



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:09 AM UTC

PDB ID : 4NP7 / pdb_00004np7
Title : Structure of phosphotriesterase mutant (S308L/Y309A) from Agrobacterium radiobacter with diethyl thiophosphate bound in the active site
Authors : Jackson, C.J.; Carr, P.D.; Sugrue, E.
Deposited on : 2013-11-20
Resolution : 1.99 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

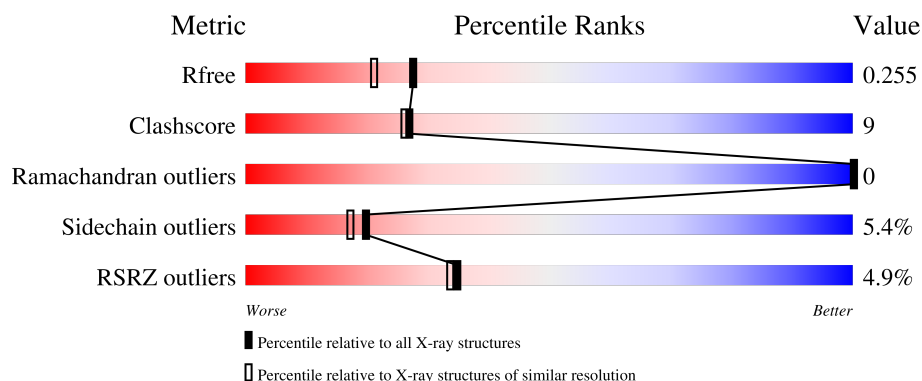
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	329	5% 57% 36% 8%

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
1	KCX	A	169	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2710 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	329	Total	C	N	O	S	0	3	0
			2536	1603	456	468	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	ALA	SER	conflict	UNP Q93LD7
A	265	ASP	ASN	conflict	UNP Q93LD7
A	308	LEU	SER	engineered mutation	UNP Q93LD7
A	309	ALA	TYR	engineered mutation	UNP Q93LD7

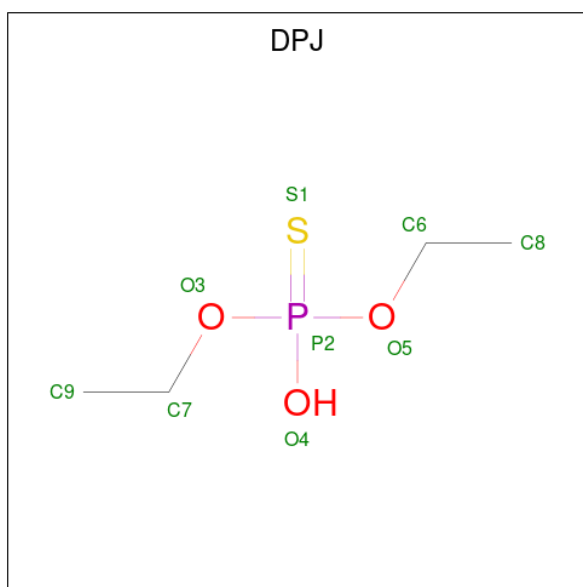
- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Co	0	0
			1	1		

- Molecule 4 is O,O-DIETHYL HYDROGEN THIOPHOSPHATE (CCD ID: DPJ) (formula: C₄H₁₁O₃PS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O	P	S	0	0
			9	4	3	1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

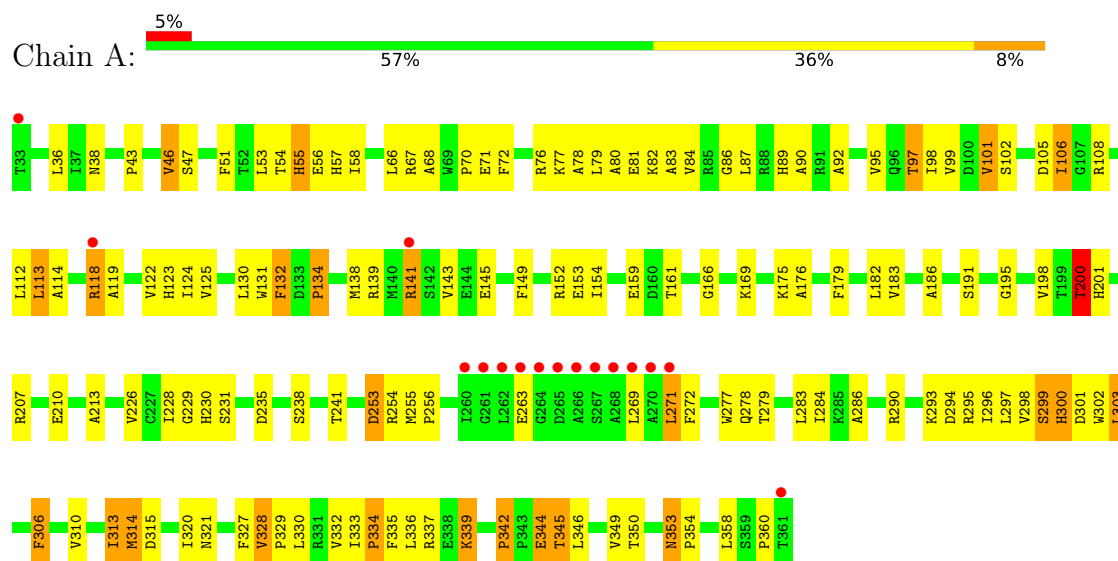
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	159	Total 159	O 159	0	0

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.13Å 109.13Å 63.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.22 – 1.99 28.22 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (28.22-1.99) 98.4 (28.22-1.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.206 , 0.251 0.216 , 0.255	Depositor DCC
R_{free} test set	1510 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2710	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: DPJ, FE2, KCX, EDO, CO

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	2.04	97/2574 (3.8%)	1.24	21/3493 (0.6%)

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	2

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	VAL	C-O	-8.69	1.17	1.24
1	A	118	ARG	C-O	-8.45	1.14	1.24
1	A	149	PHE	C-O	-8.36	1.14	1.24
1	A	353	ASN	C-O	-8.23	1.16	1.24
1	A	152	ARG	C-O	-8.08	1.14	1.24
1	A	92	ALA	C-O	-7.65	1.14	1.24
1	A	278	GLN	C-O	-7.56	1.15	1.24
1	A	77	LYS	C-O	-7.21	1.15	1.24
1	A	78	ALA	C-O	-7.20	1.15	1.24
1	A	166	GLY	C-O	-7.04	1.15	1.23
1	A	66	LEU	C-O	-6.92	1.16	1.24
1	A	283	LEU	C-O	-6.80	1.16	1.24
1	A	159	GLU	C-O	-6.79	1.17	1.24
1	A	80	ALA	C-O	-6.62	1.16	1.24
1	A	255	MET	C-O	-6.57	1.18	1.24
1	A	297	LEU	C-O	-6.55	1.16	1.24
1	A	84	VAL	C-O	-6.53	1.16	1.24
1	A	134	PRO	C-O	-6.53	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	PHE	C-O	-6.53	1.16	1.24
1	A	122	VAL	C-O	-6.51	1.17	1.24
1	A	241	THR	C-O	-6.49	1.16	1.24
1	A	334	PRO	C-O	-6.45	1.16	1.24
1	A	213	ALA	C-O	-6.39	1.16	1.24
1	A	38	ASN	C-O	-6.35	1.16	1.23
1	A	198	VAL	C-O	-6.32	1.17	1.24
1	A	89	HIS	C-O	-6.25	1.16	1.24
1	A	67	ARG	C-O	-6.20	1.17	1.24
1	A	119	ALA	C-O	-6.19	1.16	1.24
1	A	182	LEU	C-O	-6.17	1.17	1.24
1	A	296	ILE	C-O	-6.16	1.17	1.24
1	A	293	LYS	C-O	-6.14	1.16	1.24
1	A	87	LEU	C-N	-6.08	1.25	1.33
1	A	277	TRP	C-O	-6.07	1.17	1.24
1	A	90	ALA	C-O	-6.04	1.17	1.24
1	A	286	ALA	C-O	-6.02	1.17	1.24
1	A	350	THR	C-O	-6.01	1.16	1.24
1	A	207	ARG	C-O	-6.00	1.16	1.23
1	A	86	GLY	C-O	-6.00	1.16	1.23
1	A	95	VAL	C-O	-5.99	1.17	1.24
1	A	183	VAL	C-O	-5.97	1.17	1.24
1	A	114	ALA	C-O	-5.90	1.17	1.24
1	A	138	MET	C-O	-5.88	1.16	1.24
1	A	315	ASP	C-O	-5.84	1.17	1.24
1	A	210	GLU	C-O	-5.78	1.17	1.24
1	A	298	VAL	C-O	-5.76	1.18	1.24
1	A	228	ILE	C-O	-5.74	1.17	1.24
1	A	294	ASP	C-O	-5.69	1.16	1.24
1	A	102	SER	C-O	-5.62	1.17	1.24
1	A	47	SER	C-O	-5.60	1.16	1.24
1	A	112	LEU	C-O	-5.59	1.17	1.24
1	A	76	ARG	C-O	-5.54	1.17	1.24
1	A	176	ALA	C-O	-5.53	1.17	1.23
1	A	53	LEU	C-O	-5.51	1.17	1.24
1	A	301	ASP	C-O	-5.50	1.16	1.23
1	A	43	PRO	C-O	-5.45	1.17	1.23
1	A	82	LYS	C-O	-5.44	1.17	1.24
1	A	295	ARG	C-O	-5.44	1.16	1.24
1	A	179	PHE	C-O	-5.42	1.17	1.24
1	A	130	LEU	C-O	-5.42	1.17	1.23
1	A	143	VAL	C-O	-5.40	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	ILE	C-O	-5.38	1.18	1.24
1	A	108	ARG	C-O	-5.38	1.17	1.23
1	A	36	LEU	C-O	-5.37	1.17	1.23
1	A	300	HIS	C-O	-5.37	1.15	1.23
1	A	55	HIS	C-O	-5.34	1.17	1.23
1	A	342	PRO	C-O	-5.33	1.20	1.24
1	A	81	GLU	C-O	-5.32	1.17	1.24
1	A	154	ILE	C-O	-5.31	1.18	1.24
1	A	125	VAL	C-O	-5.29	1.18	1.24
1	A	290	ARG	C-O	-5.27	1.17	1.24
1	A	101	VAL	C-O	-5.27	1.17	1.24
1	A	70	PRO	C-O	-5.26	1.17	1.24
1	A	97	THR	C-O	-5.25	1.17	1.23
1	A	310	VAL	C-O	-5.25	1.17	1.24
1	A	83	ALA	C-O	-5.22	1.18	1.24
1	A	345	THR	C-O	-5.22	1.18	1.24
1	A	191	SER	C-O	-5.22	1.18	1.24
1	A	186	ALA	C-O	-5.22	1.18	1.24
1	A	284	ILE	C-O	-5.22	1.18	1.24
1	A	279	THR	C-O	-5.21	1.18	1.24
1	A	46	VAL	C-O	-5.19	1.18	1.24
1	A	153	GLU	C-O	-5.16	1.17	1.24
1	A	235	ASP	C-O	-5.11	1.17	1.24
1	A	358	LEU	C-O	-5.11	1.18	1.24
1	A	256	PRO	C-O	-5.11	1.17	1.24
1	A	336	LEU	C-O	-5.10	1.18	1.24
1	A	339	LYS	C-O	-5.09	1.17	1.24
1	A	99	VAL	C-O	-5.09	1.18	1.24
1	A	337	ARG	C-O	-5.08	1.18	1.24
1	A	123	HIS	C-O	-5.07	1.17	1.23
1	A	124	ILE	C-O	-5.07	1.18	1.24
1	A	79	LEU	C-O	-5.06	1.18	1.24
1	A	329	PRO	C-O	-5.05	1.17	1.24
1	A	231	SER	C-O	-5.04	1.17	1.24
1	A	68	ALA	C-O	-5.03	1.18	1.24
1	A	51	PHE	C-O	-5.03	1.18	1.24
1	A	139	ARG	C-O	-5.02	1.17	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	THR	N-CA-C	9.99	123.41	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	VAL	N-CA-C	8.15	118.19	110.53
1	A	68	ALA	N-CA-C	7.31	119.33	111.36
1	A	313	ILE	O-C-N	-7.08	113.80	121.80
1	A	226	VAL	N-CA-C	6.81	117.64	108.11
1	A	330	LEU	N-CA-C	6.21	117.85	111.14
1	A	272	PHE	N-CA-C	6.11	121.01	113.50
1	A	358	LEU	N-CA-C	5.85	117.74	111.36
1	A	200	THR	N-CA-C	5.75	118.43	109.52
1	A	154	ILE	N-CA-C	5.74	116.38	110.82
1	A	132	PHE	N-CA-C	5.59	119.80	113.15
1	A	106	ILE	N-CA-C	-5.56	107.07	112.29
1	A	253	ASP	O-C-N	-5.51	115.52	122.19
1	A	54	THR	N-CA-C	5.49	119.97	113.28
1	A	315	ASP	N-CA-C	5.44	117.25	111.32
1	A	299	SER	N-CA-C	5.33	115.57	108.38
1	A	349	VAL	N-CA-C	5.19	115.41	110.53
1	A	228	ILE	CA-C-N	5.04	127.00	120.64
1	A	228	ILE	C-N-CA	5.04	127.00	120.64
1	A	67	ARG	CA-C-N	5.00	127.39	120.29
1	A	67	ARG	C-N-CA	5.00	127.39	120.29

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	ILE	Mainchain

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	2536	0	2549	47	0
2	A	1	0	0	0	0
3	A	1	0	0	1	0
4	A	9	0	10	0	0
5	A	4	0	6	0	0
6	A	159	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2710	0	2565	47	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 9.

All (47) 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:314[A]:MET:HA	1:A:314[A]:MET:HE2	1.06	1.02
1:A:314[A]:MET:HE2	1:A:314[A]:MET:CA	1.91	1.00
1:A:141:ARG:HG3	1:A:141:ARG:HH11	1.29	0.97
1:A:314[A]:MET:HA	1:A:314[A]:MET:CE	1.96	0.92
1:A:131:TRP:NE1	6:A:659:HOH:O	2.06	0.87
1:A:141:ARG:NH1	1:A:145:GLU:OE1	2.12	0.81
1:A:101:VAL:HB	1:A:169:KCX:HD2	1.64	0.79
1:A:141:ARG:HG3	1:A:141:ARG:NH1	2.05	0.70
1:A:169:KCX:OQ1	6:A:659:HOH:O	2.12	0.67
1:A:230:HIS:HD2	1:A:253:ASP:OD1	1.78	0.65
1:A:344:GLU:CD	1:A:344:GLU:H	2.04	0.65
1:A:169:KCX:OQ2	3:A:402:CO:CO	1.44	0.62
1:A:169:KCX:OQ2	1:A:201:HIS:HB2	2.01	0.60
1:A:300:HIS:CE1	1:A:328:VAL:H	2.21	0.59
1:A:169:KCX:CX	6:A:659:HOH:O	2.51	0.57
1:A:200:THR:O	1:A:229:GLY:HA3	2.05	0.56
1:A:118:ARG:HG2	6:A:612:HOH:O	2.05	0.56
1:A:300:HIS:HE1	1:A:328:VAL:H	1.54	0.56
1:A:141:ARG:NH1	1:A:141:ARG:HA	2.22	0.55
1:A:306:PHE:HB2	1:A:314[A]:MET:HE3	1.89	0.54
1:A:58:ILE:HG13	1:A:113:LEU:HD12	1.90	0.53
1:A:333:ILE:HG23	1:A:346:LEU:HD13	1.91	0.51
1:A:141:ARG:HG3	1:A:145:GLU:OE1	2.10	0.51
1:A:141:ARG:NH1	1:A:141:ARG:CG	2.72	0.50
1:A:169:KCX:OQ2	1:A:230:HIS:HE1	1.95	0.49
1:A:306:PHE:HB2	1:A:314[A]:MET:CE	2.43	0.49
1:A:55:HIS:HD2	6:A:562:HOH:O	1.94	0.48
1:A:131:TRP:CD1	6:A:659:HOH:O	2.57	0.48
1:A:306:PHE:CB	1:A:314[A]:MET:HE3	2.44	0.48
1:A:342:PRO:HG2	1:A:345:THR:OG1	2.14	0.48
1:A:300:HIS:CE1	1:A:328:VAL:HG23	2.48	0.47
1:A:57:HIS:O	1:A:303:LEU:HA	2.14	0.47
1:A:106:ILE:HG22	1:A:106:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:TRP:CH2	1:A:321:ASN:HB3	2.51	0.46
1:A:353:ASN:HB2	1:A:354:PRO:HD3	1.97	0.46
1:A:132:PHE:C	1:A:134:PRO:HD3	2.41	0.45
1:A:195:GLY:O	1:A:360:PRO:HA	2.17	0.45
1:A:55:HIS:C	1:A:56:GLU:HG2	2.43	0.44
1:A:333:ILE:HB	1:A:334:PRO:HD3	2.00	0.44
1:A:169:KCX:OQ2	1:A:201:HIS:ND1	2.51	0.44
1:A:254[B]:ARG:NH2	1:A:271:LEU:O	2.51	0.43
1:A:71:GLU:H	1:A:71:GLU:CD	2.26	0.43
1:A:105:ASP:OD2	1:A:131:TRP:HB3	2.19	0.43
1:A:335:PHE:CZ	1:A:339:LYS:HE2	2.53	0.43
1:A:57:HIS:HB2	1:A:303:LEU:HB3	2.02	0.41
1:A:300:HIS:CE1	1:A:327:PHE:HB3	2.55	0.41
1:A:97:THR:HG22	1:A:98:ILE:N	2.36	0.41

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	329/329 (100%)	324 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	264/261 (101%)	249 (94%)	15 (6%)	18	15

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	VAL
1	A	113	LEU
1	A	141	ARG
1	A	175	LYS
1	A	200	THR
1	A	238	SER
1	A	263	GLU
1	A	269	LEU
1	A	271	LEU
1	A	299	SER
1	A	303	LEU
1	A	306	PHE
1	A	314[A]	MET
1	A	314[B]	MET
1	A	344	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	55	HIS
1	A	206	GLN
1	A	230	HIS
1	A	300	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	KCX	A	169	3,1,2	10,11,12	0.69	0	6,12,14	0.82	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	3,1,2	-	5/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	169	KCX	CG-CD-CE-NZ
1	A	169	KCX	CA-CB-CG-CD
1	A	169	KCX	CE-CD-CG-CB
1	A	169	KCX	OQ1-CX-NZ-CE
1	A	169	KCX	OQ2-CX-NZ-CE

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	169	KCX	7	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
4	DPJ	A	403	3,2	8,8,8	1.10	0	9,10,10	2.09	4 (44%)
5	EDO	A	404	-	3,3,3	0.47	0	2,2,2	0.56	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
4	DPJ	A	403	3,2	-	2/8/8/8	-
5	EDO	A	404	-	-	1/1/1/1	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	DPJ	O3-P2-S1	-3.50	102.97	115.86
4	A	403	DPJ	O4-P2-O3	2.83	119.27	107.09
4	A	403	DPJ	O5-P2-S1	-2.82	105.49	115.86
4	A	403	DPJ	O3-P2-O5	2.35	112.42	102.26

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	DPJ	C6-O5-P2-S1
4	A	403	DPJ	C6-O5-P2-O3
5	A	404	EDO	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	328/329 (99%)	0.43	16 (4%) 35 34	9, 21, 41, 94	3 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	LEU	6.9
1	A	260	ILE	4.9
1	A	262	LEU	4.6
1	A	267	SER	4.5
1	A	33	THR	4.5
1	A	361	THR	4.4
1	A	263	GLU	4.2
1	A	264	GLY	4.1
1	A	269	LEU	3.9
1	A	266	ALA	3.9
1	A	268	ALA	3.8
1	A	261	GLY	3.7
1	A	265	ASP	2.6
1	A	270	ALA	2.6
1	A	141	ARG	2.4
1	A	118	ARG	2.1

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	A	169	12/13	0.82	0.17	15,18,31,35	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
5	EDO	A	404	4/4	0.77	0.27	43,46,51,51	4
4	DPJ	A	403	9/9	0.91	0.15	20,27,30,31	9
2	FE2	A	401	1/1	0.99	0.02	17,17,17,17	0
3	CO	A	402	1/1	0.99	0.04	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.