



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:19 pm BST

PDB ID : 3SPE  
Title : Crystal structure of the tail sheath protein protease resistant fragment from bacteriophage phiKZ  
Authors : Aksyuk, A.A.; Kurochkina, L.P.; Fokine, A.; Mesyanzhinov, V.V.; Rossmann, M.G.  
Deposited on : 2011-07-01  
Resolution : 2.40 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](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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

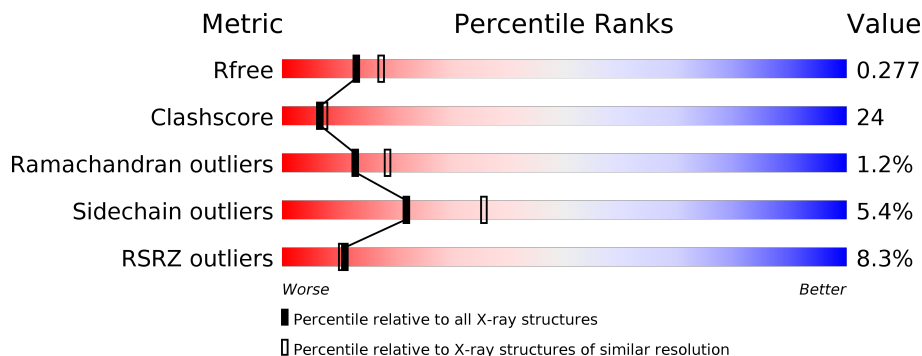
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	295	
1	B	295	

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
2	PO4	A	1	-	-	X	X
2	PO4	A	3	-	-	X	X

## 2 Entry composition [i](#)

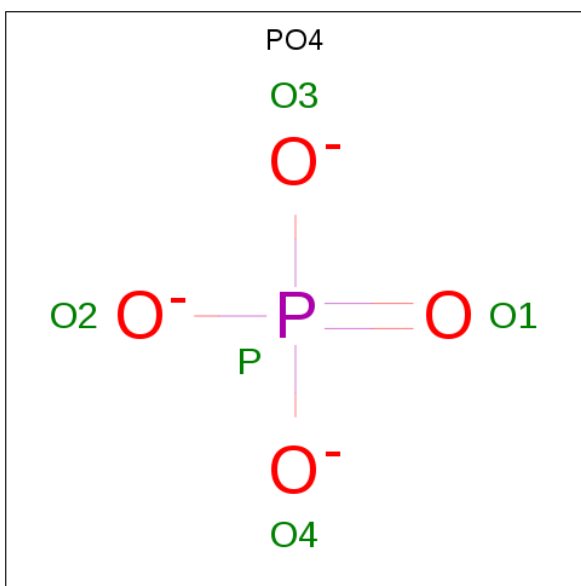
There are 4 unique types of molecules in this entry. The entry contains 4010 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHIKZ029.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	252	Total 1941	C 1234	N 309	O 393	Se 5	0	0	0
1	B	254	Total 1954	C 1242	N 311	O 396	Se 5	0	0	0

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



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

- 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	B	1	Total	C O	0	0
			6	3 3		

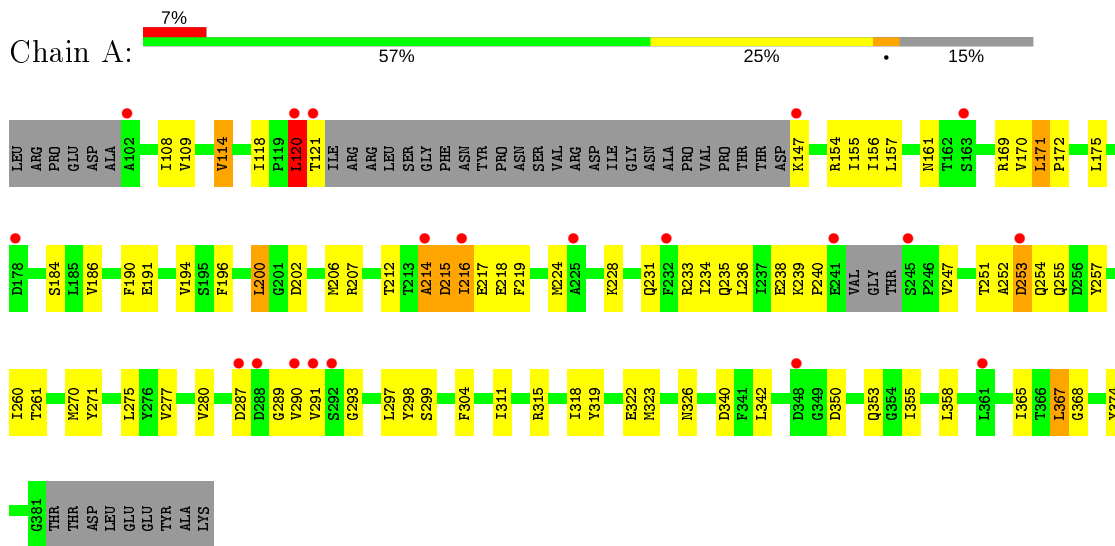
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	55	Total	O	0	0
			55	55		

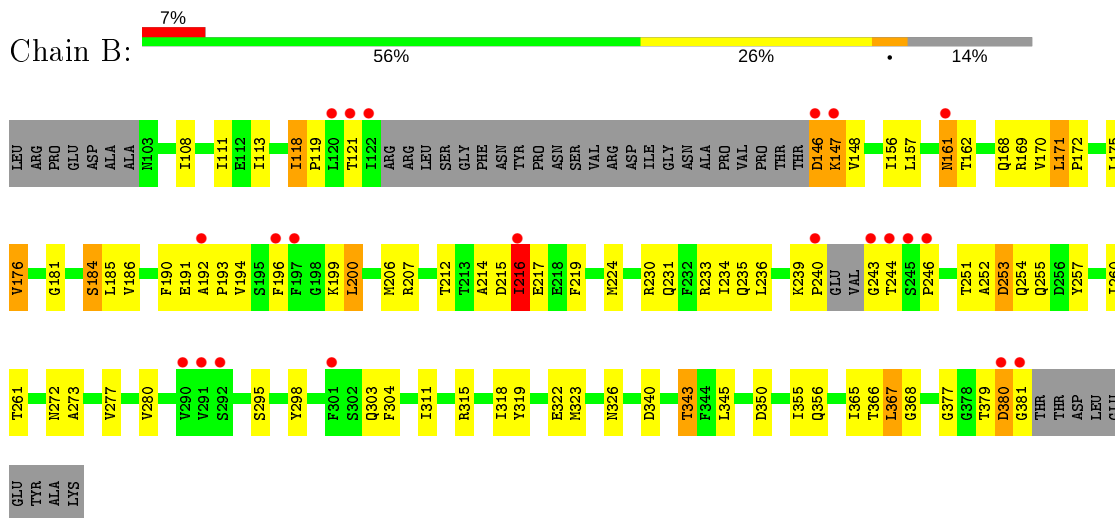
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: PHIKZ029



- Molecule 1: PHIKZ029



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.89Å 156.72Å 61.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.42 – 2.40 28.42 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.42-2.40) 98.4 (28.42-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.82 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.7_650	Depositor
R, $R_{free}$	0.256 , 0.286 0.248 , 0.277	Depositor DCC
$R_{free}$ test set	1345 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtrriage
Anisotropy	0.520	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4010	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.20% 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: GOL, PO4

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	0.50	0/1973	0.78	8/2674 (0.3%)
1	B	0.51	0/1986	0.80	7/2692 (0.3%)
All	All	0.51	0/3959	0.79	15/5366 (0.3%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	SER	CB-CA-C	-11.90	87.49	110.10
1	A	291	VAL	N-CA-CB	-8.51	92.77	111.50
1	A	215	ASP	N-CA-C	7.80	132.07	111.00
1	A	290	VAL	N-CA-C	7.39	130.97	111.00
1	A	291	VAL	N-CA-C	-6.67	93.00	111.00
1	A	214	ALA	CB-CA-C	6.43	119.75	110.10
1	A	215	ASP	N-CA-CB	-6.20	99.45	110.60
1	B	147	LYS	CB-CA-C	-6.08	98.25	110.40
1	B	216	ILE	CB-CA-C	-5.97	99.66	111.60
1	A	120	LEU	CA-CB-CG	-5.43	102.80	115.30
1	A	120	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	B	368	GLY	N-CA-C	-5.34	99.74	113.10
1	B	184	SER	N-CA-C	5.19	125.01	111.00
1	B	148	VAL	N-CA-CB	-5.13	100.21	111.50
1	B	273	ALA	N-CA-CB	-5.04	103.05	110.10

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	1941	0	1885	82	0
1	B	1954	0	1899	102	0
2	A	10	0	0	4	0
3	B	6	0	8	0	0
4	A	44	0	0	12	0
4	B	55	0	0	17	0
All	All	4010	0	3792	181	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 24.

All (181) 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:B:224:MSE:CE	1:B:231:GLN:N	1.90	1.31
1:B:224:MSE:HE2	1:B:231:GLN:CA	1.60	1.30
1:B:224:MSE:CE	1:B:230:ARG:C	2.01	1.27
1:B:224:MSE:HE3	1:B:230:ARG:C	1.56	1.24
1:B:304:PHE:HB3	4:B:29:HOH:O	1.05	1.23
1:B:170:VAL:HG23	4:B:82:HOH:O	1.40	1.22
1:B:224:MSE:HE2	1:B:231:GLN:CB	1.70	1.21
1:B:185:LEU:HB2	4:B:26:HOH:O	1.01	1.18
1:A:120:LEU:HD22	1:A:120:LEU:O	1.48	1.13
1:B:224:MSE:HE2	1:B:231:GLN:HB2	1.32	1.10
1:B:340:ASP:OD2	1:B:343:THR:HG22	1.50	1.09
1:B:224:MSE:CE	1:B:231:GLN:CA	2.31	1.06
1:B:224:MSE:HE2	1:B:231:GLN:N	1.59	1.05
1:A:367:LEU:O	4:A:391:HOH:O	1.75	1.05
1:B:162:THR:N	4:B:31:HOH:O	1.94	1.01
1:A:202:ASP:O	4:A:60:HOH:O	1.79	1.00
1:B:350:ASP:OD2	4:B:57:HOH:O	1.80	0.99
1:A:367:LEU:C	4:A:391:HOH:O	2.00	0.98
1:A:367:LEU:HB3	4:A:88:HOH:O	1.62	0.96
1:B:161:ASN:N	4:B:31:HOH:O	1.89	0.94
1:B:224:MSE:HE3	1:B:231:GLN:N	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:MSE:HE1	1:B:230:ARG:C	1.93	0.86
1:B:184:SER:O	1:B:184:SER:OG	1.86	0.85
1:B:170:VAL:N	4:B:82:HOH:O	1.91	0.84
1:A:118:ILE:O	1:A:147:LYS:HB3	1.78	0.84
1:B:224:MSE:HE1	1:B:230:ARG:O	1.77	0.83
1:B:224:MSE:HE3	1:B:230:ARG:CA	2.07	0.83
1:B:251:THR:HG22	1:B:255:GLN:H	1.43	0.82
1:A:238:GLU:OE1	4:A:79:HOH:O	1.97	0.82
1:A:247:VAL:HG21	1:B:381:GLY:HA3	1.62	0.82
1:A:120:LEU:CD2	1:A:120:LEU:O	2.30	0.79
1:B:212:THR:HG22	1:B:214:ALA:H	1.47	0.78
1:B:108:ILE:HG12	1:B:191:GLU:HG3	1.66	0.77
1:A:216:ILE:HG12	1:A:217:GLU:H	1.49	0.77
1:B:379:THR:O	1:B:380:ASP:HB2	1.84	0.76
1:A:251:THR:HG22	1:A:255:GLN:H	1.51	0.75
1:B:224:MSE:CE	1:B:231:GLN:HB2	2.16	0.75
1:B:304:PHE:CB	4:B:29:HOH:O	1.79	0.74
1:A:120:LEU:C	1:A:120:LEU:CD2	2.55	0.73
1:B:224:MSE:CE	1:B:231:GLN:HA	2.18	0.73
1:B:175:LEU:HB3	1:B:184:SER:HB3	1.71	0.72
1:B:171:LEU:HD13	1:B:172:PRO:HD2	1.71	0.72
1:A:215:ASP:HB3	2:A:3:PO4:O4	1.91	0.70
1:A:207:ARG:HD2	1:A:235:GLN:HE21	1.56	0.70
1:B:260:ILE:HB	1:B:277:VAL:HG22	1.74	0.69
1:A:260:ILE:HB	1:A:277:VAL:HG22	1.74	0.68
1:B:111:ILE:HG23	1:B:113:ILE:HD11	1.74	0.68
1:A:175:LEU:HB3	1:A:184:SER:HB3	1.75	0.68
1:B:176:VAL:HG13	4:B:67:HOH:O	1.92	0.68
1:B:304:PHE:CA	4:B:29:HOH:O	2.28	0.67
1:A:171:LEU:HD13	1:A:172:PRO:HD2	1.75	0.67
1:B:181:GLY:HA2	4:B:67:HOH:O	1.95	0.66
1:B:161:ASN:CA	4:B:31:HOH:O	2.37	0.66
1:A:200:LEU:HD12	1:A:200:LEU:C	2.17	0.65
1:A:108:ILE:HG12	1:A:191:GLU:HG3	1.78	0.65
1:B:161:ASN:OD1	1:B:377:GLY:HA3	1.96	0.65
1:B:212:THR:HG22	1:B:214:ALA:N	2.11	0.64
1:B:200:LEU:C	1:B:200:LEU:HD12	2.19	0.63
1:B:207:ARG:HD2	1:B:235:GLN:HE21	1.62	0.63
1:A:216:ILE:HG12	1:A:217:GLU:N	2.12	0.63
1:B:318:ILE:HG23	1:B:355:ILE:HD11	1.80	0.63
1:B:251:THR:CG2	1:B:255:GLN:H	2.08	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:THR:CG2	1:A:255:GLN:H	2.12	0.63
1:A:217:GLU:HA	1:A:217:GLU:OE1	1.99	0.62
1:B:212:THR:HB	1:B:215:ASP:OD1	2.00	0.62
1:A:120:LEU:HD21	1:A:353:GLN:HG2	1.82	0.61
1:A:120:LEU:C	1:A:120:LEU:HD22	2.12	0.61
1:A:239:LYS:HB3	1:A:240:PRO:HA	1.82	0.61
1:B:311:ILE:HG22	1:B:315:ARG:HD2	1.84	0.60
1:A:287:ASP:HB3	1:A:297:LEU:HB3	1.84	0.59
1:B:240:PRO:HB2	1:B:243:GLY:HA3	1.84	0.58
1:A:114:VAL:HG22	1:A:184:SER:HB3	1.84	0.58
1:A:311:ILE:HG22	1:A:315:ARG:HD2	1.86	0.57
1:B:118:ILE:O	1:B:147:LYS:HB3	2.04	0.57
1:B:224:MSE:HE1	1:B:231:GLN:HA	1.86	0.57
1:B:304:PHE:O	4:B:29:HOH:O	2.17	0.57
1:B:343:THR:HG23	1:B:345:LEU:HG	1.86	0.57
1:B:190:PHE:CD1	1:B:304:PHE:CZ	2.93	0.56
1:A:212:THR:HG22	1:A:214:ALA:N	2.21	0.56
1:B:168:GLN:HG2	4:B:4:HOH:O	2.04	0.56
1:A:298:TYR:HB3	1:B:298:TYR:CD1	2.41	0.56
1:B:207:ARG:CD	1:B:235:GLN:HE21	2.18	0.56
1:A:190:PHE:CD1	1:A:304:PHE:CZ	2.94	0.56
1:B:207:ARG:HH11	1:B:235:GLN:NE2	2.04	0.55
1:B:240:PRO:HB2	1:B:243:GLY:CA	2.36	0.55
1:A:207:ARG:HH11	1:A:235:GLN:NE2	2.03	0.55
1:B:233:ARG:HG2	1:B:257:TYR:CD2	2.42	0.55
1:A:299:SER:O	4:A:42:HOH:O	2.18	0.55
1:B:161:ASN:C	4:B:31:HOH:O	2.31	0.55
1:A:233:ARG:HG2	1:A:257:TYR:CD2	2.43	0.54
1:A:224:MSE:HB2	2:A:1:PO4:O3	2.08	0.54
1:B:157:LEU:HG	1:B:365:ILE:CD1	2.38	0.53
1:B:216:ILE:HG13	1:B:217:GLU:H	1.74	0.53
1:A:114:VAL:CG2	1:A:175:LEU:HD23	2.39	0.53
1:B:240:PRO:CG	1:B:244:THR:HA	2.39	0.53
1:B:200:LEU:O	1:B:200:LEU:HD12	2.09	0.53
1:A:154:ARG:HB3	1:A:358:LEU:HB2	1.91	0.53
1:B:251:THR:HG22	1:B:255:GLN:N	2.17	0.53
1:B:318:ILE:CG2	1:B:355:ILE:HD11	2.38	0.53
1:B:156:ILE:HD11	1:B:186:VAL:HG13	1.90	0.52
1:A:200:LEU:HD12	1:A:200:LEU:O	2.10	0.52
1:A:216:ILE:CG1	1:A:217:GLU:N	2.73	0.52
1:B:157:LEU:HG	1:B:365:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:TYR:O	1:B:323:MSE:HG2	2.11	0.51
1:A:206:MSE:HE2	1:A:236:LEU:HD22	1.93	0.51
1:A:239:LYS:HG3	1:A:374:TYR:CE2	2.46	0.51
1:A:218:GLU:OE1	1:A:218:GLU:HA	2.10	0.50
1:A:120:LEU:CD2	1:A:353:GLN:HG2	2.41	0.50
1:A:207:ARG:CD	1:A:235:GLN:HE21	2.22	0.50
1:B:366:THR:HG22	1:B:367:LEU:O	2.11	0.50
1:A:251:THR:HG22	1:A:255:GLN:N	2.25	0.49
1:B:224:MSE:HE3	1:B:230:ARG:HA	1.94	0.49
1:A:156:ILE:HD11	1:A:186:VAL:HG13	1.93	0.49
1:A:157:LEU:HG	1:A:365:ILE:CD1	2.43	0.49
1:A:280:VAL:O	1:A:280:VAL:HG12	2.12	0.49
1:A:342:LEU:HB3	1:A:367:LEU:HD23	1.95	0.49
1:B:206:MSE:HE2	1:B:236:LEU:HD22	1.93	0.49
1:A:368:GLY:CA	4:A:391:HOH:O	2.60	0.49
1:B:199:LYS:HB2	1:B:381:GLY:C	2.33	0.49
1:A:261:THR:O	1:A:277:VAL:HG23	2.13	0.49
1:B:240:PRO:HB2	1:B:243:GLY:N	2.27	0.49
1:A:114:VAL:HG22	1:A:184:SER:CB	2.43	0.48
1:B:219:PHE:HB2	1:B:231:GLN:NE2	2.28	0.48
1:A:215:ASP:HB3	2:A:3:PO4:P	2.53	0.48
1:A:206:MSE:SE	1:A:234:ILE:HD11	2.64	0.48
1:A:239:LYS:HE3	4:A:60:HOH:O	2.13	0.48
1:A:219:PHE:HB2	1:A:231:GLN:NE2	2.29	0.48
1:A:114:VAL:HG13	1:A:184:SER:HA	1.95	0.48
1:B:118:ILE:HG13	1:B:119:PRO:O	2.14	0.47
1:A:271:TYR:OH	4:A:64:HOH:O	2.14	0.47
1:B:261:THR:O	1:B:277:VAL:HG23	2.15	0.47
1:B:340:ASP:OD1	1:B:340:ASP:C	2.52	0.47
1:B:380:ASP:O	1:B:381:GLY:C	2.52	0.47
1:B:170:VAL:O	1:B:171:LEU:HD22	2.15	0.47
1:B:171:LEU:CD1	1:B:172:PRO:HD2	2.43	0.47
1:B:146:ASP:HB2	4:B:53:HOH:O	2.15	0.46
1:A:109:VAL:HG21	1:A:190:PHE:CZ	2.50	0.46
1:A:319:TYR:O	1:A:323:MSE:HG2	2.15	0.46
1:B:113:ILE:N	1:B:113:ILE:HD12	2.31	0.46
1:B:212:THR:C	1:B:214:ALA:H	2.18	0.46
1:A:170:VAL:O	1:A:171:LEU:HD22	2.16	0.46
1:A:318:ILE:CG2	1:A:355:ILE:HD11	2.46	0.45
1:B:121:THR:HG21	1:B:356:GLN:HA	1.98	0.45
1:A:212:THR:C	1:A:214:ALA:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ILE:HG13	1:A:367:LEU:HD22	1.98	0.45
1:A:206:MSE:HE2	1:A:236:LEU:CD2	2.47	0.45
1:A:367:LEU:CB	4:A:88:HOH:O	2.39	0.45
1:B:253:ASP:O	1:B:254:GLN:HB2	2.16	0.45
1:B:111:ILE:CG2	1:B:113:ILE:HD11	2.43	0.45
1:B:318:ILE:HG12	1:B:355:ILE:HD11	1.99	0.44
1:A:318:ILE:HG23	1:A:355:ILE:HD11	1.98	0.44
1:B:243:GLY:HA3	1:B:244:THR:HA	1.60	0.44
1:A:224:MSE:O	1:A:228:LYS:N	2.50	0.44
1:A:252:ALA:C	1:A:254:GLN:H	2.21	0.44
1:A:253:ASP:O	1:A:254:GLN:HB2	2.18	0.44
1:A:270:MSE:HE2	4:A:64:HOH:O	2.16	0.44
1:B:239:LYS:HE3	1:B:239:LYS:HB2	1.86	0.44
1:B:206:MSE:HE2	1:B:236:LEU:CD2	2.47	0.43
1:A:261:THR:HG22	2:A:1:PO4:O1	2.18	0.43
1:B:240:PRO:HG3	1:B:244:THR:HA	2.00	0.43
1:B:252:ALA:C	1:B:254:GLN:H	2.22	0.43
1:A:114:VAL:HG23	1:A:175:LEU:HD23	2.01	0.43
1:A:200:LEU:CD1	1:A:200:LEU:C	2.87	0.43
1:B:192:ALA:HA	1:B:193:PRO:HD2	1.93	0.43
1:B:121:THR:HG21	1:B:355:ILE:O	2.19	0.42
1:B:233:ARG:HG2	1:B:257:TYR:CE2	2.55	0.42
1:B:240:PRO:CB	1:B:243:GLY:HA3	2.48	0.42
1:B:304:PHE:N	4:B:29:HOH:O	2.46	0.42
1:A:368:GLY:HA3	4:A:391:HOH:O	2.20	0.42
1:A:289:GLY:O	1:A:293:GLY:N	2.48	0.41
1:A:194:VAL:HG12	1:A:196:PHE:H	1.86	0.41
1:A:298:TYR:HB3	1:B:298:TYR:CE1	2.54	0.41
1:A:280:VAL:O	1:A:280:VAL:CG1	2.68	0.41
1:A:350:ASP:N	1:A:350:ASP:OD1	2.30	0.41
1:B:194:VAL:HG12	1:B:196:PHE:H	1.85	0.41
1:B:206:MSE:SE	1:B:234:ILE:HD11	2.71	0.41
1:B:169:ARG:HE	1:B:169:ARG:HB2	1.42	0.41
1:B:193:PRO:HD2	1:B:303:GLN:O	2.21	0.40
1:B:280:VAL:HG12	1:B:280:VAL:O	2.21	0.40
1:A:171:LEU:CD1	1:A:172:PRO:HD2	2.48	0.40
1:A:340:ASP:OD1	1:A:340:ASP:C	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	246/295 (83%)	226 (92%)	19 (8%)	1 (0%)	34	48
1	B	248/295 (84%)	227 (92%)	16 (6%)	5 (2%)	7	9
All	All	494/590 (84%)	453 (92%)	35 (7%)	6 (1%)	13	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	380	ASP
1	A	253	ASP
1	B	253	ASP
1	B	272	ASN
1	B	367	LEU
1	B	246	PRO

### 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	213/245 (87%)	201 (94%)	12 (6%)	21	34
1	B	215/245 (88%)	204 (95%)	11 (5%)	24	39
All	All	428/490 (87%)	405 (95%)	23 (5%)	22	36

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	VAL
1	A	120	LEU
1	A	121	THR
1	A	161	ASN
1	A	169	ARG
1	A	171	LEU
1	A	200	LEU
1	A	216	ILE
1	A	275	LEU
1	A	322	GLU
1	A	326	ASN
1	A	367	LEU
1	B	118	ILE
1	B	146	ASP
1	B	161	ASN
1	B	171	LEU
1	B	176	VAL
1	B	200	LEU
1	B	216	ILE
1	B	295	SER
1	B	322	GLU
1	B	326	ASN
1	B	343	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	GLN
1	A	254	GLN
1	A	308	HIS
1	B	183	GLN
1	B	235	GLN
1	B	254	GLN
1	B	308	HIS
1	B	326	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
2	PO4	A	1	-	4,4,4	0.87	0	6,6,6	0.60	0
2	PO4	A	3	-	4,4,4	0.93	0	6,6,6	0.38	0
3	GOL	B	1	-	5,5,5	0.32	0	5,5,5	0.71	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	1	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	GOL	O1-C1-C2-C3
3	B	1	GOL	O1-C1-C2-O2



There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	PO4	2	0
2	A	3	PO4	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, 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	247/295 (83%)	0.69	20 (8%) 12 11	17, 40, 74, 119	0
1	B	249/295 (84%)	0.69	21 (8%) 11 10	20, 41, 77, 106	0
All	All	496/590 (84%)	0.69	41 (8%) 11 10	17, 41, 76, 119	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	ILE	8.6
1	A	121	THR	8.0
1	B	381	GLY	7.9
1	A	291	VAL	6.3
1	B	146	ASP	5.5
1	B	245	SER	5.4
1	A	216	ILE	5.3
1	A	241	GLU	4.4
1	A	290	VAL	4.4
1	B	122	ILE	4.2
1	B	244	THR	4.1
1	A	120	LEU	3.9
1	A	147	LYS	3.8
1	B	121	THR	3.6
1	A	253	ASP	3.3
1	A	288	ASP	3.2
1	A	361	LEU	3.0
1	A	102	ALA	3.0
1	A	245	SER	2.9
1	B	243	GLY	2.9
1	B	291	VAL	2.8
1	B	246	PRO	2.8
1	A	348	ASP	2.8
1	A	178	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	380	ASP	2.6
1	B	147	LYS	2.6
1	B	240	PRO	2.6
1	B	196	PHE	2.5
1	A	287	ASP	2.4
1	B	161	ASN	2.4
1	B	197	PHE	2.4
1	B	120	LEU	2.4
1	B	192	ALA	2.3
1	A	225	ALA	2.3
1	A	163	SER	2.2
1	A	292	SER	2.1
1	B	292	SER	2.1
1	B	301	PHE	2.1
1	A	232	PHE	2.0
1	B	290	VAL	2.0
1	A	214	ALA	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 carbohydrates 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(Å <sup>2</sup> )	Q<0.9
2	PO4	A	3	5/5	0.19	1.06	178,183,187,188	0
3	GOL	B	1	6/6	0.70	0.17	38,56,65,70	0
2	PO4	A	1	5/5	0.72	0.46	83,94,105,123	0

## 6.5 Other polymers

There are no such residues in this entry.