



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 10:19 am BST

PDB ID : 8H5J
Title : Crystal structure of PETase S121E/A180V/P181V/D186H/N233C/S242T/N246D/S282C mutant from Ideonella sakaiensis
Authors : Lee, S.H.; Seo, H.; Kim, K.-J.
Deposited on : 2022-10-13
Resolution : 1.40 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

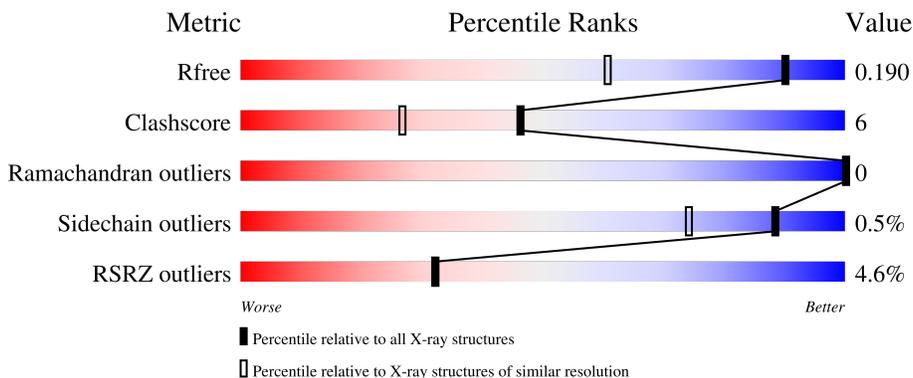
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	300	
1	B	300	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 4688 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(ethylene terephthalate) hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	2075	1275	380	402	18	0	17	0
1	B	262	2066	1267	378	403	18	0	17	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	initiating methionine	UNP A0A0K8P6T7
A	14	GLY	-	expression tag	UNP A0A0K8P6T7
A	15	SER	-	expression tag	UNP A0A0K8P6T7
A	16	SER	-	expression tag	UNP A0A0K8P6T7
A	17	HIS	-	expression tag	UNP A0A0K8P6T7
A	18	HIS	-	expression tag	UNP A0A0K8P6T7
A	19	HIS	-	expression tag	UNP A0A0K8P6T7
A	20	HIS	-	expression tag	UNP A0A0K8P6T7
A	21	HIS	-	expression tag	UNP A0A0K8P6T7
A	22	HIS	-	expression tag	UNP A0A0K8P6T7
A	23	SER	-	expression tag	UNP A0A0K8P6T7
A	24	SER	-	expression tag	UNP A0A0K8P6T7
A	25	GLY	-	expression tag	UNP A0A0K8P6T7
A	26	LEU	-	expression tag	UNP A0A0K8P6T7
A	27	VAL	-	expression tag	UNP A0A0K8P6T7
A	28	PRO	-	expression tag	UNP A0A0K8P6T7
A	29	ARG	-	expression tag	UNP A0A0K8P6T7
A	30	GLY	-	expression tag	UNP A0A0K8P6T7
A	31	SER	-	expression tag	UNP A0A0K8P6T7
A	32	HIS	-	expression tag	UNP A0A0K8P6T7
A	33	MET	-	expression tag	UNP A0A0K8P6T7
A	121	GLU	SER	engineered mutation	UNP A0A0K8P6T7
A	180	VAL	ALA	engineered mutation	UNP A0A0K8P6T7
A	181	VAL	PRO	engineered mutation	UNP A0A0K8P6T7
A	186	HIS	ASP	engineered mutation	UNP A0A0K8P6T7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	233	CYS	ASN	engineered mutation	UNP A0A0K8P6T7
A	242	THR	SER	engineered mutation	UNP A0A0K8P6T7
A	246	ASP	ASN	engineered mutation	UNP A0A0K8P6T7
A	282	CYS	SER	engineered mutation	UNP A0A0K8P6T7
A	291	LEU	-	expression tag	UNP A0A0K8P6T7
A	292	GLU	-	expression tag	UNP A0A0K8P6T7
A	293	ASP	-	expression tag	UNP A0A0K8P6T7
A	294	PRO	-	expression tag	UNP A0A0K8P6T7
A	295	ALA	-	expression tag	UNP A0A0K8P6T7
A	296	ALA	-	expression tag	UNP A0A0K8P6T7
A	297	ASN	-	expression tag	UNP A0A0K8P6T7
A	298	LYS	-	expression tag	UNP A0A0K8P6T7
A	299	ALA	-	expression tag	UNP A0A0K8P6T7
A	300	ARG	-	expression tag	UNP A0A0K8P6T7
A	301	LYS	-	expression tag	UNP A0A0K8P6T7
A	302	GLU	-	expression tag	UNP A0A0K8P6T7
A	303	ALA	-	expression tag	UNP A0A0K8P6T7
A	304	GLU	-	expression tag	UNP A0A0K8P6T7
A	305	LEU	-	expression tag	UNP A0A0K8P6T7
A	306	ALA	-	expression tag	UNP A0A0K8P6T7
A	307	ALA	-	expression tag	UNP A0A0K8P6T7
A	308	ALA	-	expression tag	UNP A0A0K8P6T7
A	309	THR	-	expression tag	UNP A0A0K8P6T7
A	310	ALA	-	expression tag	UNP A0A0K8P6T7
A	311	GLU	-	expression tag	UNP A0A0K8P6T7
A	312	GLN	-	expression tag	UNP A0A0K8P6T7
B	13	MET	-	initiating methionine	UNP A0A0K8P6T7
B	14	GLY	-	expression tag	UNP A0A0K8P6T7
B	15	SER	-	expression tag	UNP A0A0K8P6T7
B	16	SER	-	expression tag	UNP A0A0K8P6T7
B	17	HIS	-	expression tag	UNP A0A0K8P6T7
B	18	HIS	-	expression tag	UNP A0A0K8P6T7
B	19	HIS	-	expression tag	UNP A0A0K8P6T7
B	20	HIS	-	expression tag	UNP A0A0K8P6T7
B	21	HIS	-	expression tag	UNP A0A0K8P6T7
B	22	HIS	-	expression tag	UNP A0A0K8P6T7
B	23	SER	-	expression tag	UNP A0A0K8P6T7
B	24	SER	-	expression tag	UNP A0A0K8P6T7
B	25	GLY	-	expression tag	UNP A0A0K8P6T7
B	26	LEU	-	expression tag	UNP A0A0K8P6T7
B	27	VAL	-	expression tag	UNP A0A0K8P6T7
B	28	PRO	-	expression tag	UNP A0A0K8P6T7

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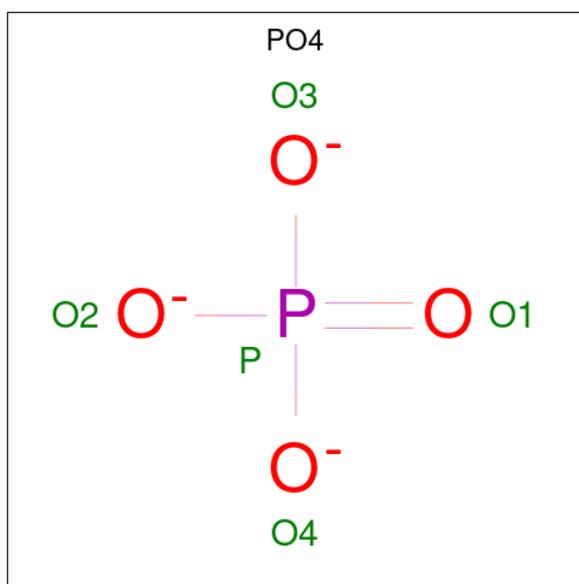
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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	ARG	-	expression tag	UNP A0A0K8P6T7
B	30	GLY	-	expression tag	UNP A0A0K8P6T7
B	31	SER	-	expression tag	UNP A0A0K8P6T7
B	32	HIS	-	expression tag	UNP A0A0K8P6T7
B	33	MET	-	expression tag	UNP A0A0K8P6T7
B	121	GLU	SER	engineered mutation	UNP A0A0K8P6T7
B	180	VAL	ALA	engineered mutation	UNP A0A0K8P6T7
B	181	VAL	PRO	engineered mutation	UNP A0A0K8P6T7
B	186	HIS	ASP	engineered mutation	UNP A0A0K8P6T7
B	233	CYS	ASN	engineered mutation	UNP A0A0K8P6T7
B	242	THR	SER	engineered mutation	UNP A0A0K8P6T7
B	246	ASP	ASN	engineered mutation	UNP A0A0K8P6T7
B	282	CYS	SER	engineered mutation	UNP A0A0K8P6T7
B	291	LEU	-	expression tag	UNP A0A0K8P6T7
B	292	GLU	-	expression tag	UNP A0A0K8P6T7
B	293	ASP	-	expression tag	UNP A0A0K8P6T7
B	294	PRO	-	expression tag	UNP A0A0K8P6T7
B	295	ALA	-	expression tag	UNP A0A0K8P6T7
B	296	ALA	-	expression tag	UNP A0A0K8P6T7
B	297	ASN	-	expression tag	UNP A0A0K8P6T7
B	298	LYS	-	expression tag	UNP A0A0K8P6T7
B	299	ALA	-	expression tag	UNP A0A0K8P6T7
B	300	ARG	-	expression tag	UNP A0A0K8P6T7
B	301	LYS	-	expression tag	UNP A0A0K8P6T7
B	302	GLU	-	expression tag	UNP A0A0K8P6T7
B	303	ALA	-	expression tag	UNP A0A0K8P6T7
B	304	GLU	-	expression tag	UNP A0A0K8P6T7
B	305	LEU	-	expression tag	UNP A0A0K8P6T7
B	306	ALA	-	expression tag	UNP A0A0K8P6T7
B	307	ALA	-	expression tag	UNP A0A0K8P6T7
B	308	ALA	-	expression tag	UNP A0A0K8P6T7
B	309	THR	-	expression tag	UNP A0A0K8P6T7
B	310	ALA	-	expression tag	UNP A0A0K8P6T7
B	311	GLU	-	expression tag	UNP A0A0K8P6T7
B	312	GLN	-	expression tag	UNP A0A0K8P6T7

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

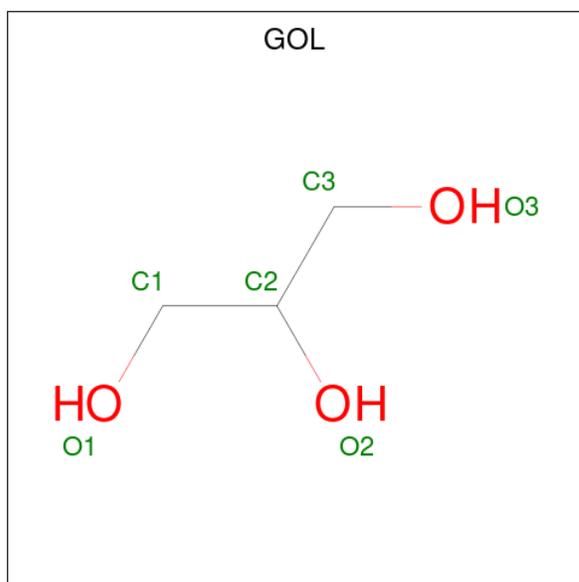
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	2	Total K 2 2	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

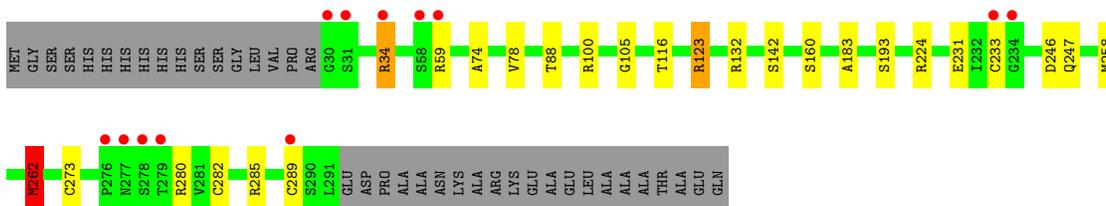
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	251	Total	O	0	0
			251	251		
5	B	272	Total	O	0	0
			272	272		

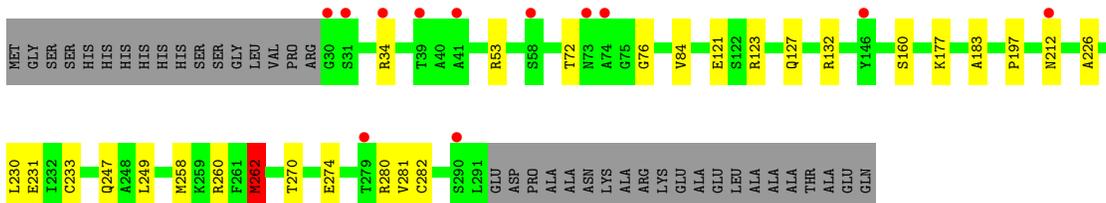
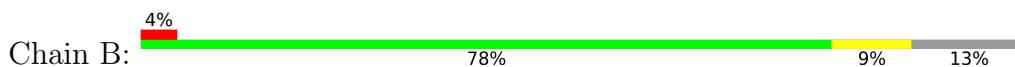
3 Residue-property plots [i](#)

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: Poly(ethylene terephthalate) hydrolase



- Molecule 1: Poly(ethylene terephthalate) hydrolase



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.22Å 50.66Å 80.85Å 90.00° 124.64° 90.00°	Depositor
Resolution (Å)	28.65 – 1.40 28.64 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (28.65-1.40) 98.1 (28.64-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 1.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0350	Depositor
R, R_{free}	0.157 , 0.190 0.158 , 0.190	Depositor DCC
R_{free} test set	4424 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.021 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4688	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 85.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3525e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, K, 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	0.59	0/2121	0.88	4/2880 (0.1%)
1	B	0.56	0/2110	0.89	3/2864 (0.1%)
All	All	0.57	0/4231	0.88	7/5744 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	262[A]	MET	CG-SD-CE	-9.57	84.89	100.20
1	B	262[B]	MET	CG-SD-CE	-9.57	84.89	100.20
1	A	123	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	A	262[A]	MET	CG-SD-CE	-6.80	89.33	100.20
1	A	262[B]	MET	CG-SD-CE	-6.80	89.33	100.20
1	A	285	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	260	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ARG	Sidechain
1	A	132[A]	ARG	Sidechain
1	A	34[A]	ARG	Sidechain
1	B	123	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	2075	0	1988	27	0
1	B	2066	0	1979	24	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	10	0	0	1	0
3	B	5	0	0	0	0
4	B	6	0	8	1	0
5	A	251	0	0	4	0
5	B	272	0	0	6	0
All	All	4688	0	3975	51	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 6.

All (51) 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:34[B]:ARG:HH12	1:A:105:GLY:HA3	1.19	1.03
1:A:231[A]:GLU:OE1	1:A:282[A]:CYS:SG	2.25	0.95
1:A:273:CYS:SG	1:A:289[A]:CYS:HB3	2.12	0.89
1:A:34[B]:ARG:NH2	1:A:74:ALA:HB1	1.90	0.87
1:B:231[B]:GLU:HG2	1:B:282[B]:CYS:SG	2.24	0.78
1:B:249:LEU:HD21	1:B:281:VAL:CG2	2.16	0.76
1:A:34[B]:ARG:NH1	1:A:105:GLY:HA3	2.01	0.74
1:A:233:CYS:SG	1:A:282[A]:CYS:HB3	2.27	0.74
1:A:34[B]:ARG:HH12	1:A:105:GLY:CA	1.98	0.73
1:A:59[A]:ARG:HD3	5:A:729:HOH:O	1.87	0.72
1:A:34[B]:ARG:NH2	1:A:34[B]:ARG:HB3	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:CYS:SG	1:B:282[B]:CYS:HB3	2.34	0.67
1:A:193:SER:HA	1:A:224:ARG:HH11	1.60	0.66
1:A:100:ARG:HH12	1:A:247[B]:GLN:NE2	1.95	0.64
1:A:59[A]:ARG:NE	5:A:503:HOH:O	2.31	0.63
1:B:53[B]:ARG:HG3	1:B:72:THR:CG2	2.29	0.62
1:A:34[B]:ARG:NH1	1:A:78:VAL:HG12	2.15	0.61
1:B:121:GLU:HB2	4:B:403:GOL:H2	1.83	0.61
1:A:100:ARG:NH1	1:A:247[B]:GLN:HE22	2.00	0.60
1:B:249:LEU:HD21	1:B:281:VAL:HG23	1.81	0.60
1:A:258:MET:O	1:A:262[A]:MET:HG3	2.01	0.60
1:A:100:ARG:NH1	1:A:247[B]:GLN:NE2	2.50	0.59
3:A:403:PO4:O3	5:A:501:HOH:O	2.17	0.59
1:A:34[B]:ARG:NH1	5:A:505:HOH:O	2.36	0.59
1:B:258:MET:O	1:B:262[A]:MET:HG3	2.03	0.58
1:A:34[B]:ARG:CZ	1:A:34[B]:ARG:CB	2.82	0.56
1:A:246:ASP:OD1	1:A:280[A]:ARG:HD3	2.08	0.55
1:B:121:GLU:CG	5:B:645:HOH:O	2.56	0.54
1:A:100:ARG:HH12	1:A:247[B]:GLN:CD	2.11	0.53
1:B:121:GLU:HB3	5:B:645:HOH:O	2.09	0.51
1:B:177:LYS:HB2	1:B:262[B]:MET:HG2	1.94	0.49
1:B:233:CYS:HB2	1:B:280[A]:ARG:NH2	2.27	0.49
1:B:233:CYS:HB2	1:B:280[A]:ARG:HH22	1.78	0.48
1:B:121:GLU:CB	5:B:645:HOH:O	2.61	0.48
1:B:230:LEU:HD21	1:B:281:VAL:HG22	1.95	0.48
1:A:34[B]:ARG:CZ	1:A:74:ALA:HB1	2.44	0.47
1:A:142:SER:HA	1:B:247:GLN:OE1	2.15	0.46
1:A:34[B]:ARG:CZ	1:A:78:VAL:HG12	2.46	0.46
1:A:160:SER:HA	1:A:183:ALA:O	2.16	0.45
1:B:121:GLU:HG2	5:B:645:HOH:O	2.16	0.44
1:A:34[B]:ARG:HB3	1:A:34[B]:ARG:CZ	2.45	0.44
1:B:132:ARG:NH1	5:B:511:HOH:O	2.49	0.44
1:A:34[B]:ARG:NH1	1:A:78:VAL:CG1	2.82	0.43
1:A:88:THR:HA	1:A:116:THR:HB	2.00	0.43
1:B:34:ARG:HE	1:B:76:GLY:HA3	1.84	0.42
1:B:270:THR:O	1:B:274:GLU:HB3	2.19	0.42
1:B:249:LEU:CD2	1:B:281:VAL:HG23	2.47	0.42
1:B:84:VAL:HG21	1:B:127:GLN:HB2	2.00	0.42
1:B:197:PRO:HA	1:B:226:ALA:O	2.21	0.41
1:B:160:SER:HA	1:B:183:ALA:O	2.22	0.40
1:B:212[A]:ASN:CG	5:B:503:HOH:O	2.60	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	277/300 (92%)	270 (98%)	7 (2%)	0	100	100
1	B	277/300 (92%)	269 (97%)	8 (3%)	0	100	100
All	All	554/600 (92%)	539 (97%)	15 (3%)	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	226/237 (95%)	224 (99%)	2 (1%)	78	58
1	B	226/237 (95%)	224 (99%)	2 (1%)	78	58
All	All	452/474 (95%)	448 (99%)	4 (1%)	88	58

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	262[A]	MET
1	A	262[B]	MET
1	B	262[A]	MET
1	B	262[B]	MET

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	PO4	A	402	-	4,4,4	1.55	1 (25%)	6,6,6	0.58	0
3	PO4	A	403	-	4,4,4	1.27	1 (25%)	6,6,6	0.71	0
4	GOL	B	403	-	5,5,5	0.26	0	5,5,5	0.73	0
3	PO4	B	402	-	4,4,4	1.99	1 (25%)	6,6,6	0.89	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	GOL	B	403	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	PO4	P-O1	3.85	1.59	1.50
3	A	403	PO4	P-O1	-2.34	1.45	1.50
3	A	402	PO4	P-O1	2.32	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	GOL	C1-C2-C3-O3
4	B	403	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	PO4	1	0
4	B	403	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	262/300 (87%)	0.01	12 (4%) 32 32	11, 17, 28, 51	0
1	B	262/300 (87%)	0.14	12 (4%) 32 32	12, 18, 28, 48	0
All	All	524/600 (87%)	0.07	24 (4%) 32 32	11, 18, 29, 51	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	ALA	5.3
1	A	30	GLY	4.0
1	B	30	GLY	3.8
1	B	58	SER	3.5
1	A	234	GLY	3.1
1	B	34	ARG	3.0
1	A	279	THR	3.0
1	A	31	SER	2.9
1	B	31	SER	2.8
1	A	58[A]	SER	2.5
1	B	73[A]	ASN	2.5
1	B	290	SER	2.4
1	B	279	THR	2.4
1	B	74	ALA	2.4
1	A	233	CYS	2.3
1	A	276	PRO	2.3
1	A	289[A]	CYS	2.2
1	A	59[A]	ARG	2.1
1	A	34[A]	ARG	2.1
1	A	278	SER	2.1
1	B	146	TYR	2.0
1	B	39	THR	2.0
1	A	277	ASN	2.0
1	B	212[A]	ASN	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 monosaccharides 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(Å ²)	Q<0.9
4	GOL	B	403	6/6	0.88	0.21	26,36,38,59	0
3	PO4	B	402	5/5	0.93	0.21	27,32,36,41	0
2	K	B	404	1/1	0.97	0.20	43,43,43,43	0
3	PO4	A	403	5/5	0.97	0.25	22,27,32,35	0
2	K	B	401	1/1	0.98	0.06	26,26,26,26	0
3	PO4	A	402	5/5	0.99	0.21	25,27,32,36	0
2	K	A	401	1/1	0.99	0.04	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.