



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:51 AM UTC

PDB ID : 2I2W / pdb_00002i2w
Title : Crystal Structure of Escherichia Coli Phosphoheptose Isomerase
Authors : DeLeon, G.; Blakely, K.; Zhang, K.; Wright, G.; Junop, M.
Deposited on : 2006-08-17
Resolution : 1.95 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

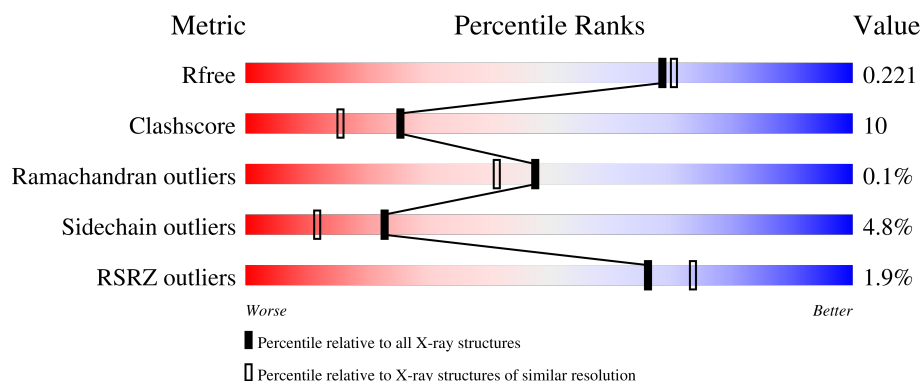
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	212	% 49% 33% 8% 9%
1	B	212	2% 49% 28% 6% 17%
1	C	212	% 51% 33% 5% 9%
1	D	212	% 55% 26% • 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6254 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 Phosphoheptose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1461	914	261	278	8			
1	B	177	Total	C	N	O	S	0	0	0
			1351	846	243	255	7			
1	C	192	Total	C	N	O	S	0	0	0
			1461	914	261	278	8			
1	D	178	Total	C	N	O	S	0	0	0
			1357	849	244	257	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P63224
A	-18	GLY	-	expression tag	UNP P63224
A	-17	SER	-	expression tag	UNP P63224
A	-16	SER	-	expression tag	UNP P63224
A	-15	HIS	-	expression tag	UNP P63224
A	-14	HIS	-	expression tag	UNP P63224
A	-13	HIS	-	expression tag	UNP P63224
A	-12	HIS	-	expression tag	UNP P63224
A	-11	HIS	-	expression tag	UNP P63224
A	-10	HIS	-	expression tag	UNP P63224
A	-9	SER	-	expression tag	UNP P63224
A	-8	SER	-	expression tag	UNP P63224
A	-7	GLY	-	expression tag	UNP P63224
A	-6	LEU	-	expression tag	UNP P63224
A	-5	VAL	-	expression tag	UNP P63224
A	-4	PRO	-	expression tag	UNP P63224
A	-3	ARG	-	expression tag	UNP P63224
A	-2	GLY	-	expression tag	UNP P63224
A	-1	SER	-	expression tag	UNP P63224
A	0	HIS	-	expression tag	UNP P63224
B	-19	MET	-	expression tag	UNP P63224

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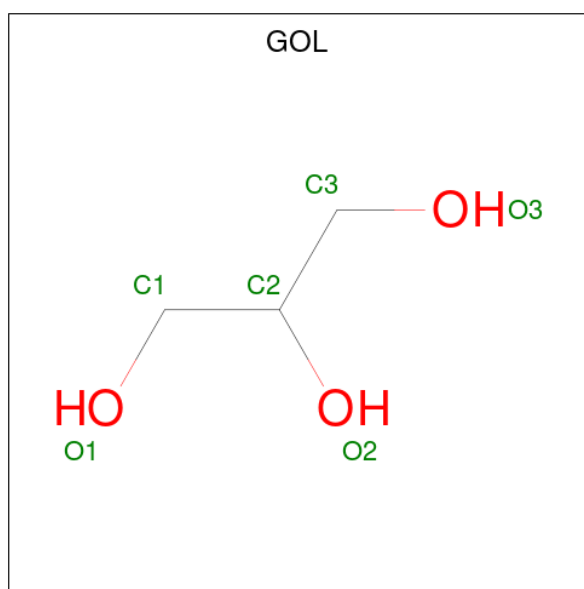
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P63224
B	-17	SER	-	expression tag	UNP P63224
B	-16	SER	-	expression tag	UNP P63224
B	-15	HIS	-	expression tag	UNP P63224
B	-14	HIS	-	expression tag	UNP P63224
B	-13	HIS	-	expression tag	UNP P63224
B	-12	HIS	-	expression tag	UNP P63224
B	-11	HIS	-	expression tag	UNP P63224
B	-10	HIS	-	expression tag	UNP P63224
B	-9	SER	-	expression tag	UNP P63224
B	-8	SER	-	expression tag	UNP P63224
B	-7	GLY	-	expression tag	UNP P63224
B	-6	LEU	-	expression tag	UNP P63224
B	-5	VAL	-	expression tag	UNP P63224
B	-4	PRO	-	expression tag	UNP P63224
B	-3	ARG	-	expression tag	UNP P63224
B	-2	GLY	-	expression tag	UNP P63224
B	-1	SER	-	expression tag	UNP P63224
B	0	HIS	-	expression tag	UNP P63224
C	-19	MET	-	expression tag	UNP P63224
C	-18	GLY	-	expression tag	UNP P63224
C	-17	SER	-	expression tag	UNP P63224
C	-16	SER	-	expression tag	UNP P63224
C	-15	HIS	-	expression tag	UNP P63224
C	-14	HIS	-	expression tag	UNP P63224
C	-13	HIS	-	expression tag	UNP P63224
C	-12	HIS	-	expression tag	UNP P63224
C	-11	HIS	-	expression tag	UNP P63224
C	-10	HIS	-	expression tag	UNP P63224
C	-9	SER	-	expression tag	UNP P63224
C	-8	SER	-	expression tag	UNP P63224
C	-7	GLY	-	expression tag	UNP P63224
C	-6	LEU	-	expression tag	UNP P63224
C	-5	VAL	-	expression tag	UNP P63224
C	-4	PRO	-	expression tag	UNP P63224
C	-3	ARG	-	expression tag	UNP P63224
C	-2	GLY	-	expression tag	UNP P63224
C	-1	SER	-	expression tag	UNP P63224
C	0	HIS	-	expression tag	UNP P63224
D	-19	MET	-	expression tag	UNP P63224
D	-18	GLY	-	expression tag	UNP P63224
D	-17	SER	-	expression tag	UNP P63224

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP P63224
D	-15	HIS	-	expression tag	UNP P63224
D	-14	HIS	-	expression tag	UNP P63224
D	-13	HIS	-	expression tag	UNP P63224
D	-12	HIS	-	expression tag	UNP P63224
D	-11	HIS	-	expression tag	UNP P63224
D	-10	HIS	-	expression tag	UNP P63224
D	-9	SER	-	expression tag	UNP P63224
D	-8	SER	-	expression tag	UNP P63224
D	-7	GLY	-	expression tag	UNP P63224
D	-6	LEU	-	expression tag	UNP P63224
D	-5	VAL	-	expression tag	UNP P63224
D	-4	PRO	-	expression tag	UNP P63224
D	-3	ARG	-	expression tag	UNP P63224
D	-2	GLY	-	expression tag	UNP P63224
D	-1	SER	-	expression tag	UNP P63224
D	0	HIS	-	expression tag	UNP P63224

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

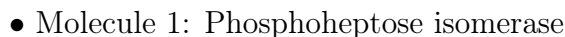


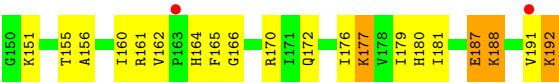
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

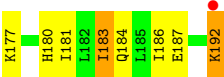
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	167	Total 167	O 167	0	0
3	B	142	Total 142	O 142	0	0
3	C	150	Total 150	O 150	0	0
3	D	159	Total 159	O 159	0	0

- Molecule 1: Phosphoheptose isomerase





● Molecule 1: Phosphoheptose isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.93Å 89.61Å 106.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.90 – 1.95 45.90 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.90-1.95) 99.6 (45.90-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.219 0.173 , 0.221	Depositor DCC
R_{free} test set	2996 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6254	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	2.34	62/1482 (4.2%)	1.73	19/1993 (1.0%)
1	B	2.22	45/1368 (3.3%)	1.81	23/1837 (1.3%)
1	C	2.33	61/1482 (4.1%)	1.78	22/1993 (1.1%)
1	D	2.22	39/1374 (2.8%)	1.74	11/1845 (0.6%)
All	All	2.28	207/5706 (3.6%)	1.77	75/7668 (1.0%)

All (207) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	162	VAL	N-CA	-13.21	1.36	1.46
1	A	25	ALA	CA-CB	12.20	1.72	1.53
1	B	125	ALA	CA-CB	10.35	1.69	1.53
1	A	18	ALA	CA-CB	9.52	1.68	1.53
1	D	71	ARG	CD-NE	-9.33	1.33	1.46
1	B	131	ILE	CA-CB	9.28	1.66	1.54
1	A	127	VAL	CA-CB	9.10	1.66	1.54
1	B	158	ILE	CA-CB	9.04	1.67	1.54
1	C	109	GLY	CA-C	9.04	1.60	1.52
1	D	156	ALA	N-CA	8.29	1.55	1.45
1	B	54	GLY	C-O	8.28	1.35	1.24
1	D	164	HIS	C-O	-8.16	1.14	1.24
1	A	109	GLY	N-CA	8.06	1.55	1.45
1	A	162	VAL	CA-CB	8.05	1.63	1.54
1	A	103	ARG	N-CA	8.05	1.56	1.46
1	A	105	VAL	N-CA	-8.02	1.36	1.46
1	C	149	GLY	N-CA	-8.00	1.32	1.45
1	B	162	VAL	CA-CB	7.70	1.61	1.53
1	A	145	THR	CA-CB	7.70	1.65	1.53
1	A	52	ASN	N-CA	7.69	1.54	1.45
1	C	48	LEU	N-CA	7.67	1.55	1.46
1	C	15	GLU	N-CA	7.64	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147	LYS	C-O	-7.62	1.17	1.24
1	B	184	GLN	C-O	7.54	1.32	1.24
1	D	2	TYR	N-CA	7.51	1.55	1.46
1	B	184	GLN	CD-NE2	7.50	1.49	1.33
1	C	114	VAL	C-O	7.49	1.31	1.24
1	C	14	ALA	N-CA	7.43	1.55	1.46
1	A	5	LEU	CA-C	7.40	1.62	1.52
1	A	6	ILE	CA-CB	-7.32	1.46	1.54
1	C	127	VAL	CA-CB	7.20	1.63	1.54
1	A	127	VAL	C-O	7.18	1.32	1.24
1	B	187	GLU	C-O	-7.17	1.15	1.24
1	C	21	LEU	C-O	-7.15	1.15	1.24
1	A	157	ASP	C-O	-7.11	1.15	1.24
1	D	43	ALA	CA-CB	7.10	1.65	1.53
1	A	14	ALA	CA-CB	7.03	1.64	1.53
1	B	82	ILE	CG1-CD1	7.00	1.79	1.51
1	C	31	GLN	CA-C	7.00	1.61	1.52
1	A	30	ILE	N-CA	6.99	1.54	1.46
1	A	1	MET	SD-CE	6.97	1.97	1.79
1	D	52	ASN	CA-C	-6.95	1.44	1.52
1	B	11	ASN	CA-C	-6.94	1.43	1.52
1	D	22	LYS	N-CA	-6.93	1.36	1.46
1	B	172	GLN	CD-NE2	6.89	1.47	1.33
1	A	25	ALA	N-CA	-6.87	1.38	1.46
1	C	3	GLN	CG-CD	6.84	1.69	1.52
1	D	105	VAL	CA-C	6.78	1.61	1.52
1	A	7	ARG	CA-C	-6.76	1.44	1.52
1	C	181	ILE	C-O	6.76	1.32	1.24
1	D	13	ALA	N-CA	6.73	1.54	1.46
1	C	147	LYS	CA-C	-6.72	1.47	1.53
1	C	64	GLU	C-O	-6.72	1.15	1.24
1	C	14	ALA	CA-CB	6.69	1.63	1.53
1	C	42	LYS	C-O	-6.64	1.15	1.24
1	D	53	GLY	C-O	6.64	1.32	1.24
1	C	3	GLN	C-O	-6.58	1.16	1.24
1	A	176	ILE	CA-C	6.57	1.62	1.52
1	A	192	LYS	CB-CG	-6.53	1.32	1.52
1	D	59	ALA	N-CA	6.52	1.54	1.46
1	D	81	ALA	CA-CB	-6.51	1.44	1.53
1	C	24	ASP	C-O	-6.49	1.15	1.24
1	D	127	VAL	CA-CB	6.49	1.62	1.54
1	A	53	GLY	CA-C	6.47	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	113	ASP	CA-C	-6.47	1.44	1.53
1	B	162	VAL	N-CA	-6.47	1.41	1.46
1	C	123	ASN	N-CA	6.46	1.53	1.46
1	C	131	ILE	CA-CB	6.44	1.61	1.54
1	A	125	ALA	N-CA	6.43	1.54	1.46
1	B	6	ILE	CA-CB	-6.43	1.46	1.54
1	D	128	ILE	C-O	6.42	1.31	1.24
1	A	43	ALA	CA-CB	6.42	1.64	1.53
1	D	160	ILE	CA-CB	6.34	1.61	1.53
1	C	47	VAL	CA-C	6.34	1.60	1.52
1	C	155	THR	CA-C	6.33	1.61	1.52
1	A	37	LEU	N-CA	-6.31	1.38	1.46
1	C	177	LYS	C-O	6.30	1.31	1.24
1	A	180	HIS	ND1-CE1	6.26	1.38	1.32
1	A	62	PHE	CA-C	6.25	1.60	1.52
1	B	134	ALA	CA-C	-6.24	1.44	1.52
1	C	161	ARG	C-O	-6.21	1.16	1.24
1	D	162	VAL	CA-CB	-6.20	1.47	1.53
1	B	169	ASP	CG-OD1	6.19	1.37	1.25
1	D	102	SER	N-CA	6.19	1.53	1.46
1	A	141	VAL	CA-CB	6.17	1.62	1.54
1	B	182	LEU	C-O	6.12	1.31	1.24
1	A	108	VAL	CA-CB	6.11	1.63	1.55
1	D	67	THR	N-CA	6.03	1.53	1.46
1	D	112	GLY	CA-C	6.03	1.59	1.51
1	B	52	ASN	N-CA	6.02	1.52	1.45
1	C	64	GLU	N-CA	5.99	1.53	1.46
1	C	118	ILE	CA-CB	5.98	1.61	1.54
1	A	110	ARG	CD-NE	5.96	1.54	1.46
1	A	3	GLN	N-CA	-5.96	1.39	1.46
1	A	158	ILE	C-O	-5.95	1.18	1.24
1	C	180	HIS	N-CA	-5.94	1.39	1.46
1	A	104	TYR	CA-C	5.92	1.60	1.52
1	D	181	ILE	CA-CB	5.91	1.62	1.54
1	A	100	ILE	CA-CB	-5.90	1.47	1.54
1	C	45	GLY	CA-C	5.88	1.59	1.52
1	D	79	ALA	C-O	5.87	1.30	1.23
1	A	72	GLU	C-O	-5.84	1.17	1.23
1	B	39	ASP	C-O	5.84	1.30	1.24
1	C	187	GLU	CA-C	5.82	1.60	1.52
1	A	178	VAL	CA-CB	5.81	1.61	1.54
1	B	112	GLY	CA-C	5.80	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	SER	CA-C	5.79	1.60	1.52
1	C	162	VAL	C-O	-5.79	1.16	1.24
1	B	183	ILE	CA-CB	5.78	1.61	1.54
1	C	103	ARG	CD-NE	-5.76	1.38	1.46
1	D	83	SER	C-O	5.75	1.35	1.23
1	B	62	PHE	N-CA	5.74	1.53	1.46
1	C	188	LYS	C-O	-5.74	1.17	1.24
1	C	84	ASP	CA-C	5.73	1.60	1.52
1	A	161	ARG	CZ-NH1	-5.72	1.24	1.32
1	A	41	PHE	CA-CB	-5.72	1.44	1.53
1	A	80	ILE	CA-C	5.71	1.59	1.52
1	D	26	ASN	C-O	-5.71	1.17	1.24
1	A	93	ASN	CG-OD1	5.71	1.34	1.23
1	A	4	ASP	CA-C	-5.70	1.45	1.52
1	A	183	ILE	CA-C	5.70	1.59	1.52
1	C	49	SER	N-CA	-5.69	1.39	1.45
1	A	109	GLY	CA-C	5.68	1.57	1.52
1	C	25	ALA	C-O	-5.67	1.17	1.24
1	C	176	ILE	CA-CB	5.66	1.62	1.54
1	A	6	ILE	C-O	-5.64	1.17	1.24
1	D	81	ALA	C-O	-5.63	1.17	1.24
1	B	72	GLU	CG-CD	5.63	1.66	1.52
1	A	176	ILE	CG1-CD1	5.62	1.73	1.51
1	A	126	ASN	N-CA	5.61	1.53	1.46
1	B	110	ARG	CD-NE	5.61	1.54	1.46
1	B	5	LEU	CA-C	5.61	1.60	1.52
1	C	156	ALA	N-CA	5.61	1.52	1.45
1	A	69	ARG	CA-C	-5.60	1.45	1.52
1	B	118	ILE	C-O	5.58	1.30	1.24
1	A	135	ARG	N-CA	5.56	1.53	1.46
1	C	5	LEU	CA-C	5.56	1.59	1.52
1	B	25	ALA	C-O	5.55	1.30	1.24
1	C	18	ALA	N-CA	5.53	1.53	1.46
1	D	69	ARG	C-O	-5.53	1.17	1.24
1	A	139	MET	C-O	5.52	1.30	1.23
1	C	38	ALA	C-O	-5.51	1.17	1.24
1	A	36	LEU	CA-CB	5.50	1.61	1.53
1	C	131	ILE	N-CA	-5.50	1.40	1.46
1	D	136	GLU	CD-OE1	5.49	1.35	1.25
1	B	52	ASN	CA-CB	-5.49	1.44	1.53
1	A	69	ARG	C-O	-5.48	1.17	1.24
1	C	15	GLU	CA-CB	-5.47	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	ILE	N-CA	5.45	1.53	1.46
1	B	101	PHE	N-CA	5.45	1.52	1.46
1	D	160	ILE	CA-C	5.43	1.59	1.52
1	D	26	ASN	CG-OD1	5.42	1.33	1.23
1	B	114	VAL	CA-CB	5.42	1.64	1.55
1	A	38	ALA	CA-CB	5.41	1.62	1.53
1	C	9	GLU	CD-OE2	5.41	1.35	1.25
1	B	137	LYS	CA-CB	5.39	1.63	1.53
1	B	53	GLY	CA-C	-5.37	1.44	1.52
1	C	103	ARG	CZ-NH2	-5.37	1.26	1.33
1	D	75	PRO	CA-C	5.36	1.59	1.52
1	A	20	PHE	CA-C	5.33	1.59	1.52
1	C	37	LEU	CA-C	5.33	1.59	1.52
1	C	25	ALA	CA-C	5.32	1.59	1.52
1	A	79	ALA	C-O	5.31	1.30	1.23
1	C	85	VAL	CA-CB	5.31	1.61	1.54
1	C	107	ALA	CA-CB	5.29	1.62	1.53
1	C	100	ILE	N-CA	-5.29	1.40	1.46
1	C	151	LYS	CE-NZ	5.29	1.65	1.49
1	B	129	LYS	CA-C	5.29	1.59	1.52
1	D	145	THR	CA-C	-5.24	1.45	1.52
1	D	180	HIS	C-O	-5.23	1.18	1.24
1	B	135	ARG	N-CA	5.22	1.52	1.46
1	C	104	TYR	CA-C	-5.21	1.46	1.52
1	C	170	ARG	N-CA	5.20	1.52	1.46
1	C	12	GLU	N-CA	-5.18	1.40	1.46
1	B	27	ILE	CA-CB	5.17	1.60	1.54
1	A	27	ILE	CA-CB	5.17	1.60	1.54
1	D	158	ILE	CA-CB	5.17	1.61	1.54
1	A	84	ASP	CA-CB	5.16	1.59	1.52
1	C	52	ASN	N-CA	5.13	1.51	1.45
1	D	177	LYS	C-O	-5.12	1.18	1.24
1	B	188	LYS	N-CA	5.12	1.52	1.46
1	B	64	GLU	CG-CD	5.11	1.64	1.52
1	A	61	HIS	CA-C	-5.11	1.46	1.52
1	C	41	PHE	C-O	-5.11	1.18	1.24
1	A	47	VAL	N-CA	5.10	1.52	1.46
1	C	40	SER	N-CA	5.09	1.52	1.46
1	D	183	ILE	N-CA	5.09	1.52	1.46
1	B	23	ASP	CA-CB	-5.08	1.46	1.53
1	B	142	ILE	C-O	5.08	1.29	1.24
1	D	25	ALA	CA-C	5.07	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	160	ILE	CA-C	5.07	1.59	1.52
1	B	137	LYS	CA-C	5.07	1.59	1.52
1	A	184	GLN	N-CA	5.06	1.52	1.46
1	D	153	ALA	CA-CB	-5.05	1.45	1.53
1	A	108	VAL	N-CA	5.04	1.50	1.46
1	C	166	GLY	CA-C	5.03	1.57	1.51
1	B	27	ILE	CA-C	5.03	1.59	1.52
1	D	55	SER	CB-OG	5.03	1.52	1.42
1	B	8	ASN	CG-OD1	5.02	1.33	1.23
1	A	82	ILE	CA-CB	5.02	1.59	1.54
1	B	43	ALA	CA-CB	-5.02	1.45	1.53
1	C	142	ILE	CA-C	5.01	1.58	1.52
1	D	145	THR	CA-CB	5.01	1.61	1.53
1	B	174	ILE	CA-CB	5.01	1.60	1.54
1	A	151	LYS	C-O	5.00	1.30	1.24
1	C	165	PHE	CA-C	-5.00	1.46	1.52
1	C	83	SER	CA-CB	5.00	1.62	1.53

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	VAL	N-CA-C	-9.65	103.27	112.83
1	C	147	LYS	CB-CA-C	-9.15	106.02	116.54
1	B	100	ILE	CB-CA-C	-8.56	101.01	111.97
1	C	42	LYS	N-CA-C	-7.82	103.00	112.54
1	B	149	GLY	N-CA-C	-7.72	104.89	114.92
1	A	182	LEU	N-CA-C	-7.66	102.87	111.07
1	A	110	ARG	NE-CZ-NH1	-7.39	114.11	121.50
1	B	130	ALA	N-CA-C	-7.30	103.40	111.36
1	A	122	GLY	N-CA-C	-7.29	105.17	115.30
1	C	172	GLN	N-CA-C	-7.11	103.61	111.36
1	C	133	ALA	N-CA-C	-7.03	103.69	111.36
1	A	2	TYR	N-CA-CB	-6.95	101.47	111.54
1	B	52	ASN	N-CA-C	6.64	120.87	110.17
1	C	122	GLY	N-CA-C	-6.58	106.25	115.32
1	B	2	TYR	N-CA-C	-6.53	103.41	112.30
1	B	82	ILE	CA-C-O	-6.51	109.73	120.80
1	C	130	ALA	N-CA-C	-6.50	104.27	111.36
1	C	71	ARG	NE-CZ-NH1	-6.46	115.05	121.50
1	C	48	LEU	N-CA-C	-6.36	98.15	108.52
1	B	112	GLY	N-CA-C	-6.24	107.27	114.69
1	D	149	GLY	N-CA-C	-6.23	107.11	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	110	ARG	NE-CZ-NH1	-6.15	115.35	121.50
1	B	132	ALA	CA-C-O	6.14	127.06	120.55
1	A	59	ALA	N-CA-C	-6.05	104.68	111.28
1	C	145	THR	CA-CB-OG1	-6.05	100.52	109.60
1	C	162	VAL	CA-C-O	6.00	122.69	119.15
1	D	183	ILE	N-CA-C	-5.97	104.53	110.62
1	A	4	ASP	N-CA-C	5.93	118.51	111.33
1	A	147	LYS	CB-CA-C	-5.92	109.73	116.54
1	B	142	ILE	CA-C-N	-5.91	113.40	122.62
1	B	142	ILE	C-N-CA	-5.91	113.40	122.62
1	A	30	ILE	N-CA-C	-5.88	105.00	110.53
1	C	66	LEU	N-CA-C	-5.87	104.96	111.36
1	C	160	ILE	N-CA-C	-5.84	97.99	107.28
1	B	140	LYS	CA-CB-CG	-5.81	102.48	114.10
1	B	102	SER	N-CA-C	5.78	118.53	111.82
1	B	104	TYR	N-CA-C	-5.77	105.08	111.36
1	B	106	GLU	N-CA-C	-5.75	104.62	111.69
1	B	40	SER	CA-CB-OG	-5.73	99.64	111.10
1	C	69	ARG	N-CA-C	5.70	119.49	112.54
1	B	160	ILE	N-CA-C	-5.66	98.99	107.37
1	C	64	GLU	CA-CB-CG	-5.65	102.80	114.10
1	B	60	MET	CA-CB-CG	-5.60	102.90	114.10
1	B	160	ILE	CA-CB-CG2	-5.56	101.05	110.50
1	D	157	ASP	CA-CB-CG	-5.51	107.09	112.60
1	D	22	LYS	N-CA-C	5.50	119.25	112.54
1	A	25	ALA	N-CA-C	-5.50	105.29	111.28
1	A	8	ASN	N-CA-C	5.47	117.24	111.28
1	A	178	VAL	CA-CB-CG2	-5.46	101.12	110.40
1	B	81	ALA	N-CA-C	-5.41	100.48	109.46
1	D	80	ILE	CA-C-O	-5.41	114.62	120.67
1	B	60	MET	CB-CA-C	-5.36	101.89	110.79
1	C	73	ASN	N-CA-C	5.35	118.82	111.54
1	A	23	ASP	N-CA-C	5.34	116.85	109.15
1	D	29	ALA	N-CA-C	-5.34	105.46	111.28
1	A	85	VAL	N-CA-C	5.33	116.69	110.62
1	B	7	ARG	CG-CD-NE	-5.32	100.31	112.00
1	C	143	THR	N-CA-C	5.31	118.40	109.95
1	A	39	ASP	N-CA-C	-5.27	105.62	111.36
1	C	100	ILE	N-CA-C	5.27	116.00	110.62
1	D	71	ARG	NE-CZ-NH2	-5.26	114.47	119.20
1	C	164	HIS	N-CA-C	5.26	118.06	110.28
1	A	95	PHE	CA-C-N	-5.21	113.92	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	PHE	C-N-CA	-5.21	113.92	122.20
1	B	58	ASP	N-CA-C	-5.19	105.53	111.14
1	D	57	CYS	CB-CA-C	-5.19	102.51	110.81
1	B	100	ILE	N-CA-CB	5.16	116.59	110.55
1	A	189	GLU	N-CA-C	5.16	116.91	111.28
1	A	51	GLY	N-CA-C	-5.13	103.26	110.91
1	C	103	ARG	CB-CA-C	-5.13	100.81	110.67
1	D	158	ILE	CB-CA-C	-5.12	103.16	110.12
1	C	110	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	C	67	THR	N-CA-C	-5.11	105.79	112.23
1	D	186	ILE	N-CA-C	-5.04	105.63	110.72
1	C	5	LEU	CD1-CG-CD2	-5.02	99.76	110.80

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	1461	0	1460	37	0
1	B	1351	0	1366	30	0
1	C	1461	0	1460	27	0
1	D	1357	0	1371	31	0
2	D	6	0	8	0	0
3	A	167	0	0	16	0
3	B	142	0	0	11	0
3	C	150	0	0	1	0
3	D	159	0	0	9	0
All	All	6254	0	5665	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (107) 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:82:ILE:CD1	1:B:82:ILE:CG1	1.79	1.59
3:A:249:HOH:O	1:D:184:GLN:HG3	1.43	1.15
1:D:98:ASN:HB2	3:D:301:HOH:O	1.46	1.13
1:B:98:ASN:HB2	3:B:324:HOH:O	1.46	1.12
1:B:100:ILE:HG12	3:B:322:HOH:O	1.60	1.01
1:C:73:ASN:HD22	1:C:73:ASN:N	1.66	0.92
1:D:169:ASP:HB2	3:D:260:HOH:O	1.79	0.82
1:B:3:GLN:HE21	1:B:3:GLN:HA	1.44	0.82
1:B:3:GLN:NE2	1:C:27:ILE:HG22	1.95	0.82
1:A:11:ASN:HB3	3:A:275:HOH:O	1.81	0.81
1:A:169:ASP:HB2	3:A:220:HOH:O	1.81	0.80
1:B:3:GLN:HA	1:B:3:GLN:NE2	1.95	0.80
1:D:183:ILE:HG21	3:D:338:HOH:O	1.82	0.78
1:B:56:HIS:ND1	3:B:326:HOH:O	2.22	0.73
1:A:184:GLN:HG2	3:A:290:HOH:O	1.91	0.70
1:C:187:GLU:OE2	1:C:187:GLU:O	2.09	0.70
1:C:73:ASN:HD22	1:C:73:ASN:H	1.39	0.70
1:C:73:ASN:N	1:C:73:ASN:ND2	2.37	0.69
1:D:1:MET:O	1:D:2:TYR:HB2	1.91	0.69
1:C:192:LYS:OXT	1:C:192:LYS:HG2	1.94	0.66
1:B:74:ARG:HD3	3:B:305:HOH:O	1.96	0.66
1:B:57:CYS:SG	1:C:60:MET:HE2	2.36	0.65
1:A:7:ARG:NH2	3:A:315:HOH:O	2.24	0.64
1:A:131:ILE:HG23	3:A:260:HOH:O	1.97	0.64
1:B:56:HIS:CE1	3:B:326:HOH:O	2.52	0.63
1:B:163:PRO:HG3	3:B:271:HOH:O	1.99	0.62
1:D:1:MET:O	1:D:2:TYR:CB	2.47	0.62
1:D:56:HIS:CD2	1:D:60:MET:HE2	2.35	0.61
1:C:188:LYS:O	1:C:191:VAL:HG22	2.00	0.61
1:D:71:ARG:HD3	3:D:349:HOH:O	2.00	0.60
1:D:28:HIS:CE1	1:D:32:ARG:HD3	2.38	0.59
1:A:28:HIS:HB3	1:A:32:ARG:HH21	1.67	0.59
1:A:108:VAL:HG12	1:B:108:VAL:HB	1.85	0.59
1:B:3:GLN:HE21	1:C:27:ILE:HG22	1.66	0.59
1:B:147:LYS:NZ	3:B:277:HOH:O	2.36	0.58
1:A:141:VAL:HG21	3:A:260:HOH:O	2.03	0.58
1:D:192:LYS:HD2	3:D:341:HOH:O	2.03	0.58
1:C:71:ARG:HG2	1:D:103:ARG:CZ	2.34	0.57
1:A:97:PHE:HA	1:A:125:ALA:HB3	1.85	0.57
1:C:1:MET:SD	1:C:3:GLN:HB2	2.46	0.56
1:A:57:CYS:SG	1:D:57:CYS:SG	3.04	0.55
1:B:7:ARG:NH2	1:C:24:ASP:OD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ILE:CD1	1:B:82:ILE:CB	2.82	0.54
1:B:3:GLN:NE2	1:B:3:GLN:CA	2.70	0.54
1:A:32:ARG:HD2	3:A:248:HOH:O	2.07	0.54
1:D:28:HIS:O	1:D:32:ARG:HG3	2.08	0.54
1:C:72:GLU:HG2	1:C:73:ASN:ND2	2.23	0.54
1:A:28:HIS:HB3	1:A:32:ARG:NH2	2.23	0.53
1:A:1:MET:HA	1:D:31:GLN:HE22	1.76	0.51
1:A:22:LYS:HG2	1:A:23:ASP:N	2.24	0.51
1:A:71:ARG:NH1	1:A:71:ARG:HG3	2.26	0.51
1:C:58:ASP:HB3	1:C:179:ILE:CD1	2.40	0.50
1:A:182:LEU:O	1:A:186:ILE:HG13	2.10	0.50
1:A:1:MET:SD	1:A:3:GLN:NE2	2.84	0.50
1:C:102:SER:O	1:C:106:GLU:HG3	2.13	0.49
1:B:19:ASN:HA	1:B:22:LYS:HD2	1.94	0.49
1:B:188:LYS:O	1:B:192:LYS:HB2	2.12	0.49
1:D:187:GLU:OE2	1:D:187:GLU:HA	2.12	0.49
1:D:192:LYS:NZ	3:D:343:HOH:O	2.45	0.49
1:A:2:TYR:OH	1:D:192:LYS:HE3	2.12	0.49
1:A:135:ARG:CZ	3:A:260:HOH:O	2.61	0.49
1:B:67:THR:O	1:B:71:ARG:HB2	2.12	0.49
1:A:1:MET:SD	1:A:3:GLN:HG2	2.54	0.48
1:C:187:GLU:OE2	1:C:191:VAL:HG13	2.14	0.48
1:B:57:CYS:CB	1:C:57:CYS:HG	2.24	0.48
1:A:2:TYR:HA	3:A:206:HOH:O	2.14	0.47
1:D:1:MET:HA	3:D:288:HOH:O	2.14	0.47
1:B:52:ASN:HB2	3:B:316:HOH:O	2.14	0.47
1:D:113:ASP:HB2	1:D:139:MET:HG2	1.97	0.47
1:C:11:ASN:O	1:C:15:GLU:HG3	2.15	0.46
1:A:38:ALA:O	1:A:42:LYS:HG3	2.15	0.46
1:B:98:ASN:N	3:B:322:HOH:O	2.48	0.46
1:A:3:GLN:OE1	1:D:27:ILE:HG22	2.15	0.46
1:C:187:GLU:OE2	1:C:187:GLU:C	2.58	0.46
1:A:135:ARG:NE	3:A:260:HOH:O	2.47	0.46
1:D:183:ILE:HD13	3:D:338:HOH:O	2.15	0.45
1:A:147:LYS:NZ	3:A:338:HOH:O	2.48	0.45
1:C:1:MET:C	1:C:1:MET:HE3	2.41	0.45
1:C:113:ASP:HB2	1:C:139:MET:HG2	1.99	0.45
1:A:2:TYR:OH	1:D:192:LYS:CE	2.65	0.45
1:A:164:HIS:HD2	3:A:340:HOH:O	1.98	0.45
1:A:3:GLN:HE22	1:D:28:HIS:HD2	1.65	0.45
1:A:65:GLU:O	1:A:69:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:NE2	1:D:3:GLN:HG3	2.32	0.44
1:B:2:TYR:H	1:C:31:GLN:NE2	2.16	0.44
1:C:50:CYS:HA	3:C:196:HOH:O	2.17	0.44
1:C:192:LYS:OXT	1:C:192:LYS:CG	2.62	0.44
1:D:1:MET:O	1:D:1:MET:HG2	2.17	0.44
1:B:66:LEU:HD23	1:B:66:LEU:HA	1.84	0.43
1:A:70:TYR:OH	1:A:187:GLU:HA	2.19	0.43
1:C:1:MET:HE2	1:C:1:MET:HB3	1.71	0.43
1:B:164:HIS:CD2	1:B:166:GLY:H	2.37	0.43
1:D:5:LEU:HD23	1:D:5:LEU:C	2.43	0.43
1:A:93:ASN:ND2	3:A:231:HOH:O	2.49	0.43
1:B:162:VAL:HA	1:B:163:PRO:HD3	1.87	0.42
1:D:1:MET:O	1:D:2:TYR:CG	2.72	0.42
1:A:8:ASN:HB3	3:A:262:HOH:O	2.20	0.42
1:D:1:MET:O	1:D:1:MET:CG	2.67	0.42
1:D:1:MET:HB3	3:D:321:HOH:O	2.18	0.42
1:B:31:GLN:HE22	1:C:1:MET:HG2	1.85	0.41
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.85	0.41
1:B:82:ILE:C	3:B:323:HOH:O	2.63	0.41
1:A:185:LEU:HD11	1:D:6:ILE:HD11	2.03	0.41
1:C:17:LEU:HD22	1:C:177:LYS:HE2	2.03	0.41
1:A:99:ASP:HB2	3:A:324:HOH:O	2.20	0.41
1:A:31:GLN:HE22	1:D:3:GLN:HG3	1.85	0.41
1:B:50:CYS:HA	3:B:326:HOH:O	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	190/212 (90%)	184 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	173/212 (82%)	171 (99%)	2 (1%)	0	100	100
1	C	190/212 (90%)	189 (100%)	1 (0%)	0	100	100
1	D	174/212 (82%)	168 (97%)	5 (3%)	1 (1%)	21	12
All	All	727/848 (86%)	712 (98%)	14 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2	TYR

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	151/168 (90%)	146 (97%)	5 (3%)	33	24
1	B	138/168 (82%)	127 (92%)	11 (8%)	11	3
1	C	151/168 (90%)	143 (95%)	8 (5%)	20	9
1	D	139/168 (83%)	135 (97%)	4 (3%)	37	29
All	All	579/672 (86%)	551 (95%)	28 (5%)	23	12

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	57	CYS
1	A	73	ASN
1	A	74	ARG
1	A	147	LYS
1	B	1	MET
1	B	3	GLN
1	B	5	LEU
1	B	57	CYS
1	B	60	MET

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Mol	Chain	Res	Type
1	B	72	GLU
1	B	100	ILE
1	B	108	VAL
1	B	136	GLU
1	B	191	VAL
1	B	192	LYS
1	C	1	MET
1	C	5	LEU
1	C	21	LEU
1	C	22	LYS
1	C	71	ARG
1	C	73	ASN
1	C	108	VAL
1	C	192	LYS
1	D	21	LEU
1	D	100	ILE
1	D	129	LYS
1	D	192	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	26	ASN
1	A	31	GLN
1	A	93	ASN
1	A	164	HIS
1	A	184	GLN
1	B	3	GLN
1	B	11	ASN
1	B	26	ASN
1	B	31	GLN
1	B	56	HIS
1	B	61	HIS
1	C	11	ASN
1	C	26	ASN
1	C	31	GLN
1	C	61	HIS
1	C	73	ASN
1	C	164	HIS
1	C	184	GLN
1	D	26	ASN

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Mol	Chain	Res	Type
1	D	28	HIS
1	D	61	HIS
1	D	164	HIS

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 ⓘ

1 ligand is 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	GOL	D	196	-	5,5,5	0.96	0	5,5,5	2.66	3 (60%)

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	GOL	D	196	-	-	2/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	196	GOL	O1-C1-C2	-3.87	92.96	110.38
2	D	196	GOL	O2-C2-C1	3.55	123.86	109.18
2	D	196	GOL	O2-C2-C3	2.67	120.24	109.18

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	196	GOL	O2-C2-C3-O3
2	D	196	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	192/212 (90%)	-0.18	3 (1%) 70 77	26, 38, 62, 102	0
1	B	177/212 (83%)	-0.19	5 (2%) 55 62	26, 36, 62, 92	0
1	C	192/212 (90%)	-0.24	3 (1%) 70 77	24, 34, 63, 96	0
1	D	178/212 (83%)	-0.36	3 (1%) 69 76	25, 33, 55, 83	0
All	All	739/848 (87%)	-0.24	14 (1%) 66 74	24, 35, 62, 102	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	83	SER	3.8
1	D	1	MET	3.8
1	B	1	MET	3.7
1	A	191	VAL	3.5
1	A	1	MET	3.4
1	C	1	MET	3.2
1	B	167	TYR	3.1
1	C	191	VAL	3.1
1	D	192	LYS	2.5
1	B	53	GLY	2.4
1	B	191	VAL	2.3
1	C	163	PRO	2.2
1	A	192	LYS	2.1
1	B	74	ARG	2.1

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
2	GOL	D	196	6/6	0.90	0.12	44,51,53,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.