



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 03:56 AM UTC

PDB ID : 5WJ0 / pdb_00005wj0
Title : Phosphotriesterase variant S5+254R
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Deposited on : 2017-07-21
Resolution : 1.65 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

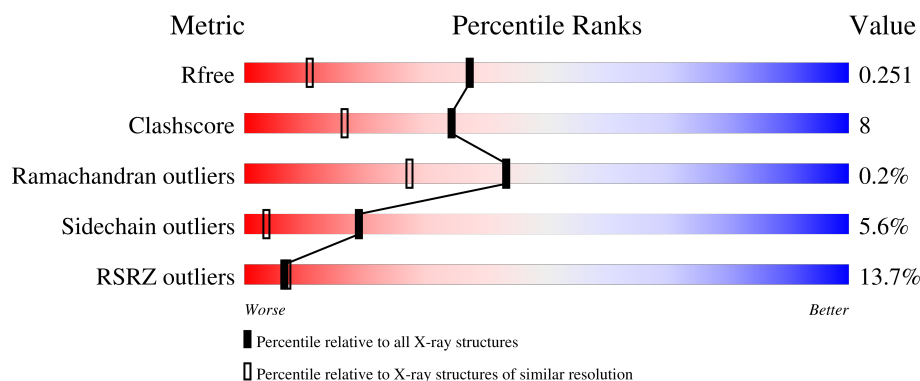
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	333	
1	G	333	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CAC	A	2406	-	X	-	-
4	CAC	G	406	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5200 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 Phosphotriesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	4	0
			2444	1544	442	452	6			
1	G	315	Total	C	N	O	S	0	9	0
			2489	1572	453	458	6			

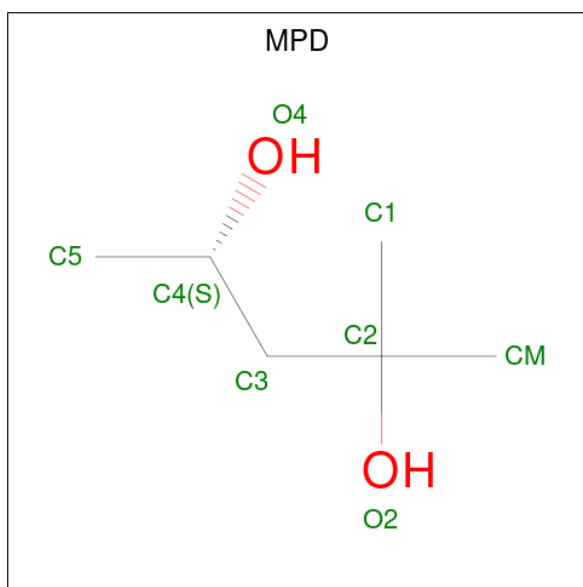
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	LEU	PHE	conflict	UNP A0A060GZX0
A	233	ALA	ASP	conflict	UNP A0A060GZX0
A	271	HIS	LEU	conflict	UNP A0A060GZX0
A	293	THR	MET	conflict	UNP A0A060GZX0
A	306	ILE	PHE	conflict	UNP A0A060GZX0
A	320	GLY	VAL	conflict	UNP A0A060GZX0
G	216	LEU	PHE	conflict	UNP A0A060GZX0
G	233	ALA	ASP	conflict	UNP A0A060GZX0
G	271	HIS	LEU	conflict	UNP A0A060GZX0
G	293	THR	MET	conflict	UNP A0A060GZX0
G	306	ILE	PHE	conflict	UNP A0A060GZX0
G	320	GLY	VAL	conflict	UNP A0A060GZX0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

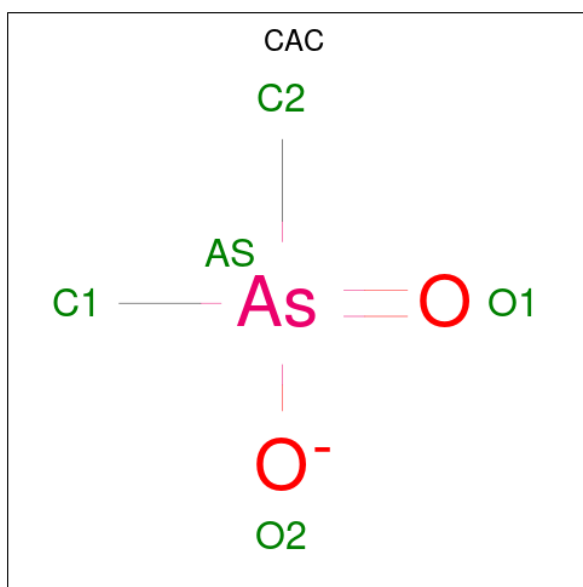
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	G	2	Total	Zn	0	0
			2	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	G	1	Total	As	C	O	0	0
			5	1	2	2		

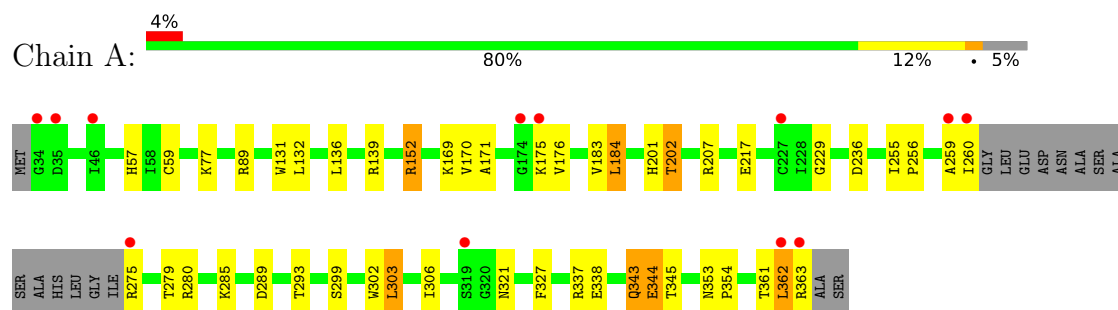
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	113	Total	O	0	0
			113	113		
5	G	92	Total	O	0	0
			92	92		

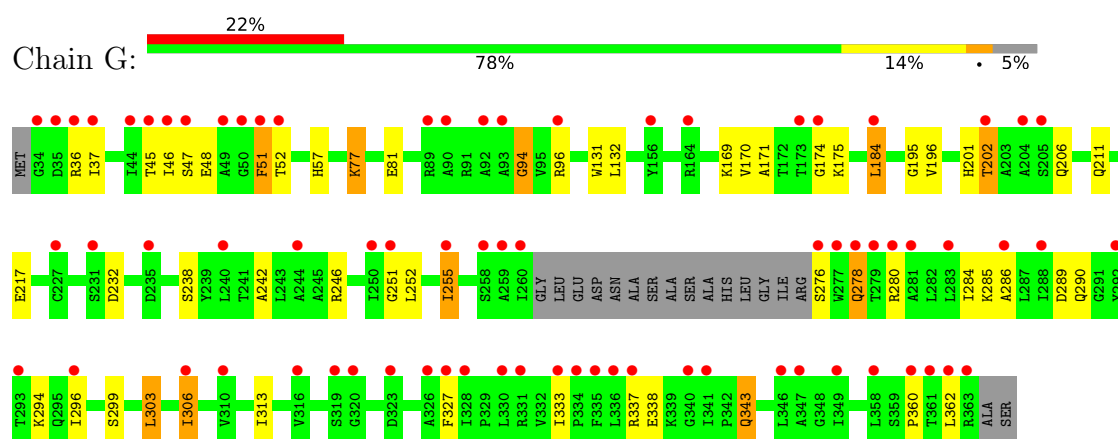
3 Residue-property plots [i](#)

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: Phosphotriesterase



• Molecule 1: Phosphotriesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.33Å 85.78Å 88.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.43 – 1.65 29.43 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.43-1.65) 99.9 (29.43-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.65Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.215 , 0.248 0.216 , 0.251	Depositor DCC
R_{free} test set	4054 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k 0.012 for -l,-k,-h 0.013 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5200	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, KCX, ZN, MPD

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	0.43	0/2474	0.63	0/3358
1	G	0.40	1/2520 (0.0%)	0.61	1/3418 (0.0%)
All	All	0.42	1/4994 (0.0%)	0.62	1/6776 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	333	ILE	CA-CB	-5.78	1.51	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	94	GLY	N-CA-C	5.69	121.26	114.48

There are no chirality outliers.

There are no planarity outliers.

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	2444	0	2484	36	0
1	G	2489	0	2523	39	0
2	A	2	0	0	0	0
2	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	24	0	42	2	0
3	G	24	0	42	2	0
4	A	5	0	0	0	0
4	G	5	0	0	0	0
5	A	113	0	0	5	0
5	G	92	0	0	4	0
All	All	5200	0	5091	77	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 8.

All (77) 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:170[B]:VAL:HG11	1:A:184:LEU:HD13	1.55	0.89
1:G:170[B]:VAL:HG11	1:G:184:LEU:HD13	1.61	0.82
1:A:170[B]:VAL:HG11	1:A:184:LEU:CD1	2.12	0.80
1:G:170[B]:VAL:HG11	1:G:184:LEU:CD1	2.14	0.78
1:G:202:THR:HG21	5:G:522:HOH:O	1.94	0.67
1:G:251:GLY:HA3	5:G:547:HOH:O	1.96	0.64
1:G:276:SER:HB2	1:G:278[A]:GLN:HE21	1.63	0.62
1:G:36:ARG:HH11	1:G:45:THR:HG23	1.64	0.61
1:A:202:THR:HG21	5:A:2515:HOH:O	2.00	0.61
1:G:217:GLU:OE2	1:G:246[B]:ARG:NH1	2.35	0.60
1:G:57:HIS:HB2	1:G:303:LEU:HB3	1.84	0.59
1:G:284:ILE:HG23	1:G:296:ILE:HG21	1.85	0.58
1:A:131:TRP:CG	1:A:132:LEU:H	2.22	0.58
1:G:303:LEU:HD13	1:G:306[A]:ILE:HG12	1.86	0.57
1:A:57:HIS:HB2	1:A:303:LEU:HB3	1.88	0.56
1:G:51:PHE:HD1	1:G:52:THR:N	2.04	0.56
1:G:131:TRP:CG	1:G:132:LEU:H	2.23	0.56
3:A:2403:MPD:O4	3:A:2403:MPD:O2	2.24	0.54
1:A:361:THR:HG22	1:A:363:ARG:H	1.73	0.54
1:A:362:LEU:HD23	5:A:2605:HOH:O	2.08	0.53
1:G:337:ARG:HH21	1:G:343:GLN:HG2	1.74	0.52
1:G:174:GLY:O	1:G:211:GLN:NE2	2.43	0.52
1:A:170[A]:VAL:HG21	1:A:184:LEU:CD1	2.40	0.51
1:A:337:ARG:HH12	1:A:343:GLN:HG2	1.75	0.51
1:A:170[B]:VAL:CG1	1:A:184:LEU:HD13	2.34	0.51
1:A:59:CYS:HB3	5:A:2593:HOH:O	2.11	0.50
1:G:57:HIS:O	1:G:303:LEU:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:HD13	1:A:280:ARG:HB3	1.94	0.50
1:A:337:ARG:HH22	1:A:343:GLN:HG2	1.76	0.50
3:G:401:MPD:O4	3:G:401:MPD:O2	2.08	0.50
1:G:51:PHE:C	1:G:51:PHE:CD1	2.89	0.50
1:G:51:PHE:HD1	1:G:51:PHE:C	2.21	0.48
1:A:259:ALA:O	1:A:260:ILE:HB	2.13	0.48
1:G:285:LYS:NZ	1:G:289:ASP:OD2	2.46	0.48
1:A:275:ARG:HH21	1:A:279:THR:HG22	1.79	0.48
1:A:255:ILE:HG12	5:A:2502:HOH:O	2.13	0.47
1:A:57:HIS:O	1:A:303:LEU:HA	2.14	0.47
1:A:337:ARG:HH22	1:A:343:GLN:CG	2.26	0.47
1:A:256:PRO:HG3	1:A:327:PHE:CD1	2.50	0.47
1:A:89:ARG:HG3	5:A:2538:HOH:O	2.14	0.46
1:G:37:ILE:HG13	1:G:46:ILE:HG22	1.96	0.46
1:G:174:GLY:HA3	1:G:206:GLN:OE1	2.15	0.46
1:G:303:LEU:HD22	1:G:306[B]:ILE:HG23	1.97	0.46
1:G:232:ASP:OD2	1:G:280:ARG:NH1	2.48	0.45
1:A:302:TRP:CH2	1:A:321:ASN:HB3	2.52	0.45
1:A:217:GLU:HG2	3:A:2405:MPD:H53	1.98	0.45
1:G:306[B]:ILE:CD1	1:G:313:ILE:HG23	2.47	0.44
1:G:303:LEU:HD22	1:G:306[B]:ILE:CG2	2.48	0.44
1:G:242:ALA:O	1:G:246[B]:ARG:HG3	2.18	0.44
1:G:286:ALA:O	1:G:290:GLN:HG2	2.18	0.44
1:A:207:ARG:NE	1:A:236:ASP:OD2	2.50	0.44
1:A:255:ILE:HB	1:A:256:PRO:HD3	1.99	0.44
1:A:344:GLU:CD	1:A:344:GLU:H	2.25	0.43
1:G:252:LEU:HD12	1:G:284:ILE:HG12	2.01	0.43
1:G:232:ASP:HB3	1:G:252:LEU:HA	2.01	0.43
1:A:285:LYS:NZ	1:A:289:ASP:OD2	2.41	0.42
1:G:77:LYS:HE2	1:G:77:LYS:HB3	1.58	0.42
1:G:171:ALA:HA	1:G:201:HIS:HB3	2.01	0.42
1:A:170[B]:VAL:HG13	1:A:183:VAL:HG12	2.02	0.42
1:A:152:ARG:O	1:A:152:ARG:HG2	2.20	0.42
1:A:136:LEU:HG	1:A:139:ARG:NH2	2.35	0.41
1:A:171:ALA:HA	1:A:201:HIS:HB3	2.02	0.41
1:A:184:LEU:HA	1:A:184:LEU:HD12	1.78	0.41
1:G:94:GLY:O	1:G:96[B]:ARG:NE	2.49	0.41
1:A:131:TRP:CG	1:A:132:LEU:N	2.89	0.41
1:A:303:LEU:HD11	1:A:306[A]:ILE:HD11	2.02	0.41
1:A:353:ASN:HB2	1:A:354:PRO:HD3	2.01	0.41
1:G:81:GLU:HG2	3:G:401:MPD:O2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:PHE:HB2	1:G:96[B]:ARG:HH21	1.85	0.41
1:G:251:GLY:CA	5:G:547:HOH:O	2.60	0.41
1:G:77:LYS:HD2	1:G:81:GLU:CD	2.45	0.41
1:G:48:GLU:HG2	5:G:588:HOH:O	2.21	0.41
1:G:255:ILE:HB	1:G:327[B]:PHE:HE1	1.85	0.41
1:G:195:GLY:O	1:G:360:PRO:HA	2.21	0.41
1:A:202:THR:HG22	1:A:229:GLY:O	2.21	0.40
1:A:293:THR:HG21	1:A:345:THR:HG23	2.04	0.40
1:G:131:TRP:CG	1:G:132:LEU:N	2.90	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	315/333 (95%)	303 (96%)	11 (4%)	1 (0%)	36	21
1	G	319/333 (96%)	309 (97%)	10 (3%)	0	100	100
All	All	634/666 (95%)	612 (96%)	21 (3%)	1 (0%)	43	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	256/264 (97%)	245 (96%)	11 (4%)	26	6
1	G	260/264 (98%)	241 (93%)	19 (7%)	13	2
All	All	516/528 (98%)	486 (94%)	30 (6%)	19	3

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LYS
1	A	152	ARG
1	A	175	LYS
1	A	184	LEU
1	A	202	THR
1	A	299	SER
1	A	303	LEU
1	A	338	GLU
1	A	343	GLN
1	A	344	GLU
1	A	362	LEU
1	G	47	SER
1	G	51	PHE
1	G	77	LYS
1	G	175	LYS
1	G	184	LEU
1	G	196	VAL
1	G	202	THR
1	G	238	SER
1	G	255	ILE
1	G	278[A]	GLN
1	G	278[B]	GLN
1	G	294	LYS
1	G	299	SER
1	G	303	LEU
1	G	306[A]	ILE
1	G	306[B]	ILE
1	G	338	GLU
1	G	343	GLN
1	G	362	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	KCX	A	169	2,1	10,11,12	1.65	2 (20%)	6,12,14	2.01	2 (33%)
1	KCX	G	169	2,1	10,11,12	2.37	2 (20%)	6,12,14	0.61	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
1	KCX	A	169	2,1	-	1/9/10/12	-
1	KCX	G	169	2,1	-	1/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	169	KCX	CX-NZ	5.87	1.45	1.35
1	A	169	KCX	CX-NZ	4.18	1.42	1.35
1	G	169	KCX	OQ1-CX	4.02	1.29	1.21
1	A	169	KCX	OQ1-CX	2.15	1.25	1.21

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	KCX	OQ1-CX-NZ	-3.56	119.52	124.92
1	A	169	KCX	CE-NZ-CX	-2.25	118.16	121.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	169	KCX	C-CA-CB-CG
1	G	169	KCX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
3	MPD	A	2405	-	7,7,7	0.73	0	9,10,10	0.64	0
3	MPD	G	402	-	7,7,7	0.76	0	9,10,10	0.25	0
3	MPD	A	2404	-	7,7,7	0.79	0	9,10,10	0.64	0
4	CAC	A	2406	2	2,4,4	2.41	2 (100%)	4,6,6	3.08	2 (50%)
4	CAC	G	406	2	2,4,4	2.91	2 (100%)	4,6,6	2.16	2 (50%)
3	MPD	G	405	-	7,7,7	0.81	0	9,10,10	0.64	0
3	MPD	A	2403	-	7,7,7	0.64	0	9,10,10	0.56	0
3	MPD	G	401	-	7,7,7	0.70	0	9,10,10	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	A	2405	-	-	1/5/5/5	-
3	MPD	G	402	-	-	3/5/5/5	-
3	MPD	A	2404	-	-	1/5/5/5	-
3	MPD	G	405	-	-	1/5/5/5	-
3	MPD	A	2403	-	-	5/5/5/5	-
3	MPD	G	401	-	-	3/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	406	CAC	AS-C1	3.02	1.97	1.90
4	G	406	CAC	AS-C2	2.80	1.96	1.90
4	A	2406	CAC	AS-C1	2.53	1.96	1.90
4	A	2406	CAC	AS-C2	2.29	1.95	1.90

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2406	CAC	O1-AS-C1	-5.55	104.60	111.50
4	G	406	CAC	O2-AS-C1	3.09	113.33	105.84
4	A	2406	CAC	O2-AS-C1	2.24	111.26	105.84
4	G	406	CAC	O2-AS-C2	2.10	110.92	105.84

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2403	MPD	C2-C3-C4-C5
3	G	402	MPD	O2-C2-C3-C4
3	G	402	MPD	C2-C3-C4-O4
3	A	2403	MPD	C1-C2-C3-C4
3	A	2403	MPD	CM-C2-C3-C4
3	A	2405	MPD	C2-C3-C4-C5
3	G	401	MPD	C2-C3-C4-C5
3	G	402	MPD	C2-C3-C4-C5
3	G	405	MPD	C2-C3-C4-C5
3	A	2403	MPD	O2-C2-C3-C4
3	A	2403	MPD	C2-C3-C4-O4
3	G	401	MPD	C2-C3-C4-O4
3	A	2404	MPD	C1-C2-C3-C4
3	G	401	MPD	CM-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2405	MPD	1	0
3	A	2403	MPD	1	0
3	G	401	MPD	2	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	315/333 (94%)	0.31	12 (3%)	44 48	7, 20, 39, 64	4 (1%)
1	G	314/333 (94%)	1.23	74 (23%)	2 2	10, 30, 50, 74	9 (2%)
All	All	629/666 (94%)	0.77	86 (13%)	6 7	7, 26, 46, 74	13 (2%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	260	ILE	8.1
1	G	362	LEU	5.8
1	G	37	ILE	5.0
1	A	260	ILE	5.0
1	A	34	GLY	4.7
1	G	34	GLY	4.4
1	A	362	LEU	4.2
1	G	259	ALA	4.0
1	G	276	SER	3.9
1	G	92	ALA	3.9
1	G	277	TRP	3.6
1	G	251	GLY	3.5
1	G	45	THR	3.5
1	A	275	ARG	3.5
1	G	363	ARG	3.3
1	G	204	ALA	3.3
1	G	328	ILE	3.2
1	G	51	PHE	3.2
1	G	278[A]	GLN	3.2
1	G	320	GLY	3.2
1	G	156	TYR	3.1
1	G	306[A]	ILE	3.1
1	A	174	GLY	3.1
1	A	175	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	35	ASP	3.1
1	G	184	LEU	3.0
1	G	319	SER	3.0
1	G	361	THR	3.0
1	G	46	ILE	2.9
1	G	286	ALA	2.9
1	G	36	ARG	2.9
1	G	227	CYS	2.9
1	G	173	THR	2.8
1	G	35	ASP	2.8
1	G	346	LEU	2.7
1	G	349	ILE	2.7
1	A	363	ARG	2.7
1	G	335	PHE	2.7
1	G	330	LEU	2.7
1	G	90	ALA	2.7
1	G	280	ARG	2.7
1	G	327[A]	PHE	2.7
1	G	337	ARG	2.7
1	G	244	ALA	2.7
1	G	331	ARG	2.6
1	G	358	LEU	2.6
1	G	49	ALA	2.6
1	G	326	ALA	2.6
1	G	347	ALA	2.6
1	G	44	ILE	2.6
1	G	96[A]	ARG	2.6
1	G	310	VAL	2.5
1	A	319	SER	2.5
1	G	174	GLY	2.5
1	G	288	ILE	2.5
1	G	279	THR	2.5
1	G	323	ASP	2.4
1	G	255	ILE	2.4
1	G	281	ALA	2.3
1	A	46	ILE	2.3
1	G	316	VAL	2.3
1	G	231	SER	2.3
1	G	235	ASP	2.3
1	G	341	ILE	2.3
1	G	333	ILE	2.2
1	G	89	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	292	TYR	2.2
1	G	52	THR	2.2
1	G	47	SER	2.2
1	G	258	SER	2.2
1	A	259	ALA	2.2
1	G	283	LEU	2.2
1	G	293	THR	2.2
1	G	240	LEU	2.1
1	G	336	LEU	2.1
1	G	202	THR	2.1
1	G	360	PRO	2.1
1	G	296	ILE	2.1
1	G	340	GLY	2.1
1	G	334	PRO	2.1
1	G	50	GLY	2.0
1	G	93	ALA	2.0
1	G	205	SER	2.0
1	A	227	CYS	2.0
1	G	164[A]	ARG	2.0
1	G	250	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	KCX	G	169	12/13	0.91	0.10	20,23,28,30	0
1	KCX	A	169	12/13	0.96	0.06	9,13,15,16	0

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	MPD	G	402	8/8	0.20	0.31	57,61,62,62	0
3	MPD	A	2404	8/8	0.30	0.31	54,60,63,69	0
3	MPD	A	2405	8/8	0.34	0.30	27,48,52,56	0
3	MPD	G	401	8/8	0.47	0.26	35,43,49,51	0
3	MPD	G	405	8/8	0.62	0.23	54,55,56,58	0
4	CAC	A	2406	5/5	0.77	0.32	11,37,40,43	5
3	MPD	A	2403	8/8	0.80	0.15	40,44,50,54	0
4	CAC	G	406	5/5	0.82	0.26	19,32,41,43	5
2	ZN	G	403	1/1	0.94	0.06	21,21,21,21	0
2	ZN	G	404	1/1	0.96	0.06	27,27,27,27	0
2	ZN	A	2401	1/1	0.97	0.05	14,14,14,14	0
2	ZN	A	2402	1/1	0.97	0.04	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.