



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:08 AM UTC

PDB ID : 8ADK / pdb_00008adk
Title : Poly(ADP-ribose) glycohydrolase (PARG) from *Drosophila melanogaster*
Authors : Ariza, A.; Fontana, P.
Deposited on : 2022-07-08
Resolution : 2.47 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

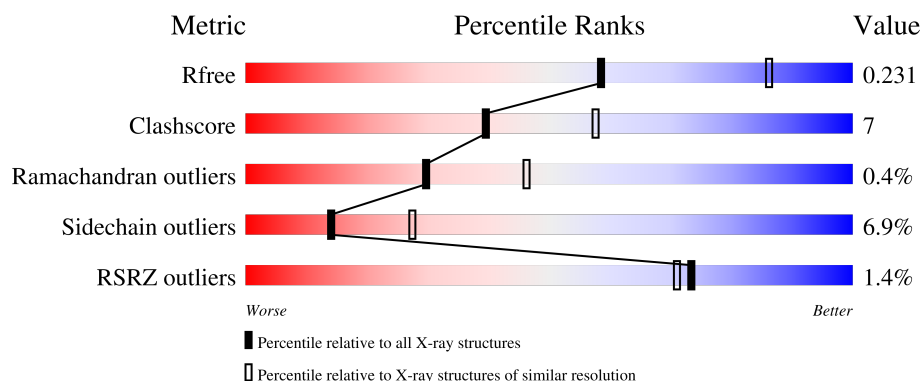
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	578	% 69% 17% • • 11%
1	B	578	2% 68% 17% • • 11%
1	C	578	% 70% 15% • 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12923 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 Poly(ADP-ribose) glycohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	1	0
			4192	2671	738	763	20			
1	B	517	Total	C	N	O	S	0	1	0
			4192	2671	738	763	20			
1	C	517	Total	C	N	O	S	0	1	0
			4192	2671	738	763	20			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O46043
A	-18	GLY	-	expression tag	UNP O46043
A	-17	SER	-	expression tag	UNP O46043
A	-16	SER	-	expression tag	UNP O46043
A	-15	HIS	-	expression tag	UNP O46043
A	-14	HIS	-	expression tag	UNP O46043
A	-13	HIS	-	expression tag	UNP O46043
A	-12	HIS	-	expression tag	UNP O46043
A	-11	HIS	-	expression tag	UNP O46043
A	-10	HIS	-	expression tag	UNP O46043
A	-9	SER	-	expression tag	UNP O46043
A	-8	SER	-	expression tag	UNP O46043
A	-7	GLY	-	expression tag	UNP O46043
A	-6	LEU	-	expression tag	UNP O46043
A	-5	VAL	-	expression tag	UNP O46043
A	-4	PRO	-	expression tag	UNP O46043
A	-3	ARG	-	expression tag	UNP O46043
A	-2	GLY	-	expression tag	UNP O46043
A	-1	SER	-	expression tag	UNP O46043
A	0	HIS	-	expression tag	UNP O46043
B	-19	MET	-	initiating methionine	UNP O46043
B	-18	GLY	-	expression tag	UNP O46043
B	-17	SER	-	expression tag	UNP O46043

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP O46043
B	-15	HIS	-	expression tag	UNP O46043
B	-14	HIS	-	expression tag	UNP O46043
B	-13	HIS	-	expression tag	UNP O46043
B	-12	HIS	-	expression tag	UNP O46043
B	-11	HIS	-	expression tag	UNP O46043
B	-10	HIS	-	expression tag	UNP O46043
B	-9	SER	-	expression tag	UNP O46043
B	-8	SER	-	expression tag	UNP O46043
B	-7	GLY	-	expression tag	UNP O46043
B	-6	LEU	-	expression tag	UNP O46043
B	-5	VAL	-	expression tag	UNP O46043
B	-4	PRO	-	expression tag	UNP O46043
B	-3	ARG	-	expression tag	UNP O46043
B	-2	GLY	-	expression tag	UNP O46043
B	-1	SER	-	expression tag	UNP O46043
B	0	HIS	-	expression tag	UNP O46043
C	-19	MET	-	initiating methionine	UNP O46043
C	-18	GLY	-	expression tag	UNP O46043
C	-17	SER	-	expression tag	UNP O46043
C	-16	SER	-	expression tag	UNP O46043
C	-15	HIS	-	expression tag	UNP O46043
C	-14	HIS	-	expression tag	UNP O46043
C	-13	HIS	-	expression tag	UNP O46043
C	-12	HIS	-	expression tag	UNP O46043
C	-11	HIS	-	expression tag	UNP O46043
C	-10	HIS	-	expression tag	UNP O46043
C	-9	SER	-	expression tag	UNP O46043
C	-8	SER	-	expression tag	UNP O46043
C	-7	GLY	-	expression tag	UNP O46043
C	-6	LEU	-	expression tag	UNP O46043
C	-5	VAL	-	expression tag	UNP O46043
C	-4	PRO	-	expression tag	UNP O46043
C	-3	ARG	-	expression tag	UNP O46043
C	-2	GLY	-	expression tag	UNP O46043
C	-1	SER	-	expression tag	UNP O46043
C	0	HIS	-	expression tag	UNP O46043

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



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	89	Total	O	0	0
			89	89		

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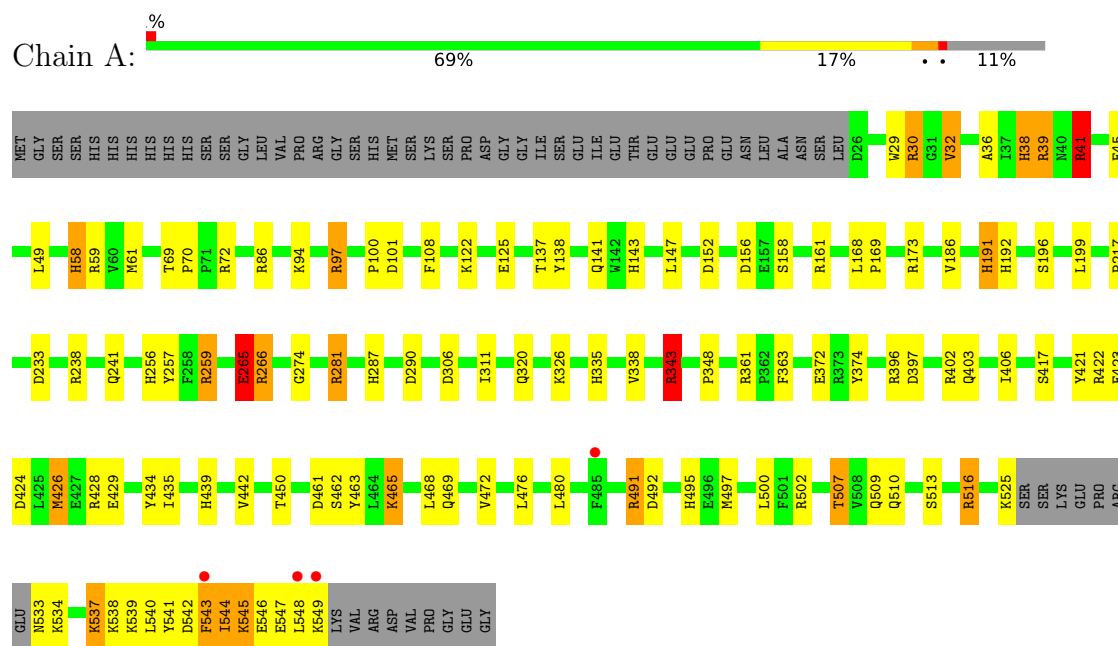
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	80	Total	O	0	0
			80	80		

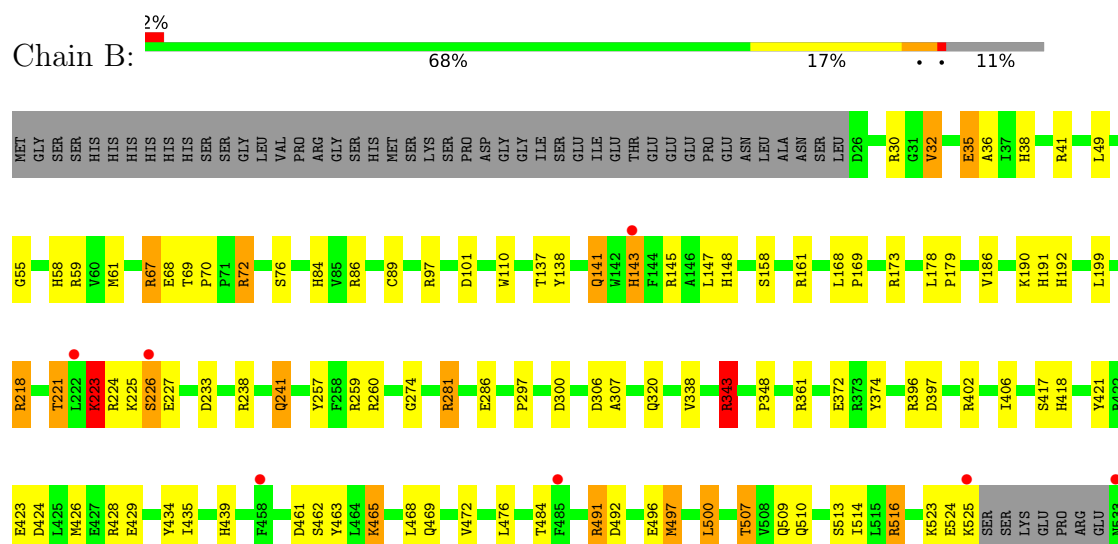
3 Residue-property plots

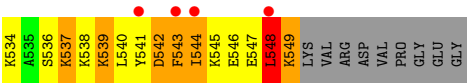
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Poly(ADP-ribose) glycohydrolase

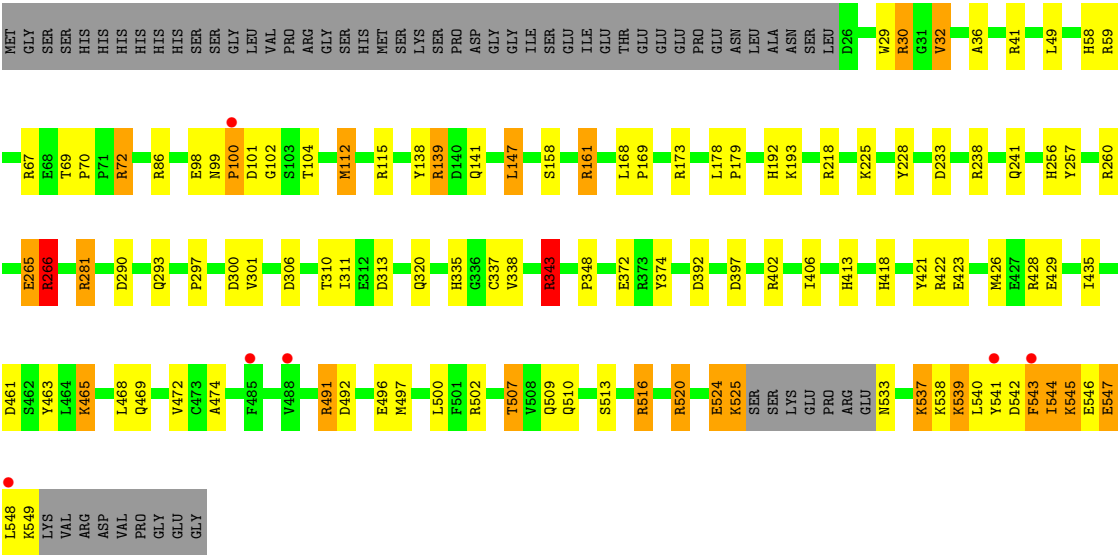


- Molecule 1: Poly(ADP-ribose) glycohydrolase





● Molecule 1: Poly(ADP-ribose) glycohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.43Å 115.62Å 122.91Å 90.00° 112.21° 90.00°	Depositor
Resolution (Å)	59.02 – 2.47 59.02 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.2 (59.02-2.47) 99.2 (59.02-2.47)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.177 , 0.228 0.183 , 0.231	Depositor DCC
R_{free} test set	4167 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12923	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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, SO4, CL

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	0.89	11/4305 (0.3%)	1.30	12/5837 (0.2%)
1	B	0.88	10/4305 (0.2%)	1.31	13/5837 (0.2%)
1	C	0.87	6/4305 (0.1%)	1.28	10/5837 (0.2%)
All	All	0.88	27/12915 (0.2%)	1.29	35/17511 (0.2%)

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	15
1	B	0	21
1	C	0	17
All	All	0	53

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	HIS	CE1-NE2	9.17	1.41	1.32
1	B	418	HIS	CE1-NE2	8.17	1.40	1.32
1	C	192	HIS	CE1-NE2	8.03	1.40	1.32
1	C	335	HIS	CE1-NE2	7.83	1.40	1.32
1	B	439	HIS	CE1-NE2	7.50	1.40	1.32
1	A	38	HIS	CE1-NE2	7.07	1.39	1.32
1	B	191	HIS	CE1-NE2	6.76	1.39	1.32
1	B	192	HIS	CE1-NE2	6.72	1.39	1.32
1	A	192	HIS	CE1-NE2	6.70	1.39	1.32
1	A	191	HIS	CE1-NE2	6.66	1.39	1.32
1	B	148	HIS	CE1-NE2	6.64	1.39	1.32
1	A	58	HIS	CE1-NE2	6.61	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	58	HIS	CE1-NE2	6.54	1.39	1.32
1	A	143	HIS	CE1-NE2	6.48	1.39	1.32
1	B	543	PHE	C-N	6.06	1.41	1.33
1	C	543	PHE	C-N	6.05	1.41	1.33
1	B	58	HIS	CE1-NE2	6.04	1.38	1.32
1	C	418	HIS	CE1-NE2	5.97	1.38	1.32
1	A	287	HIS	CE1-NE2	5.54	1.38	1.32
1	C	256	HIS	CE1-NE2	5.49	1.38	1.32
1	A	335	HIS	CE1-NE2	5.20	1.37	1.32
1	B	38	HIS	CE1-NE2	5.19	1.37	1.32
1	B	542	ASP	C-N	5.18	1.41	1.33
1	B	84	HIS	CE1-NE2	5.17	1.37	1.32
1	A	439	HIS	CE1-NE2	5.14	1.37	1.32
1	A	543	PHE	C-N	5.09	1.40	1.33
1	A	495	HIS	CE1-NE2	5.01	1.37	1.32

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	ASP	CA-CB-CG	7.30	119.90	112.60
1	A	233	ASP	CA-CB-CG	7.04	119.64	112.60
1	A	137	THR	CA-CB-OG1	-6.82	99.37	109.60
1	A	152	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	424	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	306	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	403	GLN	OE1-CD-NE2	5.92	128.52	122.60
1	B	397	ASP	CA-CB-CG	5.91	118.51	112.60
1	B	141	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	B	223	LYS	CB-CA-C	5.64	119.08	109.72
1	B	424	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	306	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	290	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	233	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	76	SER	N-CA-CB	5.53	116.91	111.10
1	B	35	GLU	CB-CA-C	-5.52	99.75	110.46
1	B	190	LYS	O-C-N	5.51	129.11	122.94
1	C	392	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	265	GLU	CB-CG-CD	5.44	121.85	112.60
1	C	260	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	A	156	ASP	CA-CB-CG	5.36	117.95	112.60
1	C	413	HIS	CA-CB-CG	5.30	119.11	113.80
1	B	35	GLU	N-CA-CB	5.30	118.51	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ARG	CB-CA-C	5.29	119.05	109.37
1	B	221	THR	CA-CB-CG2	5.28	119.48	110.50
1	B	536	SER	N-CA-CB	5.28	117.88	110.12
1	A	397	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	426	MET	N-CA-C	-5.22	106.06	112.90
1	C	397	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	293	GLN	CB-CA-C	-5.20	101.39	110.17
1	C	306	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	217	PRO	N-CA-CB	5.13	108.11	103.34
1	B	143	HIS	CA-CB-CG	5.10	118.90	113.80
1	C	104	THR	CA-CB-OG1	-5.02	102.06	109.60
1	C	72	ARG	CB-CA-C	5.01	117.53	109.41

There are no chirality outliers.

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Sidechain
1	A	173	ARG	Sidechain
1	A	238	ARG	Sidechain
1	A	259	ARG	Sidechain
1	A	281[A]	ARG	Sidechain
1	A	281[B]	ARG	Sidechain
1	A	343	ARG	Sidechain
1	A	39	ARG	Sidechain
1	A	402	ARG	Sidechain
1	A	422	ARG	Sidechain
1	A	491	ARG	Sidechain
1	A	502	ARG	Sidechain
1	A	516	ARG	Sidechain
1	A	72	ARG	Sidechain
1	A	97	ARG	Sidechain
1	B	145	ARG	Sidechain
1	B	161	ARG	Sidechain
1	B	173	ARG	Sidechain
1	B	218	ARG	Sidechain
1	B	224	ARG	Sidechain
1	B	226	SER	Peptide
1	B	238	ARG	Sidechain
1	B	259	ARG	Sidechain
1	B	260	ARG	Sidechain
1	B	281[A]	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	281[B]	ARG	Sidechain
1	B	343	ARG	Sidechain
1	B	361	ARG	Sidechain
1	B	402	ARG	Sidechain
1	B	41	ARG	Sidechain
1	B	491	ARG	Sidechain
1	B	516	ARG	Sidechain
1	B	548	LEU	Peptide
1	B	67	ARG	Sidechain
1	B	72	ARG	Sidechain
1	B	86	ARG	Sidechain
1	C	139	ARG	Sidechain
1	C	161	ARG	Sidechain
1	C	173	ARG	Sidechain
1	C	218	ARG	Sidechain
1	C	266	ARG	Sidechain
1	C	281[A]	ARG	Sidechain
1	C	281[B]	ARG	Sidechain
1	C	343	ARG	Sidechain
1	C	402	ARG	Sidechain
1	C	41	ARG	Sidechain
1	C	422	ARG	Sidechain
1	C	491	ARG	Sidechain
1	C	502	ARG	Sidechain
1	C	516	ARG	Sidechain
1	C	520	ARG	Sidechain
1	C	67	ARG	Sidechain
1	C	72	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4192	0	4121	57	0
1	B	4192	0	4121	55	0
1	C	4192	0	4121	57	0
2	A	18	0	24	3	0
2	B	12	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	12	0	16	1	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	1	0
4	A	2	0	0	1	0
4	B	1	0	0	1	0
5	A	108	0	0	2	0
5	B	89	0	0	3	0
5	C	80	0	0	1	0
All	All	12923	0	12419	169	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 7.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ARG:HB3	1:A:266:ARG:HH11	1.10	1.10
1:A:266:ARG:HH11	1:A:266:ARG:CB	1.72	1.03
1:B:227:GLU:HG2	5:B:708:HOH:O	1.62	0.98
1:B:539:LYS:HE2	1:B:543:PHE:CD1	2.05	0.92
1:C:539:LYS:HE3	1:C:543:PHE:CD1	2.04	0.92
1:C:266:ARG:HA	5:C:712:HOH:O	1.70	0.91
1:A:539:LYS:HE2	1:A:543:PHE:CD1	2.09	0.87
1:A:266:ARG:HB3	1:A:266:ARG:NH1	1.93	0.84
1:C:539:LYS:HE3	1:C:543:PHE:CE1	2.16	0.81
1:C:32:VAL:HG13	1:C:36:ALA:HB3	1.67	0.77
1:A:32:VAL:HG13	1:A:36:ALA:HB3	1.67	0.77
1:B:32:VAL:HG13	1:B:36:ALA:HB3	1.68	0.76
1:C:540:LEU:O	1:C:544:ILE:HB	1.87	0.73
1:B:138:TYR:HA	1:B:141:GLN:HE21	1.54	0.72
1:B:540:LEU:O	1:B:544:ILE:HB	1.88	0.72
1:A:540:LEU:O	1:A:544:ILE:HB	1.89	0.72
1:A:41:ARG:CB	1:A:41:ARG:HH11	2.03	0.72
1:C:281[B]:ARG:HH21	1:C:281[B]:ARG:CG	2.05	0.70
1:A:545:LYS:HA	1:A:548:LEU:HD12	1.75	0.69
1:C:545:LYS:HA	1:C:548:LEU:HD12	1.76	0.68
1:B:545:LYS:HA	1:B:548:LEU:HD12	1.75	0.68
1:C:281[A]:ARG:HD3	1:C:435:ILE:O	1.95	0.66
1:B:549:LYS:O	1:B:549:LYS:HG2	1.95	0.66
1:B:539:LYS:CE	1:B:543:PHE:CD1	2.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:MET:HE3	1:B:537:LYS:HG2	1.79	0.65
1:C:525:LYS:HE3	1:C:525:LYS:C	2.22	0.64
1:A:41:ARG:HH11	1:A:41:ARG:HB3	1.63	0.64
1:A:265:GLU:HG2	1:A:266:ARG:N	2.11	0.64
1:A:86:ARG:HH12	2:A:601:GOL:H31	1.62	0.64
1:A:539:LYS:CE	1:A:543:PHE:CD1	2.80	0.64
1:A:542:ASP:O	1:A:546:GLU:HG3	1.98	0.63
1:B:500:LEU:HD23	1:B:544:ILE:HG21	1.80	0.63
1:B:223:LYS:HD3	1:B:225:LYS:H	1.64	0.63
1:A:97:ARG:NE	4:A:606:CL:CL	2.69	0.62
1:B:143:HIS:HB3	5:B:722:HOH:O	1.99	0.62
1:A:281[A]:ARG:HD3	1:A:435:ILE:O	1.99	0.62
1:A:41:ARG:HB3	1:A:45:GLU:OE1	1.99	0.62
1:C:86:ARG:HH22	2:C:601:GOL:H11	1.64	0.62
1:B:281[A]:ARG:HD3	1:B:435:ILE:O	2.00	0.61
1:A:497:MET:HE3	1:A:537:LYS:CG	2.31	0.61
1:C:421:TYR:OH	1:C:461:ASP:OD2	2.19	0.61
1:C:265:GLU:HG3	1:C:266:ARG:N	2.15	0.60
1:C:539:LYS:CE	1:C:543:PHE:CD1	2.82	0.60
1:C:497:MET:HE3	1:C:537:LYS:CG	2.32	0.59
1:C:421:TYR:HA	1:C:426:MET:HE3	1.85	0.59
1:B:421:TYR:HA	1:B:426:MET:HE3	1.83	0.58
1:B:68:GLU:OE1	1:B:72:ARG:HD2	2.02	0.58
1:A:463:TYR:CD2	1:A:537:LYS:HD2	2.38	0.58
1:B:497:MET:HE3	1:B:537:LYS:CG	2.33	0.58
1:B:421:TYR:OH	1:B:461:ASP:OD2	2.22	0.57
1:C:497:MET:HE3	1:C:537:LYS:HG2	1.86	0.57
1:C:542:ASP:O	1:C:546:GLU:HG3	2.04	0.57
1:A:463:TYR:HD2	1:A:537:LYS:HD2	1.69	0.57
1:B:463:TYR:HD2	1:B:537:LYS:HD2	1.69	0.57
1:C:463:TYR:CD2	1:C:537:LYS:HD2	2.40	0.57
1:A:266:ARG:CB	1:A:266:ARG:NH1	2.56	0.56
1:B:538:LYS:O	1:B:541:TYR:HB2	2.06	0.56
1:C:538:LYS:O	1:C:541:TYR:HB2	2.06	0.56
1:A:86:ARG:NH1	2:A:601:GOL:H31	2.21	0.55
1:A:421:TYR:HA	1:A:426:MET:HE3	1.87	0.55
1:A:497:MET:HE3	1:A:537:LYS:HG2	1.89	0.55
1:A:538:LYS:O	1:A:541:TYR:HB2	2.06	0.55
1:B:463:TYR:CD2	1:B:537:LYS:HD2	2.42	0.54
1:C:463:TYR:HD2	1:C:537:LYS:HD2	1.73	0.54
1:B:423:GLU:OE1	1:B:516:ARG:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:TYR:OH	1:A:461:ASP:OD2	2.24	0.53
1:B:542:ASP:O	1:B:546:GLU:HG3	2.08	0.53
1:C:297:PRO:HG2	1:C:300:ASP:OD2	2.09	0.53
1:A:320:GLN:OE1	1:A:343:ARG:NH2	2.39	0.52
1:A:290:ASP:HA	5:A:704:HOH:O	2.08	0.52
1:C:281[B]:ARG:HH21	1:C:281[B]:ARG:HG3	1.73	0.52
1:B:281[B]:ARG:HH21	1:B:281[B]:ARG:HG3	1.75	0.52
1:B:257:TYR:HB2	1:B:348:PRO:HG2	1.93	0.51
1:C:168:LEU:HB3	1:C:169:PRO:HD3	1.91	0.51
1:B:61:MET:HE2	1:B:186:VAL:HG22	1.93	0.51
1:A:38:HIS:C	1:A:39:ARG:HG2	2.36	0.51
1:A:266:ARG:HH11	1:A:266:ARG:CG	2.22	0.51
1:A:423:GLU:OE1	1:A:516:ARG:HG2	2.11	0.50
1:A:428:ARG:NH1	1:A:429:GLU:OE1	2.44	0.50
1:B:320:GLN:OE1	1:B:343:ARG:NH2	2.44	0.49
1:B:428:ARG:NH1	1:B:429:GLU:OE1	2.45	0.49
1:A:257:TYR:HB2	1:A:348:PRO:HG2	1.95	0.48
1:B:168:LEU:HB3	1:B:169:PRO:HD3	1.95	0.48
1:C:138:TYR:HA	1:C:141:GLN:HE21	1.77	0.48
1:B:468:LEU:O	1:B:472:VAL:HG23	2.14	0.48
1:C:98:GLU:OE2	1:C:102:GLY:HA2	2.13	0.48
1:C:265:GLU:HG3	1:C:266:ARG:H	1.78	0.48
1:C:539:LYS:O	1:C:539:LYS:HD3	2.13	0.48
1:C:112:MET:HE2	1:C:115:ARG:NH2	2.28	0.48
1:C:257:TYR:HB2	1:C:348:PRO:HG2	1.96	0.48
1:A:259:ARG:HD2	5:A:742:HOH:O	2.14	0.48
1:C:428:ARG:NH1	1:C:429:GLU:OE1	2.46	0.47
1:A:138:TYR:HA	1:A:141:GLN:HE21	1.79	0.47
1:A:497:MET:HE3	1:A:537:LYS:HG3	1.97	0.47
1:C:69:THR:HA	1:C:70:PRO:C	2.40	0.46
1:C:320:GLN:OE1	1:C:343:ARG:NH2	2.44	0.46
1:A:311:ILE:CG2	1:A:320:GLN:HB3	2.46	0.46
1:A:41:ARG:CB	1:A:41:ARG:NH1	2.77	0.46
1:A:94:LYS:HE2	1:A:108:PHE:CE1	2.51	0.46
1:B:137:THR:HB	1:B:138:TYR:CD2	2.50	0.46
1:A:86:ARG:HH12	2:A:601:GOL:C3	2.27	0.46
1:C:310:THR:OG1	1:C:313:ASP:HB2	2.15	0.46
1:A:468:LEU:O	1:A:472:VAL:HG23	2.16	0.46
1:C:320:GLN:O	1:C:406:ILE:HA	2.15	0.46
1:B:32:VAL:HG13	1:B:36:ALA:CB	2.43	0.45
1:C:139:ARG:HG3	1:C:139:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:GLU:OE1	1:C:516:ARG:HG2	2.15	0.45
1:A:320:GLN:O	1:A:406:ILE:HA	2.16	0.45
1:B:465:LYS:O	1:B:469:GLN:HG3	2.16	0.45
1:C:281[B]:ARG:HH21	1:C:281[B]:ARG:HG2	1.81	0.45
1:C:228:TYR:O	3:C:604:SO4:O3	2.33	0.45
1:C:147:LEU:HD12	1:C:147:LEU:HA	1.84	0.45
1:B:549:LYS:O	1:B:549:LYS:CG	2.62	0.45
1:B:320:GLN:O	1:B:406:ILE:HA	2.17	0.45
1:C:539:LYS:O	1:C:539:LYS:CD	2.64	0.45
1:B:297:PRO:HG2	1:B:300:ASP:OD2	2.17	0.44
1:A:465:LYS:O	1:A:469:GLN:HG3	2.17	0.44
1:B:372:GLU:HB3	1:B:374:TYR:CE2	2.52	0.44
1:B:274:GLY:HA3	1:B:396:ARG:NH1	2.32	0.44
1:C:547:GLU:OE1	1:C:547:GLU:HA	2.15	0.44
1:A:513:SER:HA	1:A:516:ARG:HH11	1.83	0.44
1:C:524:GLU:HA	1:C:524:GLU:OE1	2.17	0.44
1:C:468:LEU:O	1:C:472:VAL:HG23	2.17	0.44
1:B:507:THR:HG22	1:B:510:GLN:CG	2.48	0.43
1:A:168:LEU:HB3	1:A:169:PRO:HD3	2.01	0.43
1:C:428:ARG:C	1:C:428:ARG:HD3	2.43	0.43
1:A:69:THR:HA	1:A:70:PRO:C	2.42	0.43
1:C:491:ARG:NH1	1:C:492:ASP:OD1	2.51	0.43
1:B:218:ARG:HH22	2:B:601:GOL:C3	2.30	0.43
1:B:434:TYR:CE1	1:B:476:LEU:HD21	2.53	0.43
1:C:465:LYS:O	1:C:469:GLN:HG3	2.19	0.43
1:C:507:THR:HG22	1:C:510:GLN:CG	2.49	0.43
1:A:147:LEU:HD12	1:A:147:LEU:HA	1.82	0.42
1:B:514:ILE:CG2	1:B:540:LEU:HD22	2.49	0.42
1:A:61:MET:HE2	1:A:186:VAL:HG22	2.00	0.42
1:B:143:HIS:O	1:B:241:GLN:HG3	2.20	0.42
1:B:514:ILE:HG22	1:B:540:LEU:HD22	2.02	0.42
1:A:507:THR:HG22	1:A:510:GLN:CG	2.49	0.42
1:B:178:LEU:N	1:B:179:PRO:HD2	2.34	0.42
1:C:99:ASN:O	1:C:100:PRO:C	2.62	0.42
1:A:372:GLU:HB3	1:A:374:TYR:CE2	2.55	0.42
1:B:69:THR:HA	1:B:70:PRO:C	2.45	0.41
1:B:89:CYS:HA	1:B:110:TRP:CG	2.55	0.41
1:B:97:ARG:HD3	4:B:604:CL:CL	2.57	0.41
1:B:491:ARG:NH1	1:B:492:ASP:OD1	2.53	0.41
1:C:301:VAL:CG2	1:C:474:ALA:HA	2.51	0.41
1:C:311:ILE:CG2	1:C:320:GLN:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:HH21	1:B:97:ARG:CB	2.33	0.41
1:B:218:ARG:HH22	2:B:601:GOL:H31	1.85	0.41
1:A:539:LYS:HE3	1:A:543:PHE:CE1	2.56	0.41
1:C:178:LEU:N	1:C:179:PRO:HD2	2.35	0.41
1:A:29:TRP:O	1:A:30:ARG:HD3	2.20	0.41
1:B:513:SER:HA	1:B:516:ARG:HH11	1.85	0.41
1:B:547:GLU:C	1:B:549:LYS:N	2.79	0.41
1:A:434:TYR:CE1	1:A:476:LEU:HD21	2.56	0.41
1:A:491:ARG:NH1	1:A:492:ASP:OD1	2.54	0.41
1:B:307:ALA:HA	1:B:484:THR:OG1	2.19	0.41
1:C:32:VAL:HG13	1:C:36:ALA:CB	2.45	0.41
1:C:372:GLU:HB3	1:C:374:TYR:CE2	2.56	0.41
1:C:524:GLU:OE1	1:C:524:GLU:CA	2.69	0.41
1:C:513:SER:HA	1:C:516:ARG:HH11	1.85	0.41
1:A:274:GLY:HA3	1:A:396:ARG:NH1	2.36	0.40
1:B:147:LEU:HD12	1:B:147:LEU:HA	1.89	0.40
1:C:29:TRP:O	1:C:30:ARG:HD3	2.21	0.40
1:C:112:MET:HE2	1:C:115:ARG:HH22	1.86	0.40
1:A:58:HIS:CG	1:A:196:SER:HB2	2.57	0.40
1:A:450:THR:HG22	1:A:480:LEU:HD11	2.04	0.40
1:B:55:GLY:HA3	5:B:766:HOH:O	2.21	0.40
1:A:191:HIS:CE1	1:A:361:ARG:HH21	2.40	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	514/578 (89%)	495 (96%)	17 (3%)	2 (0%)	30	46
1	B	514/578 (89%)	493 (96%)	19 (4%)	2 (0%)	30	46
1	C	514/578 (89%)	495 (96%)	17 (3%)	2 (0%)	30	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1542/1734 (89%)	1483 (96%)	53 (3%)	6 (0%)	30	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	548	LEU
1	C	100	PRO
1	A	100	PRO
1	B	338	VAL
1	A	338	VAL
1	C	338	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	455/507 (90%)	424 (93%)	31 (7%)	14	28
1	B	455/507 (90%)	424 (93%)	31 (7%)	14	28
1	C	455/507 (90%)	423 (93%)	32 (7%)	14	27
All	All	1365/1521 (90%)	1271 (93%)	94 (7%)	14	27

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	32	VAL
1	A	41	ARG
1	A	49	LEU
1	A	59	ARG
1	A	101	ASP
1	A	122	LYS
1	A	125	GLU
1	A	158	SER
1	A	199	LEU

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Mol	Chain	Res	Type
1	A	241	GLN
1	A	265	GLU
1	A	266	ARG
1	A	326	LYS
1	A	343	ARG
1	A	363	PHE
1	A	417	SER
1	A	442	VAL
1	A	462	SER
1	A	465	LYS
1	A	500	LEU
1	A	507	THR
1	A	509	GLN
1	A	525	LYS
1	A	533	ASN
1	A	534	LYS
1	A	537	LYS
1	A	544	ILE
1	A	545	LYS
1	A	547	GLU
1	A	549	LYS
1	B	30	ARG
1	B	32	VAL
1	B	35	GLU
1	B	49	LEU
1	B	59	ARG
1	B	67	ARG
1	B	101	ASP
1	B	158	SER
1	B	199	LEU
1	B	221	THR
1	B	223	LYS
1	B	226	SER
1	B	241	GLN
1	B	286	GLU
1	B	343	ARG
1	B	417	SER
1	B	462	SER
1	B	465	LYS
1	B	496	GLU
1	B	497	MET
1	B	500	LEU

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Mol	Chain	Res	Type
1	B	507	THR
1	B	509	GLN
1	B	523	LYS
1	B	524	GLU
1	B	525	LYS
1	B	534	LYS
1	B	537	LYS
1	B	539	LYS
1	B	544	ILE
1	B	549	LYS
1	C	30	ARG
1	C	32	VAL
1	C	49	LEU
1	C	59	ARG
1	C	101	ASP
1	C	112	MET
1	C	147	LEU
1	C	158	SER
1	C	161	ARG
1	C	193	LYS
1	C	225	LYS
1	C	238	ARG
1	C	241	GLN
1	C	265	GLU
1	C	266	ARG
1	C	337	CYS
1	C	343	ARG
1	C	465	LYS
1	C	496	GLU
1	C	500	LEU
1	C	507	THR
1	C	509	GLN
1	C	520	ARG
1	C	524	GLU
1	C	525	LYS
1	C	533	ASN
1	C	537	LYS
1	C	539	LYS
1	C	544	ILE
1	C	545	LYS
1	C	547	GLU
1	C	549	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	141	GLN
1	A	149	GLN
1	A	416	GLN
1	A	533	ASN
1	B	141	GLN
1	B	143	HIS
1	B	183	GLN
1	B	376	ASN
1	B	418	HIS
1	B	533	ASN
1	C	56	ASN
1	C	99	ASN
1	C	141	GLN
1	C	439	HIS
1	C	533	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	B	601	-	5,5,5	0.16	0	5,5,5	0.69	0
3	SO4	C	604	-	4,4,4	0.87	0	6,6,6	0.59	0
3	SO4	C	603	-	4,4,4	0.20	0	6,6,6	1.23	0
2	GOL	A	603	-	5,5,5	0.62	0	5,5,5	1.29	0
2	GOL	B	602	-	5,5,5	0.39	0	5,5,5	0.68	0
3	SO4	A	605	-	4,4,4	1.43	1 (25%)	6,6,6	0.88	0
2	GOL	C	602	-	5,5,5	0.56	0	5,5,5	0.99	0
2	GOL	A	602	-	5,5,5	0.20	0	5,5,5	0.39	0
2	GOL	C	601	-	5,5,5	0.18	0	5,5,5	0.35	0
3	SO4	B	603	-	4,4,4	0.33	0	6,6,6	0.67	0
3	SO4	A	604	-	4,4,4	0.41	0	6,6,6	0.76	0
2	GOL	A	601	-	5,5,5	0.38	0	5,5,5	1.11	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	GOL	B	601	-	-	2/4/4/4	-
2	GOL	A	603	-	-	4/4/4/4	-
2	GOL	B	602	-	-	3/4/4/4	-
2	GOL	C	602	-	-	4/4/4/4	-
2	GOL	A	602	-	-	0/4/4/4	-
2	GOL	C	601	-	-	3/4/4/4	-
2	GOL	A	601	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	SO4	O2-S	2.22	1.58	1.44

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	C1-C2-C3-O3
2	A	603	GOL	C1-C2-C3-O3
2	A	603	GOL	O2-C2-C3-O3
2	B	602	GOL	C1-C2-C3-O3
2	C	602	GOL	O1-C1-C2-O2
2	C	602	GOL	O1-C1-C2-C3
2	C	602	GOL	C1-C2-C3-O3
2	C	602	GOL	O2-C2-C3-O3
2	B	601	GOL	O2-C2-C3-O3
2	A	601	GOL	O1-C1-C2-C3
2	A	603	GOL	O1-C1-C2-C3
2	B	601	GOL	C1-C2-C3-O3
2	C	601	GOL	O1-C1-C2-C3
2	B	602	GOL	O2-C2-C3-O3
2	B	602	GOL	O1-C1-C2-O2
2	C	601	GOL	O2-C2-C3-O3
2	A	601	GOL	O2-C2-C3-O3
2	A	603	GOL	O1-C1-C2-O2
2	C	601	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GOL	2	0
3	C	604	SO4	1	0
2	C	601	GOL	1	0
2	A	601	GOL	3	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	517/578 (89%)	-0.19	4 (0%) 82 80	29, 60, 111, 158	1 (0%)
1	B	517/578 (89%)	-0.10	11 (2%) 63 60	29, 67, 113, 158	1 (0%)
1	C	517/578 (89%)	-0.12	6 (1%) 76 74	27, 64, 118, 152	1 (0%)
All	All	1551/1734 (89%)	-0.14	21 (1%) 73 71	27, 64, 113, 158	3 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	LEU	4.6
1	A	543	PHE	3.5
1	B	525	LYS	3.3
1	B	543	PHE	3.3
1	B	485	PHE	3.0
1	B	533	ASN	3.0
1	B	548	LEU	2.8
1	C	543	PHE	2.8
1	B	458	PHE	2.8
1	C	548	LEU	2.7
1	B	544	ILE	2.7
1	C	485	PHE	2.5
1	A	548	LEU	2.4
1	A	485	PHE	2.4
1	C	488	VAL	2.4
1	B	143	HIS	2.3
1	B	226	SER	2.2
1	A	549	LYS	2.2
1	C	100	PRO	2.1
1	B	541	TYR	2.1
1	C	541	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 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	C	602	6/6	0.80	0.20	57,79,89,96	0
2	GOL	B	601	6/6	0.83	0.13	88,94,98,100	0
2	GOL	B	602	6/6	0.85	0.18	96,104,106,122	0
2	GOL	A	602	6/6	0.87	0.13	77,101,109,111	0
3	SO4	C	604	5/5	0.87	0.15	65,72,160,165	0
2	GOL	A	603	6/6	0.89	0.14	48,76,80,82	0
3	SO4	B	603	5/5	0.91	0.11	46,68,121,141	0
3	SO4	A	605	5/5	0.92	0.11	56,60,61,160	0
2	GOL	C	601	6/6	0.92	0.10	83,91,95,98	0
3	SO4	C	603	5/5	0.92	0.10	58,65,74,83	0
2	GOL	A	601	6/6	0.92	0.09	60,69,78,82	0
4	CL	A	607	1/1	0.94	0.13	75,75,75,75	0
4	CL	B	604	1/1	0.96	0.09	85,85,85,85	0
3	SO4	A	604	5/5	0.97	0.05	45,45,55,66	0
4	CL	A	606	1/1	0.98	0.05	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.