	N-CA	-5.57	1.40	1.47
1	B	281	GLU	N-CA	5.54	1.53	1.46
1	A	50	TYR	CA-C	-5.54	1.46	1.52
1	B	172	HIS	C-O	-5.50	1.17	1.24
1	B	279	LEU	N-CA	-5.43	1.39	1.46
1	A	245	LEU	C-O	5.42	1.30	1.24
1	A	70	ASN	C-O	-5.39	1.17	1.24
1	D	33	GLY	CA-C	5.36	1.56	1.51
1	A	320	PRO	C-O	-5.28	1.16	1.24
1	D	330	LYS	N-CA	5.26	1.52	1.46
1	D	485	HIS	CA-C	-5.23	1.46	1.52
1	B	211	GLN	N-CA	-5.18	1.39	1.46
1	B	278	LEU	C-O	-5.16	1.18	1.24
1	B	655	PHE	N-CA	-5.15	1.40	1.46
1	B	22	GLU	N-CA	5.11	1.52	1.46
1	D	170	VAL	N-CA	-5.11	1.40	1.46
1	A	34	ILE	N-CA	-5.10	1.40	1.46
1	A	165	VAL	C-O	-5.10	1.18	1.24
1	A	387	ALA	CA-C	-5.09	1.46	1.52
1	D	242	ILE	C-O	-5.09	1.18	1.24
1	B	271	GLU	C-O	-5.07	1.17	1.24
1	A	452	ILE	C-O	-5.03	1.18	1.24
1	A	683	TRP	C-O	-5.01	1.18	1.24
1	D	717	SER	N-CA	-5.00	1.39	1.46

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	658	THR	CB-CA-C	-8.37	96.62	110.85
1	B	259	VAL	CB-CA-C	-7.64	101.82	112.14
1	C	350	LEU	CA-C-N	-7.52	111.01	119.28
1	C	350	LEU	C-N-CA	-7.52	111.01	119.28
1	D	743	GLY	N-CA-C	7.41	122.28	111.24
1	A	755	ILE	N-CA-C	7.40	117.47	111.62
1	D	259	VAL	N-CA-CB	6.71	122.30	111.23
1	A	259	VAL	CB-CA-C	-6.34	103.85	111.97
1	B	643	VAL	CB-CA-C	-6.29	103.83	111.88
1	D	653	ILE	CB-CA-C	-6.19	103.68	112.22
1	C	733	ASN	N-CA-C	6.19	119.28	109.81
1	D	658	THR	N-CA-CB	6.13	118.96	110.07
1	D	95	ARG	NE-CZ-NH2	6.03	124.63	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63	THR	N-CA-CB	6.01	118.95	110.36
1	C	658	THR	N-CA-CB	5.97	119.00	110.16
1	C	590	ASN	N-CA-C	5.89	119.57	112.38
1	D	658	THR	CB-CA-C	-5.87	101.63	110.90
1	A	704	ASN	CA-C-N	5.86	125.76	119.85
1	A	704	ASN	C-N-CA	5.86	125.76	119.85
1	A	259	VAL	N-CA-C	5.85	116.03	110.42
1	D	95	ARG	NE-CZ-NH1	-5.85	115.65	121.50
1	C	571	GLU	N-CA-C	5.71	117.74	109.07
1	D	480	GLY	CA-C-N	5.65	125.76	119.32
1	D	480	GLY	C-N-CA	5.65	125.76	119.32
1	B	269	GLU	N-CA-C	-5.63	105.22	111.36
1	B	703	VAL	N-CA-C	5.60	115.65	107.37
1	A	666	ASN	N-CA-C	5.59	119.72	113.01
1	D	546	ILE	CB-CA-C	-5.53	104.83	111.18
1	C	84	ASN	CA-C-N	5.50	125.58	119.32
1	C	84	ASN	C-N-CA	5.50	125.58	119.32
1	D	165	VAL	CA-C-N	5.44	124.90	119.24
1	D	165	VAL	C-N-CA	5.44	124.90	119.24
1	D	163	LYS	N-CA-C	5.36	118.61	111.75
1	A	30	GLY	N-CA-C	-5.33	107.98	114.92
1	B	263	CYS	N-CA-C	5.32	117.50	111.11
1	B	733	ASN	N-CA-C	5.32	116.36	108.86
1	B	338	LYS	CB-CA-C	-5.28	103.16	111.51
1	C	124	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	D	32	ILE	CA-C-N	5.26	125.22	121.65
1	D	32	ILE	C-N-CA	5.26	125.22	121.65
1	B	255	ASN	N-CA-C	5.24	118.61	111.39
1	C	686	LEU	CB-CA-C	-5.23	101.95	110.85
1	D	177	LYS	N-CA-C	5.07	116.78	109.07
1	C	707	LEU	CA-C-N	-5.04	114.59	119.78
1	C	707	LEU	C-N-CA	-5.04	114.59	119.78
1	C	58	SER	CB-CA-C	-5.03	110.76	116.54
1	B	607	LEU	CA-C-N	5.02	125.55	119.98
1	B	607	LEU	C-N-CA	5.02	125.55	119.98
1	D	210	ASN	N-CA-C	5.00	118.50	111.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	551	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	51	0
1	B	6187	0	6119	61	0
1	C	6187	0	6120	62	0
1	D	6187	0	6119	71	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	1	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	4	0
5	D	321	0	0	10	0
All	All	26306	0	24646	244	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 (244) 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:1:MET:HE3	1:B:103:ILE:HD11	1.31	1.11
1:B:303:ALA:HB2	1:B:656:MET:HE1	1.29	1.09

Continued on next page...

Continued from previous page...

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:CB	1:B:656:MET:HE1	2.06	0.85
1:B:303:ALA:HB2	1:B:656:MET:CE	2.07	0.84
1:D:709:GLU:CD	1:D:709:GLU:H	1.88	0.81
1:C:10:ILE:HD12	1:C:99:LEU:HD21	1.65	0.78
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:B:1:MET:HE3	1:B:103:ILE:CD1	2.16	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: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:1:MET:HE1	1:B:3:LEU:HA	1.80	0.63
1:B:755:ILE:HD13	1:B:755:ILE:N	2.15	0.62
1:D:723:ASN:OD1	1:D:742:LYS:N	2.25	0.62
1:B:197:LYS:HE3	1:B:259:VAL:CG2	2.29	0.62
1:C:696:GLU:OE2	1:C:696:GLU:HA	1.98	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: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:1:MET:HE2	1:B:101:GLN:HE22	1.68	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:D:1:MET:HE3	1:D:103:ILE:HD13	1.86	0.57
1:B:581:PRO:O	1:B:584:VAL:HG13	2.04	0.57
1:A:628:MET:HE2	1:A:628:MET:HA	1.85	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:308:LYS:HE3	5:D:1105:HOH:O	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:693:ILE:HG23	1:D:701:LEU:HD22	1.85	0.57
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:C:741:GLU:O	1:C:742:LYS:HG2	2.06	0.56
1:D:258:ASP:O	1:D:259:VAL:HG13	2.05	0.56
1:D:310:ASN:HA	1:D:679:LEU:HD22	1.86	0.56
1:C:467:ASN:OD1	1:C:469:GLU:HG3	2.06	0.56
1:D:740:VAL:HG22	1:D:741:GLU:N	2.21	0.56
1:D:56:ASP:C	1:D:63:THR:HG22	2.31	0.55
1:A:317:MET:HE3	1:A:327:LEU:HD13	1.89	0.55
1:C:640:LEU:C	1:C:640:LEU:HD23	2.30	0.55
1:C:746:LYS:NZ	1:C:753:GLU:OE2	2.39	0.55
1:B:1:MET:HE1	1:B:3:LEU:HD23	1.89	0.55
1:C:7:GLU:CD	1:C:7:GLU:H	2.15	0.55
1:C:10:ILE:CD1	1:C:309:PHE:CD1	2.89	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:D:756:ILE:C	1:D:756:ILE:HD12	2.31	0.54
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:A:273:LYS:NZ	5:A:1117:HOH:O	2.41	0.52
1:C:744:ASN:N	1:C:744:ASN:OD1	2.42	0.52
1:C:414:ARG:NH1	1:C:415:ILE:O	2.43	0.52
1:D:746:LYS:HG2	1:D:755:ILE:CD1	2.40	0.52
1:C:136:GLN:HB3	1:C:138:TYR:CE2	2.45	0.52
1:D:496:TYR:CD1	1:D:603:LEU:CD2	2.93	0.52
1:D:496:TYR:CE1	1:D:603:LEU:HD21	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: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: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:OD1	1:C:255:ASN:N	2.42	0.50
1:C:310:ASN:HA	1:C:679:LEU:HD22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:39:GLU:OE2	1:D:138:TYR:OH	2.21	0.49
1:D:313:HIS:O	1:D:317:MET:HB2	2.12	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:B:189:ILE:HD12	1:B:189:ILE:C	2.38	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:C:472:ARG:NH1	5:C:1057:HOH:O	2.31	0.48
1:C:628:MET:HB3	1:C:630:LYS:HG2	1.95	0.48
1:D:142:CYS:HB3	1:D:145:TYR:CE2	2.48	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:79:ASN:O	1:A:80:ARG:HB2	2.11	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:B:317:MET:HE1	1:B:679:LEU:HD12	1.97	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:B:420:ILE:HB	1:B:478:VAL:HA	1.96	0.47
1:C:696:GLU:OE2	1:C:696:GLU:CA	2.63	0.47
1:D:653:ILE:O	1:D:657:ARG:HG3	2.14	0.47
1:D:741:GLU:N	5:D:912:HOH:O	2.46	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:C:693:ILE:HD13	1:C:703:VAL:HG13	1.97	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:A:430:TYR:HA	1:A:500:TRP:CH2	2.50	0.47
1:B:15:LEU:HD21	1:B:85:PRO:HB2	1.97	0.47
1:B:755:ILE:HD13	1:B:755:ILE:H	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:GLN:NE2	1:A:622:TYR:OH	2.45	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:302:VAL:O	1:B:306:SER:OG	2.22	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:224:TYR:OH	4:B:805:PO4:O3	2.23	0.46
1:B:696:GLU:OE1	1:B:696:GLU:HA	2.15	0.46
1:C:189:ILE:C	1:C:189:ILE:HD12	2.41	0.46
1:A:68:LEU:HB3	1:A:69:PRO:HD2	1.96	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:391:TRP:HB2	5:D:1104:HOH:O	2.15	0.46
1:D:704:ASN:OD1	1:D:750:LYS:HA	2.15	0.46
1:D:390:PRO:HG2	1:D:393:SER:HB2	1.98	0.46
1:D:490:ASN:ND2	1:D:559:GLU:OE1	2.47	0.46
1:D:650:ARG:HB2	1:D:653:ILE:HD11	1.98	0.45
1:B:124:ARG:HA	1:B:135:VAL:O	2.16	0.45
1:D:577:MET:SD	1:D:657:ARG:HD2	2.56	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:C:10:ILE:HD11	1:C:99:LEU:HD11	1.98	0.45
1:B:1:MET:CE	1:B:103:ILE:HD11	2.23	0.45
1:B:344:ASP:O	1:B:348:PHE:HB2	2.16	0.45
1:D:746:LYS:O	1:D:747:LEU:HD23	2.16	0.45
1:A:344:ASP:O	1:A:348:PHE:HB2	2.16	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:D:409:LEU:HD23	1:D:587:ASP:OD1	2.17	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:C:653:ILE:HD13	1:C:653:ILE:O	2.18	0.44
1:D:648:THR:CG2	1:D:706:TRP:CZ2	3.00	0.44
1:C:111:LYS:HE2	1:C:115:GLY:HA2	2.00	0.44
1:D:717:SER:OG	1:D:726:ASP:OD1	2.33	0.44
1:A:11:GLU:CG	1:A:96:VAL:HG12	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:624:GLU:OE1	1:A:650:ARG:NH1	2.50	0.44
1:D:142:CYS:HB3	1:D:145:TYR:CZ	2.53	0.44
1:D:408:TYR:C	1:D:409:LEU:HD13	2.43	0.44
1:B:110:LEU:O	1:B:117:ILE:HA	2.18	0.43
1:C:467:ASN:OD1	1:C:467:ASN:C	2.60	0.43
1:A:569:ILE:HG12	1:A:628:MET:HE3	1.99	0.43
1:B:109:ARG:NE	1:B:143:GLU:OE1	2.51	0.43
1:B:324:HIS:CG	3:B:803:GOL:H11	2.53	0.43
1:B:648:THR:HG21	1:B:706:TRP:CD2	2.53	0.43
1:D:518:LYS:NZ	5:D:966:HOH:O	2.50	0.43
1:B:337:TYR:C	1:B:338:LYS:HG2	2.42	0.43
1:B:695:ILE:HD13	1:B:701:LEU:HD12	2.01	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:A:15:LEU:HD21	1:A:85:PRO:HB2	2.01	0.43
1:C:330:LYS:HA	1:C:674:ILE:O	2.18	0.43
1:A:508:LEU:O	1:A:512:LEU:HD23	2.18	0.43
1:B:593:GLN:OE1	1:B:622:TYR:OH	2.25	0.43
1:C:337:TYR:OH	4:C:805:PO4:O2	2.37	0.43
1:D:407:ASP:OD1	1:D:407:ASP:C	2.62	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:513:LEU:O	1:A:517:PRO:HB3	2.18	0.42
1:A:645:VAL:HG23	1:A:647:GLU:HB2	2.01	0.42
1:B:163:LYS:HA	1:B:169:ARG:HG3	2.01	0.42
1:B:1:MET:HE2	1:B:101:GLN:NE2	2.34	0.42
1:C:180:ASP:OD2	1:C:180:ASP:C	2.62	0.42
1:C:247:VAL:C	1:C:248:LEU:HD12	2.44	0.42
1:D:466:TYR:HB2	1:D:473:TYR:CE1	2.54	0.42
1:A:533:GLU:HB2	1:A:534:PRO:HD3	2.01	0.42
1:B:100:LYS:HE3	5:B:1058:HOH:O	2.18	0.42
1:A:346:GLU:HB3	1:A:431:ALA:HB2	2.02	0.42
1:A:569:ILE:HG12	1:A:628:MET:CE	2.50	0.42
1:D:204:THR:OG1	1:D:244:LYS:HG3	2.20	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:D:1:MET:CE	1:D:103:ILE:HD13	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:255:ASN:C	1:C:256:VAL:HG22	2.45	0.41
1:C:329:ALA:HB2	1:C:342:PHE:CD2	2.55	0.41
1:C:690:PHE:CD1	1:C:708:PRO:HD3	2.55	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:C:116:ARG:NH1	5:C:1113:HOH:O	2.53	0.41
1:D:554:LEU:HD13	1:D:618:ILE:HG22	2.02	0.41
1:D:698:ASP:OD1	1:D:700:VAL:HG23	2.20	0.41
1:D:756:ILE:HD12	1:D:756:ILE:O	2.19	0.41
1:A:68:LEU:HB3	1:A:69:PRO:CD	2.51	0.41
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:480:GLY:O	1:C:481:PRO:C	2.63	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:A:295:ILE:HG21	1:A:686:LEU:HD13	2.02	0.41
1:D:609:GLU:CD	1:D:609:GLU:H	2.29	0.41
1:D:430:TYR:HA	1:D:500:TRP:CH2	2.56	0.41
1:A:643:VAL:HG21	1:A:690:PHE:CD1	2.56	0.41
1:A:650:ARG:HH11	1:A:650:ARG:HB3	1.86	0.41
1:B:515:LYS:N	1:B:515:LYS:CD	2.83	0.41
1:C:496:TYR:CD1	1:C:546:ILE:HD12	2.56	0.41
1:D:78:ILE:CD1	1:D:149:LEU:CD2	2.98	0.41
1:D:206:VAL:HG12	1:D:213:CYS:SG	2.61	0.41
1:C:114:LYS:HG3	5:C:1012:HOH:O	2.21	0.41
1:A:71:PRO:HB2	1:A:246:THR:HG21	2.04	0.40
1:A:364:MET:O	1:A:367:TYR:HB3	2.21	0.40
1:B:648:THR:HG21	1:B:706:TRP:CE2	2.57	0.40
1:D:169:ARG:NH2	3:D:805:GOL:H2	2.36	0.40
1:A:288:ARG:NH2	5:A:1176:HOH:O	2.42	0.40
1:B:648:THR:HB	1:B:706:TRP:CZ2	2.56	0.40
1:B:12:GLN:OE1	1:B:95:ARG:HD3	2.22	0.40
1:A:189:ILE:HD12	1:A:189:ILE:C	2.47	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

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	754/764 (99%)	724 (96%)	27 (4%)	3 (0%)	30	22
1	B	754/764 (99%)	729 (97%)	23 (3%)	2 (0%)	36	30
1	C	754/764 (99%)	726 (96%)	23 (3%)	5 (1%)	18	10
1	D	754/764 (99%)	717 (95%)	33 (4%)	4 (0%)	24	16
All	All	3016/3056 (99%)	2896 (96%)	106 (4%)	14 (0%)	24	16

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%)	643 (96%)	26 (4%)	28	23
1	B	669/676 (99%)	643 (96%)	26 (4%)	28	23
1	C	669/676 (99%)	633 (95%)	36 (5%)	20	12
1	D	669/676 (99%)	628 (94%)	41 (6%)	17	10
All	All	2676/2704 (99%)	2547 (95%)	129 (5%)	23	16

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	119	THR
1	A	163	LYS
1	A	205	LYS
1	A	207	LEU
1	A	211	GLN
1	A	259	VAL
1	A	321	GLU
1	A	413	VAL
1	A	465	LYS
1	A	472	ARG
1	A	551	ASP
1	A	571	GLU
1	A	576	ASN
1	A	579	VAL
1	A	582	GLU
1	A	640	LEU
1	A	647	GLU
1	A	648	THR
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	179	LYS
1	B	195	LYS
1	B	197	LYS
1	B	205	LYS
1	B	259	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	268	LYS
1	B	288	ARG
1	B	338	LYS
1	B	342	PHE
1	B	403	LYS
1	B	470	LYS
1	B	508	LEU
1	B	515	LYS
1	B	522	LYS
1	B	525	LYS
1	B	584	VAL
1	B	610	GLU
1	B	653	ILE
1	B	698	ASP
1	B	715	LYS
1	B	734	VAL
1	B	737	LYS
1	B	755	ILE
1	B	756	ILE
1	C	44	GLU
1	C	114	LYS
1	C	170	VAL
1	C	174	GLU
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	532	GLU
1	C	539	GLU
1	C	553	LYS
1	C	582	GLU
1	C	609	GLU
1	C	614	GLN
1	C	625	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	715	LYS
1	C	731	LYS
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	119	THR
1	D	137	LYS
1	D	197	LYS
1	D	239	ARG
1	D	243	GLU
1	D	254	LYS
1	D	342	PHE
1	D	409	LEU
1	D	442	ILE
1	D	468	LYS
1	D	469	GLU
1	D	470	LYS
1	D	521	GLU
1	D	532	GLU
1	D	552	LYS
1	D	554	LEU
1	D	566	ASP
1	D	590	ASN
1	D	609	GLU
1	D	610	GLU
1	D	648	THR
1	D	650	ARG
1	D	653	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	658	THR
1	D	696	GLU
1	D	701	LEU
1	D	702	SER
1	D	709	GLU
1	D	731	LYS
1	D	732	ASP
1	D	734	VAL
1	D	740	VAL
1	D	746	LYS
1	D	750	LYS
1	D	756	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	210	ASN
1	A	382	ASN
1	A	593	GLN
1	A	597	GLN
1	A	752	GLN
1	B	101	GLN
1	B	130	ASN
1	B	132	ASN
1	B	324	HIS
1	B	382	ASN
1	B	575	ASN
1	B	614	GLN
1	C	130	ASN
1	C	136	GLN
1	D	130	ASN
1	D	378	ASN
1	D	538	GLN
1	D	549	HIS
1	D	597	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	802	-	12,12,12	0.60	0	17,17,17	1.85	5 (29%)
3	GOL	C	804	-	5,5,5	0.42	0	5,5,5	0.29	0
4	PO4	B	805	-	4,4,4	1.28	0	6,6,6	1.21	1 (16%)
3	GOL	D	805	-	5,5,5	1.16	1 (20%)	5,5,5	1.03	0
4	PO4	A	805	-	4,4,4	0.62	0	6,6,6	1.26	1 (16%)
3	GOL	A	804	-	5,5,5	0.86	0	5,5,5	1.26	1 (20%)
4	PO4	D	807	-	4,4,4	0.94	0	6,6,6	1.11	1 (16%)
2	BGC	D	801	-	12,12,12	0.66	0	17,17,17	1.00	1 (5%)
2	BGC	B	801	-	12,12,12	1.18	1 (8%)	17,17,17	1.19	2 (11%)
4	PO4	C	806	-	4,4,4	1.00	0	6,6,6	0.91	0
2	BGC	D	802	-	12,12,12	1.29	2 (16%)	17,17,17	1.71	6 (35%)
3	GOL	B	803	-	5,5,5	0.49	0	5,5,5	1.03	0
3	GOL	A	803	-	5,5,5	0.79	0	5,5,5	0.62	0
3	GOL	C	803	-	5,5,5	0.72	0	5,5,5	0.48	0
2	BGC	B	802	-	12,12,12	0.58	0	17,17,17	1.22	2 (11%)
4	PO4	C	805	-	4,4,4	0.91	0	6,6,6	1.42	1 (16%)
3	GOL	D	803	-	5,5,5	0.76	0	5,5,5	0.44	0
3	GOL	D	804	-	5,5,5	0.81	0	5,5,5	1.15	0
2	BGC	C	801	-	12,12,12	0.53	0	17,17,17	1.34	2 (11%)
3	GOL	D	806	-	5,5,5	0.63	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	A	801	-	12,12,12	0.68	0	17,17,17	1.57	5 (29%)
4	PO4	B	804	-	4,4,4	1.94	2 (50%)	6,6,6	1.60	1 (16%)
2	BGC	C	802	-	12,12,12	1.03	1 (8%)	17,17,17	1.07	2 (11%)

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	B	802	-	-	0/2/22/22	0/1/1/1
2	BGC	C	801	-	-	0/2/22/22	0/1/1/1
2	BGC	A	802	-	-	0/2/22/22	0/1/1/1
3	GOL	D	806	-	-	4/4/4/4	-
2	BGC	D	801	-	-	0/2/22/22	0/1/1/1
3	GOL	D	803	-	-	1/4/4/4	-
3	GOL	C	804	-	-	2/4/4/4	-
2	BGC	A	801	-	-	0/2/22/22	0/1/1/1
2	BGC	B	801	-	-	0/2/22/22	0/1/1/1
3	GOL	D	805	-	-	2/4/4/4	-
2	BGC	D	802	-	-	0/2/22/22	0/1/1/1
3	GOL	A	804	-	-	1/4/4/4	-
3	GOL	B	803	-	-	3/4/4/4	-
3	GOL	D	804	-	-	2/4/4/4	-
3	GOL	A	803	-	-	0/4/4/4	-
2	BGC	C	802	-	-	0/2/22/22	0/1/1/1
3	GOL	C	803	-	-	4/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	804	PO4	P-O1	3.13	1.57	1.50
2	D	802	BGC	O5-C5	-3.11	1.36	1.44
3	D	805	GOL	O2-C2	2.46	1.50	1.43
2	B	801	BGC	O4-C4	2.46	1.49	1.43
2	C	802	BGC	O1-C1	2.44	1.47	1.39
2	D	802	BGC	O1-C1	2.27	1.46	1.39
4	B	804	PO4	P-O3	-2.04	1.48	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	BGC	O2-C2-C1	-3.54	101.07	109.25
4	B	804	PO4	O4-P-O3	3.44	118.62	107.91
2	B	802	BGC	O1-C1-O5	-3.23	100.82	110.41
2	C	801	BGC	C4-C3-C2	-3.13	105.33	110.83
2	D	802	BGC	C1-C2-C3	3.09	116.66	110.36
2	B	801	BGC	C1-O5-C5	3.04	119.53	113.65
2	D	802	BGC	O2-C2-C1	-3.03	102.24	109.25
2	A	801	BGC	C4-C3-C2	-2.96	105.63	110.83
4	C	805	PO4	O4-P-O2	2.94	117.06	107.91
2	D	801	BGC	C4-C3-C2	-2.90	105.74	110.83
2	A	802	BGC	O4-C4-C3	2.88	117.17	110.38
2	B	802	BGC	O5-C1-C2	2.71	115.07	110.30
2	A	802	BGC	O5-C5-C4	2.56	114.32	109.70
2	D	802	BGC	O5-C5-C6	-2.49	100.26	106.44
2	A	802	BGC	O3-C3-C4	2.49	116.25	110.38
2	A	801	BGC	O3-C3-C4	-2.43	104.64	110.38
2	C	801	BGC	O1-C1-O5	-2.42	103.22	110.41
2	A	801	BGC	C3-C4-C5	2.34	114.48	110.23
2	D	802	BGC	C1-O5-C5	2.34	118.17	113.65
2	D	802	BGC	O5-C5-C4	2.28	113.81	109.70
2	C	802	BGC	C1-O5-C5	2.28	118.06	113.65
2	C	802	BGC	O2-C2-C1	-2.24	104.07	109.25
2	D	802	BGC	C6-C5-C4	2.20	118.41	113.02
3	A	804	GOL	O2-C2-C1	2.19	118.23	109.18
2	A	802	BGC	C1-C2-C3	2.18	114.81	110.36
4	A	805	PO4	O3-P-O1	-2.10	103.51	110.95
2	A	801	BGC	O2-C2-C3	2.09	115.29	110.38
2	A	801	BGC	O5-C5-C4	-2.05	106.00	109.70
2	B	801	BGC	O2-C2-C3	2.05	115.20	110.38
4	D	807	PO4	O4-P-O1	-2.03	103.76	110.95
4	B	805	PO4	O4-P-O2	2.01	114.15	107.91

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	804	GOL	O1-C1-C2-C3
3	D	804	GOL	O1-C1-C2-C3
3	D	805	GOL	O1-C1-C2-C3
3	D	806	GOL	O1-C1-C2-C3
3	D	804	GOL	O1-C1-C2-O2
3	B	803	GOL	O1-C1-C2-C3
3	C	803	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	803	GOL	C1-C2-C3-O3
3	D	803	GOL	O1-C1-C2-C3
3	D	806	GOL	C1-C2-C3-O3
3	C	803	GOL	O1-C1-C2-O2
3	C	804	GOL	O1-C1-C2-O2
3	D	805	GOL	O1-C1-C2-O2
3	D	806	GOL	O1-C1-C2-O2
3	B	803	GOL	O2-C2-C3-O3
3	A	804	GOL	O2-C2-C3-O3
3	D	806	GOL	O2-C2-C3-O3
3	B	803	GOL	C1-C2-C3-O3
3	C	803	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	756/764 (98%)	0.13	19 (2%) 58 60	13, 27, 53, 93	0
1	B	756/764 (98%)	0.08	11 (1%) 72 73	13, 26, 51, 69	0
1	C	756/764 (98%)	0.22	13 (1%) 69 70	17, 30, 54, 72	0
1	D	756/764 (98%)	0.24	17 (2%) 62 64	16, 30, 55, 75	0
All	All	3024/3056 (98%)	0.17	60 (1%) 65 67	13, 29, 53, 93	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	550	PRO	4.2
1	A	548	TYR	4.0
1	D	408	TYR	3.7
1	A	755	ILE	3.5
1	D	496	TYR	3.5
1	D	256	VAL	3.5
1	B	755	ILE	3.3
1	C	256	VAL	3.3
1	A	706	TRP	3.2
1	D	743	GLY	3.0
1	A	609	GLU	3.0
1	D	756	ILE	3.0
1	D	740	VAL	2.9
1	D	547	PRO	2.9
1	C	740	VAL	2.9
1	A	547	PRO	2.9
1	C	572	TYR	2.9
1	A	546	ILE	2.8
1	C	756	ILE	2.8
1	B	568	VAL	2.8
1	A	756	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	549	HIS	2.7
1	A	640	LEU	2.7
1	A	650	ARG	2.7
1	B	408	TYR	2.7
1	D	532	GLU	2.6
1	B	756	ILE	2.6
1	D	653	ILE	2.6
1	B	409	LEU	2.6
1	C	408	TYR	2.5
1	B	706	TRP	2.5
1	A	488	CYS	2.5
1	B	743	GLY	2.5
1	A	568	VAL	2.4
1	D	572	TYR	2.4
1	C	257	GLY	2.4
1	A	551	ASP	2.4
1	D	568	VAL	2.4
1	D	567	PHE	2.3
1	D	586	LEU	2.3
1	A	611	PHE	2.3
1	C	409	LEU	2.3
1	D	258	ASP	2.3
1	C	433	MET	2.2
1	A	408	TYR	2.2
1	C	653	ILE	2.2
1	A	383	GLY	2.2
1	C	586	LEU	2.2
1	D	549	HIS	2.1
1	C	496	TYR	2.1
1	C	743	GLY	2.1
1	B	550	PRO	2.1
1	A	743	GLY	2.1
1	C	280	PHE	2.1
1	A	163	LYS	2.1
1	D	409	LEU	2.1
1	B	649	ASN	2.0
1	B	488	CYS	2.0
1	B	609	GLU	2.0
1	D	113	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	804	6/6	0.61	0.26	55,57,60,64	0
3	GOL	C	803	6/6	0.71	0.20	46,55,59,62	0
3	GOL	D	803	6/6	0.72	0.19	44,54,61,61	0
3	GOL	A	804	6/6	0.81	0.18	33,35,40,41	0
3	GOL	A	803	6/6	0.82	0.15	29,41,45,47	0
3	GOL	D	805	6/6	0.83	0.13	27,36,38,50	0
3	GOL	D	806	6/6	0.84	0.13	46,47,49,49	0
3	GOL	C	804	6/6	0.87	0.11	47,49,50,55	0
4	PO4	B	805	5/5	0.89	0.13	42,43,47,47	0
3	GOL	B	803	6/6	0.90	0.14	30,40,42,42	0
4	PO4	C	806	5/5	0.90	0.12	45,46,46,50	0
2	BGC	D	802	12/12	0.94	0.07	21,26,27,27	0
2	BGC	A	801	12/12	0.94	0.06	19,21,23,24	0
2	BGC	A	802	12/12	0.94	0.07	21,26,29,32	0
2	BGC	B	802	12/12	0.94	0.07	19,26,29,31	0
2	BGC	B	801	12/12	0.95	0.06	20,22,24,26	0
2	BGC	C	801	12/12	0.95	0.06	19,24,25,25	0
2	BGC	C	802	12/12	0.95	0.06	20,25,29,30	0
2	BGC	D	801	12/12	0.95	0.06	21,24,25,25	0
4	PO4	B	804	5/5	0.98	0.04	18,21,23,26	0
4	PO4	D	807	5/5	0.98	0.06	22,25,27,28	0
4	PO4	A	805	5/5	0.99	0.05	20,20,23,24	0
4	PO4	C	805	5/5	0.99	0.06	22,24,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.