



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 03:39 PM EST

PDB ID : 3KDR  
Title : The Crystal Structure of a HK97 Family Phage Portal Protein from *Corynebacterium diphtheriae* to 2.9Å  
Authors : Nocek, B.; Stein, A.J.; Mulligan, R.; Duggan, E.; Abdullah, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2009-10-23  
Resolution : 2.90 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

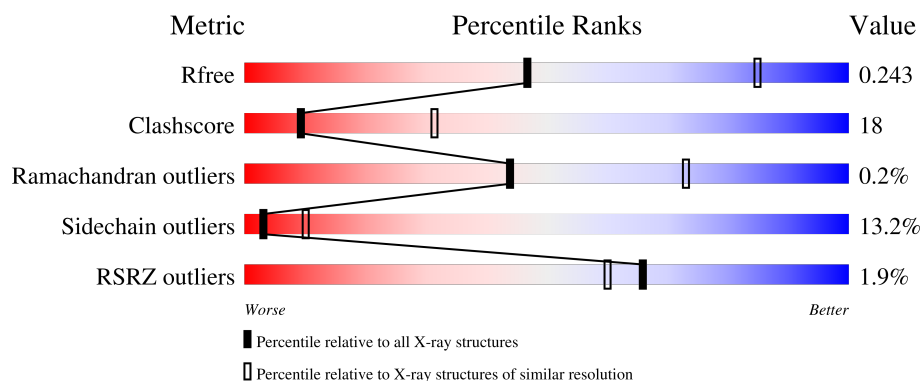
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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  $\geq 3$ , 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	310	<div> <div>2%</div> <div>64% 22% 5% 8%</div> </div>
1	B	310	<div> <div>%</div> <div>57% 29% 5% 9%</div> </div>
1	C	310	<div> <div>2%</div> <div>65% 23% • 7%</div> </div>

## 2 Entry composition [i](#)

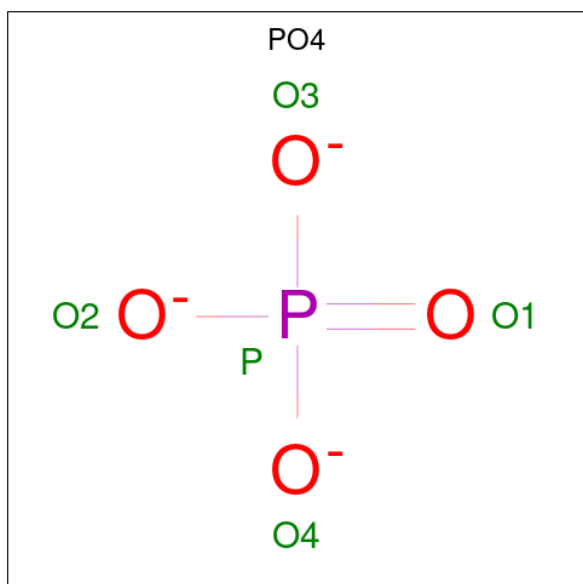
There are 5 unique types of molecules in this entry. The entry contains 6311 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HK97 Family Phage Portal Protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	Se	0	0	0
			2087	1305	373	397	4	8			
1	B	283	Total	C	N	O	S	Se	0	0	0
			2085	1303	375	395	4	8			
1	C	287	Total	C	N	O	S	Se	0	0	0
			2106	1317	377	400	4	8			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



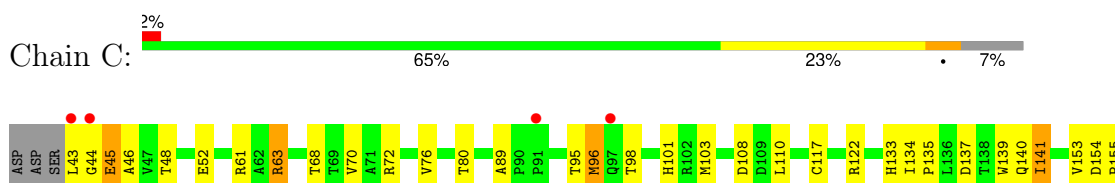
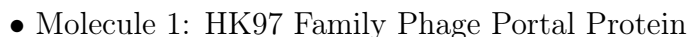
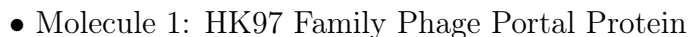
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

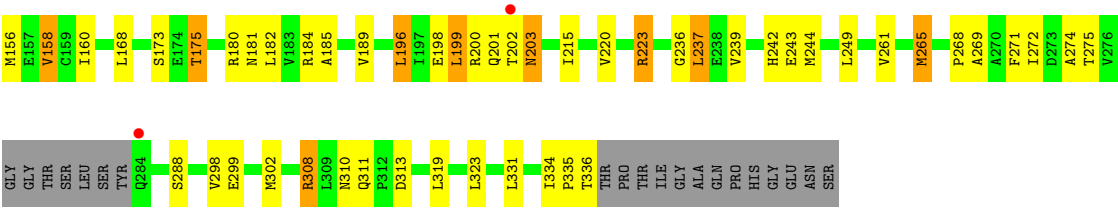
- Molecule 5 is water.

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



- Molecule 1: HK97 Family Phage Portal Protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	F 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	340.07Å 340.07Å 340.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.25 – 2.90 36.25 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (36.25-2.90) 98.4 (36.25-2.90)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.90Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0102	Depositor
R, $R_{free}$	0.198 , 0.245 0.198 , 0.243	Depositor DCC
$R_{free}$ test set	1854 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 29.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6311	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, GOL, SO4

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	0.97	0/2117	0.91	2/2886 (0.1%)
1	B	1.03	1/2113 (0.0%)	0.91	1/2878 (0.0%)
1	C	1.05	0/2136	0.91	1/2911 (0.0%)
All	All	1.02	1/6366 (0.0%)	0.91	4/8675 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77	CYS	CB-SG	-8.47	1.67	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	154	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	211	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	C	141	ILE	CB-CA-C	-5.20	101.19	111.60

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	2087	0	2049	91	0
1	B	2085	0	2052	88	0
1	C	2106	0	2071	72	0
2	A	5	0	0	1	0
2	C	5	0	0	1	0
3	A	6	0	8	2	0
3	B	6	0	8	3	0
4	B	5	0	0	0	0
4	C	5	0	0	1	0
5	A	1	0	0	0	0
All	All	6311	0	6188	223	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 18.

All (223) 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:C:202:THR:HG22	1:C:236:GLY:O	1.36	1.21
1:A:201:GLN:HG2	1:B:234:SER:O	1.42	1.14
1:B:97:GLN:HE22	1:B:133:HIS:N	1.51	1.07
1:B:97:GLN:NE2	1:B:133:HIS:H	1.56	1.03
1:C:43:LEU:HD12	1:C:52:GLU:HG2	1.49	0.94
1:A:97:GLN:HE22	1:A:133:HIS:H	0.95	0.92
1:B:310:ASN:HD21	1:B:323:LEU:H	1.17	0.90
1:B:285:ASN:HD22	1:B:285:ASN:H	1.21	0.87
1:A:201:GLN:CG	1:B:234:SER:O	2.22	0.86
1:B:69:THR:O	1:B:73:THR:HG23	1.75	0.84
1:A:227:ASN:O	1:A:230:VAL:HG23	1.77	0.83
1:C:43:LEU:HD12	1:C:52:GLU:CG	2.08	0.82
1:C:98:THR:OG1	1:C:101:HIS:HD2	1.62	0.82
1:B:185:ALA:O	1:B:189:VAL:HG13	1.81	0.81
1:C:215:ILE:HD12	1:C:237:LEU:HD22	1.62	0.80
1:C:199:LEU:HD23	1:C:237:LEU:HD21	1.63	0.79
1:A:97:GLN:NE2	1:A:133:HIS:H	1.77	0.79
1:A:310:ASN:HD21	1:A:323:LEU:H	1.32	0.77
1:B:64:ASN:O	1:B:68:THR:HB	1.86	0.76
1:A:97:GLN:HE22	1:A:133:HIS:N	1.80	0.76
1:A:235:SER:OG	1:C:201:GLN:HB3	1.85	0.76
1:C:269:ALA:HB1	1:C:274:ALA:HB3	1.68	0.75
1:B:285:ASN:HD22	1:B:285:ASN:N	1.83	0.75
1:C:223:ARG:HH11	1:C:223:ARG:HG2	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ARG:HD2	1:C:243:GLU:OE2	1.87	0.74
1:B:315:HIS:HE1	1:B:321:ASN:O	1.69	0.74
1:C:95:THR:HG23	1:C:95:THR:O	1.88	0.73
1:A:165:HIS:HD2	1:A:167:GLY:H	1.36	0.73
1:B:299:GLU:OE2	1:B:302:MSE:HE3	1.89	0.72
1:C:43:LEU:HB3	1:C:44:GLY:HA3	1.72	0.72
1:B:299:GLU:CD	1:B:302:MSE:CE	2.58	0.72
1:A:180:ARG:O	1:A:183:VAL:HG12	1.90	0.72
1:B:299:GLU:OE2	1:B:302:MSE:CE	2.38	0.71
1:A:299:GLU:CD	1:A:302:MSE:CE	2.59	0.70
1:B:226:ARG:C	1:B:227:ASN:HD22	1.95	0.70
1:C:98:THR:OG1	1:C:101:HIS:CD2	2.45	0.69
1:A:201:GLN:NE2	1:B:234:SER:O	2.26	0.68
1:A:216:ILE:O	1:A:220:VAL:HG23	1.93	0.68
1:A:182:LEU:CD2	1:A:254:ARG:HA	2.22	0.68
1:A:240:HIS:HD2	3:A:350:GOL:H2	1.59	0.68
1:B:301:LEU:O	1:B:305:ILE:HG13	1.95	0.67
1:B:97:GLN:HE22	1:B:133:HIS:H	0.75	0.67
1:B:299:GLU:CD	1:B:302:MSE:HE2	2.14	0.67
1:C:43:LEU:O	1:C:184:ARG:NH2	2.28	0.67
1:A:202:THR:OG1	1:A:236:GLY:C	2.34	0.66
1:B:232:PHE:CE2	1:B:234:SER:HA	2.31	0.66
1:B:268:PRO:HG2	1:B:271:PHE:CD2	2.32	0.65
1:C:45:GLU:HG2	1:C:46:ALA:N	2.10	0.65
1:A:165:HIS:CD2	1:A:167:GLY:H	2.13	0.65
1:B:213:ASP:O	1:B:217:ASN:ND2	2.25	0.65
1:B:216:ILE:O	1:B:220:VAL:HG23	1.97	0.65
1:A:227:ASN:O	1:A:230:VAL:CG2	2.45	0.65
1:B:148:VAL:HG23	1:B:153:VAL:HG21	1.78	0.65
1:A:243:GLU:OE1	1:B:223:ARG:NH1	2.30	0.64
1:C:45:GLU:O	1:C:180:ARG:NH2	2.30	0.64
1:B:123:ASP:O	1:B:124:GLU:C	2.36	0.64
1:A:287:ALA:O	1:A:291:ILE:HG13	1.97	0.63
1:A:63:ARG:HH11	1:A:64:ASN:ND2	1.96	0.63
1:A:57:PRO:HG3	1:C:175:THR:HG21	1.80	0.62
1:A:299:GLU:HA	1:A:302:MSE:HE2	1.79	0.62
1:B:199:LEU:HB3	1:B:237:LEU:HD21	1.82	0.61
1:A:208:SER:H	1:A:211:ASP:HB2	1.64	0.61
1:C:261:VAL:O	1:C:265:MSE:HG3	2.01	0.60
1:A:201:GLN:HG2	1:B:234:SER:C	2.21	0.60
1:B:50:ARG:HD2	1:B:112:PHE:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASP:OD1	1:A:155:PRO:HD2	2.01	0.60
1:A:122:ARG:NH2	1:A:313:ASP:O	2.35	0.60
1:B:69:THR:O	1:B:73:THR:CG2	2.50	0.59
1:A:209:PRO:O	1:A:213:ASP:HB2	2.01	0.59
1:B:299:GLU:HA	1:B:302:MSE:HE2	1.85	0.58
1:B:285:ASN:H	1:B:285:ASN:ND2	1.99	0.58
1:A:290:MSE:O	1:A:294:VAL:HG23	2.04	0.58
1:B:310:ASN:HD21	1:B:323:LEU:N	1.94	0.58
1:B:168:LEU:CD1	1:B:265:MSE:HE3	2.34	0.58
1:A:63:ARG:HH11	1:A:64:ASN:HD22	1.51	0.58
1:C:201:GLN:HG2	1:C:237:LEU:HD12	1.85	0.58
1:C:154:ASP:OD2	1:C:155:PRO:HD2	2.05	0.56
1:A:214:ARG:O	1:A:217:ASN:HB2	2.05	0.56
1:C:133:HIS:ND1	4:C:3:SO4:O1	2.34	0.56
1:A:299:GLU:CD	1:A:302:MSE:HE2	2.25	0.56
2:A:1:PO4:O1	2:C:2:PO4:O4	2.23	0.56
1:C:63:ARG:NH2	1:C:108:ASP:OD2	2.39	0.56
1:A:182:LEU:HD21	1:A:254:ARG:N	2.21	0.55
1:B:240:HIS:HD2	3:B:2:GOL:H32	1.71	0.55
1:B:240:HIS:HD2	3:B:2:GOL:C3	2.19	0.55
1:A:240:HIS:CD2	3:A:350:GOL:H2	2.42	0.55
1:C:223:ARG:HG2	1:C:223:ARG:NH1	2.17	0.55
1:C:202:THR:CG2	1:C:236:GLY:O	2.31	0.55
1:A:234:SER:O	1:A:236:GLY:N	2.25	0.55
1:A:195:ALA:HB2	1:B:191:GLN:O	2.08	0.54
1:B:73:THR:HG22	1:B:330:LEU:HD11	1.89	0.54
1:C:199:LEU:CD2	1:C:237:LEU:HD21	2.34	0.54
1:A:189:VAL:HG12	1:C:249:LEU:CD1	2.37	0.54
1:A:311:GLN:NE2	1:B:96:MSE:HE2	2.21	0.54
1:B:202:THR:OG1	1:B:236:GLY:O	2.23	0.54
1:A:97:GLN:HE21	1:A:102:ARG:HB2	1.73	0.54
1:B:180:ARG:HD3	1:B:184:ARG:CZ	2.38	0.54
1:A:57:PRO:CG	1:C:175:THR:HG21	2.38	0.53
1:C:168:LEU:HD11	1:C:265:MSE:HE3	1.90	0.53
1:A:235:SER:OG	1:C:201:GLN:CB	2.55	0.53
1:B:134:ILE:HD12	1:B:138:THR:HG22	1.89	0.53
1:B:285:ASN:N	1:B:285:ASN:ND2	2.55	0.53
1:C:117:CYS:SG	1:C:158:VAL:HG22	2.48	0.53
1:A:331:LEU:CD1	1:B:335:PRO:HB2	2.39	0.53
1:A:148:VAL:O	1:A:148:VAL:CG2	2.56	0.52
1:A:96:MSE:HE1	1:C:311:GLN:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ASP:OD2	1:B:313:ASP:N	2.42	0.52
1:A:83:PRO:HB2	1:A:129:ILE:HA	1.92	0.52
1:A:319:LEU:HD12	1:A:319:LEU:H	1.75	0.52
1:A:234:SER:C	1:A:236:GLY:H	2.08	0.52
1:A:182:LEU:HD23	1:A:254:ARG:HA	1.90	0.52
1:B:315:HIS:CE1	1:B:321:ASN:O	2.59	0.52
1:B:189:VAL:HG23	1:B:189:VAL:O	2.09	0.51
1:C:299:GLU:CD	1:C:302:MSE:CE	2.79	0.51
1:B:63:ARG:HD3	1:B:63:ARG:C	2.30	0.51
1:B:144:ASN:C	1:B:144:ASN:OD1	2.50	0.51
1:C:117:CYS:HB2	1:C:139:TRP:CE2	2.46	0.50
1:A:242:HIS:NE2	1:B:239:VAL:HG22	2.26	0.50
1:B:82:PRO:HG3	1:B:315:HIS:CD2	2.47	0.50
1:A:202:THR:N	1:A:236:GLY:O	2.31	0.50
1:B:137:ASP:C	1:B:137:ASP:OD1	2.50	0.50
1:B:227:ASN:N	1:B:227:ASN:ND2	2.59	0.50
1:A:202:THR:OG1	1:A:236:GLY:HA2	2.11	0.50
1:B:235:SER:O	1:B:235:SER:OG	2.30	0.50
1:A:242:HIS:CE1	1:B:239:VAL:HG22	2.47	0.50
1:C:185:ALA:O	1:C:189:VAL:HG23	2.12	0.50
1:B:240:HIS:CD2	3:B:2:GOL:H32	2.47	0.49
1:B:73:THR:CG2	1:B:330:LEU:HD11	2.42	0.49
1:B:168:LEU:HD11	1:B:265:MSE:HE3	1.93	0.49
1:A:146:VAL:O	1:A:153:VAL:HG12	2.11	0.49
1:C:308:ARG:NH2	1:C:313:ASP:OD2	2.38	0.49
1:B:141:ILE:HG22	1:B:142:GLU:O	2.12	0.49
1:C:45:GLU:HG2	1:C:46:ALA:H	1.76	0.49
1:A:276:VAL:O	1:A:277:GLY:C	2.52	0.49
1:A:85:VAL:HB	1:A:86:PRO:HD3	1.95	0.49
1:A:218:GLY:O	1:A:221:ALA:HB3	2.13	0.49
1:B:175:THR:HG21	1:B:260:ASP:HB3	1.95	0.48
1:B:233:SER:HB3	1:B:237:LEU:HB3	1.94	0.48
1:C:45:GLU:CG	1:C:46:ALA:H	2.26	0.48
1:C:48:THR:N	1:C:52:GLU:OE1	2.38	0.48
1:C:334:ILE:HG22	1:C:335:PRO:O	2.13	0.48
1:C:299:GLU:HA	1:C:302:MSE:HE2	1.96	0.48
1:A:68:THR:O	1:A:72:ARG:HG3	2.14	0.47
1:A:202:THR:OG1	1:A:236:GLY:CA	2.62	0.47
1:B:203:ASN:OD1	1:B:203:ASN:C	2.51	0.47
1:A:299:GLU:N	1:A:300:PRO:HD2	2.29	0.47
1:B:310:ASN:ND2	1:B:323:LEU:H	2.00	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLN:HA	1:A:236:GLY:O	2.15	0.47
1:C:95:THR:O	1:C:95:THR:CG2	2.57	0.47
1:C:43:LEU:CD1	1:C:52:GLU:OE2	2.63	0.47
1:A:233:SER:HB2	1:C:200:ARG:HA	1.97	0.47
1:B:308:ARG:HD2	1:B:308:ARG:HA	1.73	0.47
1:C:45:GLU:CG	1:C:46:ALA:N	2.77	0.47
1:C:202:THR:HG22	1:C:236:GLY:C	2.25	0.47
1:A:195:ALA:HB3	1:A:243:GLU:HB2	1.96	0.46
1:A:219:TYR:OH	1:C:196:LEU:HD22	2.15	0.46
1:A:269:ALA:HB1	1:A:274:ALA:HB3	1.97	0.46
1:A:204:ASN:OD1	1:A:204:ASN:N	2.47	0.46
1:B:267:VAL:HG23	1:B:268:PRO:HD2	1.98	0.46
1:B:182:LEU:HD22	1:B:254:ARG:HA	1.97	0.46
1:A:96:MSE:HE3	1:C:311:GLN:CD	2.36	0.46
1:A:299:GLU:OE1	1:A:302:MSE:CE	2.62	0.46
1:C:68:THR:O	1:C:72:ARG:HG3	2.15	0.46
1:C:298:VAL:HG12	1:C:302:MSE:HG3	1.98	0.46
1:A:238:GLU:OE1	1:A:240:HIS:HE1	1.99	0.46
1:A:82:PRO:HA	1:A:83:PRO:HD3	1.86	0.45
1:A:201:GLN:CD	1:B:234:SER:O	2.55	0.45
1:B:139:TRP:O	1:B:140:GLN:HG2	2.16	0.45
1:C:122:ARG:NH1	1:C:156:MSE:HG3	2.30	0.45
1:B:84:PHE:CE2	1:B:314:MSE:HE3	2.51	0.45
1:C:201:GLN:HE22	1:C:203:ASN:HB2	1.82	0.45
1:B:135:PRO:O	1:B:138:THR:HB	2.16	0.45
1:B:123:ASP:CB	1:B:129:ILE:HD11	2.46	0.45
1:B:139:TRP:C	1:B:140:GLN:HG2	2.37	0.45
1:A:148:VAL:HG23	1:A:149:ASN:ND2	2.32	0.45
1:A:195:ALA:HB3	1:A:243:GLU:CB	2.47	0.45
1:A:219:TYR:CE2	1:C:196:LEU:HD22	2.51	0.45
1:A:299:GLU:CD	1:A:302:MSE:HE1	2.37	0.45
1:C:70:VAL:HG12	1:C:103:MSE:HG3	1.99	0.45
1:A:182:LEU:HD21	1:A:254:ARG:CA	2.47	0.44
1:B:223:ARG:C	1:B:225:GLY:H	2.21	0.44
1:C:61:ARG:HG3	1:C:272:ILE:HG22	1.99	0.44
1:A:96:MSE:HE3	1:C:311:GLN:OE1	2.16	0.44
1:A:311:GLN:HE21	1:B:96:MSE:HE2	1.82	0.44
1:A:331:LEU:HD11	1:B:335:PRO:HB2	1.99	0.44
1:A:141:ILE:O	1:A:141:ILE:HG23	2.17	0.44
1:B:54:LEU:HD22	1:B:60:LEU:HD13	1.99	0.44
1:A:96:MSE:CE	1:C:311:GLN:CD	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:TYR:CZ	1:C:196:LEU:HD22	2.53	0.44
1:B:227:ASN:HD22	1:B:227:ASN:N	2.14	0.44
1:C:96:MSE:HE2	1:C:96:MSE:HB3	1.85	0.43
1:C:198:GLU:OE1	1:C:242:HIS:HE1	2.02	0.43
1:A:219:TYR:CE2	1:C:196:LEU:CD2	3.02	0.43
1:C:265:MSE:HE2	1:C:265:MSE:HB3	1.85	0.43
1:B:97:GLN:NE2	1:B:133:HIS:N	2.35	0.43
1:B:294:VAL:O	1:B:299:GLU:HB2	2.18	0.43
1:B:50:ARG:HD2	1:B:112:PHE:CG	2.54	0.42
1:A:110:LEU:HD23	1:A:110:LEU:HA	1.93	0.42
1:C:140:GLN:HG3	1:C:141:ILE:N	2.34	0.42
1:B:117:CYS:HB2	1:B:139:TRP:CE2	2.54	0.42
1:B:267:VAL:HG22	1:B:268:PRO:N	2.35	0.42
1:C:122:ARG:NH1	1:C:156:MSE:O	2.47	0.42
1:C:268:PRO:O	1:C:271:PHE:HB2	2.19	0.42
1:A:122:ARG:HH22	1:A:313:ASP:HB2	1.85	0.42
1:A:58:ALA:HB1	1:A:272:ILE:HD12	2.02	0.42
1:C:160:ILE:O	1:C:308:ARG:HD3	2.19	0.42
1:C:201:GLN:NE2	1:C:203:ASN:HB2	2.35	0.42
1:C:299:GLU:CD	1:C:302:MSE:HE2	2.41	0.42
1:B:169:LEU:HD23	1:B:169:LEU:HA	1.86	0.41
1:B:290:MSE:O	1:B:294:VAL:HG23	2.19	0.41
1:C:310:ASN:HD21	1:C:323:LEU:H	1.67	0.41
1:B:134:ILE:O	1:B:134:ILE:HG13	2.19	0.41
1:C:89:ALA:CB	1:C:95:THR:O	2.68	0.41
1:A:285:ASN:O	1:A:286:ALA:C	2.60	0.41
1:C:181:ASN:HD22	1:C:181:ASN:HA	1.67	0.41
1:A:238:GLU:OE1	1:A:240:HIS:CE1	2.74	0.40
1:B:142:GLU:O	1:B:143:GLU:C	2.57	0.40
1:B:269:ALA:HB1	1:B:274:ALA:HB3	2.03	0.40
1:A:94:ALA:O	1:C:308:ARG:NH1	2.54	0.40
1:A:285:ASN:ND2	1:A:285:ASN:H	2.19	0.40
1:B:89:ALA:HA	1:B:90:PRO:HD3	1.85	0.40
1:C:134:ILE:HA	1:C:135:PRO:HD3	1.90	0.40
1:A:299:GLU:OE1	1:A:302:MSE:HE2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	281/310 (91%)	264 (94%)	16 (6%)	1 (0%)	30	60
1	B	277/310 (89%)	263 (95%)	13 (5%)	1 (0%)	30	60
1	C	283/310 (91%)	274 (97%)	9 (3%)	0	100	100
All	All	841/930 (90%)	801 (95%)	38 (4%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	SER
1	B	142	GLU

### 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	214/235 (91%)	190 (89%)	24 (11%)	5	16
1	B	215/235 (92%)	181 (84%)	34 (16%)	2	6
1	C	216/235 (92%)	189 (88%)	27 (12%)	3	12
All	All	645/705 (92%)	560 (87%)	85 (13%)	3	10

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	PRO

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Mol	Chain	Res	Type
1	A	63	ARG
1	A	81	LEU
1	A	87	VAL
1	A	96	MSE
1	A	125	SER
1	A	147	ARG
1	A	148	VAL
1	A	175	THR
1	A	180	ARG
1	A	201	GLN
1	A	202	THR
1	A	204	ASN
1	A	206	GLN
1	A	207	LEU
1	A	208	SER
1	A	214	ARG
1	A	216	ILE
1	A	223	ARG
1	A	234	SER
1	A	275	THR
1	A	285	ASN
1	A	319	LEU
1	A	323	LEU
1	B	50	ARG
1	B	65	LEU
1	B	73	THR
1	B	76	VAL
1	B	80	THR
1	B	96	MSE
1	B	115	VAL
1	B	120	LEU
1	B	122	ARG
1	B	127	THR
1	B	129	ILE
1	B	138	THR
1	B	140	GLN
1	B	141	ILE
1	B	144	ASN
1	B	147	ARG
1	B	158	VAL
1	B	175	THR
1	B	182	LEU

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Mol	Chain	Res	Type
1	B	200	ARG
1	B	208	SER
1	B	210	ASP
1	B	212	VAL
1	B	227	ASN
1	B	228	SER
1	B	235	SER
1	B	237	LEU
1	B	239	VAL
1	B	275	THR
1	B	276	VAL
1	B	285	ASN
1	B	288	SER
1	B	336	THR
1	B	337	THR
1	C	45	GLU
1	C	63	ARG
1	C	76	VAL
1	C	80	THR
1	C	96	MSE
1	C	110	LEU
1	C	137	ASP
1	C	153	VAL
1	C	158	VAL
1	C	173	SER
1	C	175	THR
1	C	182	LEU
1	C	196	LEU
1	C	199	LEU
1	C	203	ASN
1	C	220	VAL
1	C	223	ARG
1	C	237	LEU
1	C	239	VAL
1	C	244	MSE
1	C	265	MSE
1	C	275	THR
1	C	288	SER
1	C	308	ARG
1	C	319	LEU
1	C	331	LEU
1	C	336	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	97	GLN
1	A	149	ASN
1	A	165	HIS
1	A	171	HIS
1	A	206	GLN
1	A	240	HIS
1	A	285	ASN
1	A	310	ASN
1	A	311	GLN
1	A	321	ASN
1	B	97	GLN
1	B	149	ASN
1	B	192	ASN
1	B	201	GLN
1	B	227	ASN
1	B	240	HIS
1	B	285	ASN
1	B	310	ASN
1	B	315	HIS
1	C	64	ASN
1	C	101	HIS
1	C	181	ASN
1	C	242	HIS
1	C	310	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

6 ligands 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	$\# Z  > 2$
3	GOL	B	2	-	5,5,5	0.59	0	5,5,5	1.52	0
2	PO4	A	1	-	4,4,4	0.94	0	6,6,6	1.17	1 (16%)
4	SO4	B	4	-	4,4,4	0.34	0	6,6,6	0.38	0
3	GOL	A	350	-	5,5,5	0.57	0	5,5,5	1.12	1 (20%)
4	SO4	C	3	-	4,4,4	0.30	0	6,6,6	0.50	0
2	PO4	C	2	-	4,4,4	0.84	0	6,6,6	1.04	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	GOL	B	2	-	-	2/4/4/4	-
3	GOL	A	350	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	PO4	O4-P-O2	2.32	115.13	107.91
3	A	350	GOL	O2-C2-C3	2.02	117.53	109.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2	GOL	C1-C2-C3-O3
3	A	350	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	350	GOL	C1-C2-C3-O3
3	B	2	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	GOL	3	0
2	A	1	PO4	1	0
3	A	350	GOL	2	0
4	C	3	SO4	1	0
2	C	2	PO4	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	277/310 (89%)	-0.32	6 (2%) 62 55	2, 16, 27, 32	0
1	B	275/310 (88%)	-0.51	4 (1%) 71 66	2, 14, 25, 34	0
1	C	279/310 (90%)	-0.48	6 (2%) 62 55	2, 16, 24, 34	0
All	All	831/930 (89%)	-0.44	16 (1%) 66 60	2, 16, 26, 34	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	44	GLY	4.1
1	C	43	LEU	4.0
1	A	272	ILE	3.9
1	C	91	PRO	3.0
1	B	94	ALA	2.9
1	C	202	THR	2.8
1	C	284	GLN	2.7
1	A	230	VAL	2.4
1	B	97	GLN	2.4
1	A	150	GLY	2.3
1	B	121	ASP	2.2
1	A	204	ASN	2.2
1	A	143	GLU	2.1
1	A	284	GLN	2.1
1	B	142	GLU	2.1
1	C	97	GLN	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, 95<sup>th</sup> 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	GOL	A	350	6/6	0.75	0.24	58,61,62,62	0
2	PO4	A	1	5/5	0.78	0.19	78,79,82,83	0
2	PO4	C	2	5/5	0.79	0.15	77,77,78,81	0
4	SO4	B	4	5/5	0.84	0.23	101,101,102,102	0
4	SO4	C	3	5/5	0.91	0.13	76,78,80,80	0
3	GOL	B	2	6/6	0.92	0.14	45,47,51,55	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.