



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:48 AM GMT

PDB ID : 2O8R
Title : Crystal Structure of Polyphosphate Kinase from Porphyromonas Gingivalis
Authors : Patskovsky, Y.; Toro, R.; Sauder, J.M.; Dickey, M.; Adams, J.M.; Ozyurt, S.; Wasserman, S.R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-12-12
Resolution : 2.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

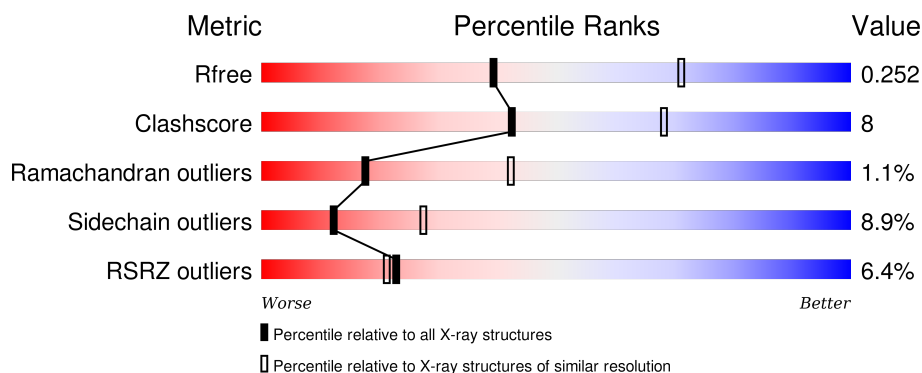
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	705	
1	B	705	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10452 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 Polyphosphate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	648	Total	C	N	O	S	Se	0	4	0
			5344	3412	935	972	7	18			
1	B	605	Total	C	N	O	S	Se	0	3	0
			4987	3189	867	907	5	19			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	CLONING ARTIFACT	UNP Q7MTR1
A	0	SER	-	CLONING ARTIFACT	UNP Q7MTR1
A	1	LEU	MET	ENGINEERED	UNP Q7MTR1
A	13	MSE	MET	ENGINEERED	UNP Q7MTR1
A	24	MSE	MET	ENGINEERED	UNP Q7MTR1
A	144	MSE	MET	ENGINEERED	UNP Q7MTR1
A	225	MSE	MET	ENGINEERED	UNP Q7MTR1
A	268	MSE	MET	ENGINEERED	UNP Q7MTR1
A	273	MSE	MET	ENGINEERED	UNP Q7MTR1
A	306	MSE	MET	ENGINEERED	UNP Q7MTR1
A	335	MSE	MET	ENGINEERED	UNP Q7MTR1
A	360	MSE	MET	ENGINEERED	UNP Q7MTR1
A	420	MSE	MET	ENGINEERED	UNP Q7MTR1
A	431	MSE	MET	ENGINEERED	UNP Q7MTR1
A	478	MSE	MET	ENGINEERED	UNP Q7MTR1
A	514	MSE	MET	ENGINEERED	UNP Q7MTR1
A	537	MSE	MET	ENGINEERED	UNP Q7MTR1
A	541	MSE	MET	ENGINEERED	UNP Q7MTR1
A	577	MSE	MET	ENGINEERED	UNP Q7MTR1
A	591	MSE	MET	ENGINEERED	UNP Q7MTR1
A	617	MSE	MET	ENGINEERED	UNP Q7MTR1
A	635	THR	ALA	ENGINEERED	UNP Q7MTR1
A	690	THR	ALA	ENGINEERED	UNP Q7MTR1
A	696	GLU	-	CLONING ARTIFACT	UNP Q7MTR1
A	697	GLY	-	CLONING ARTIFACT	UNP Q7MTR1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	698	HIS	-	EXPRESSION TAG	UNP Q7MTR1
A	699	HIS	-	EXPRESSION TAG	UNP Q7MTR1
A	700	HIS	-	EXPRESSION TAG	UNP Q7MTR1
A	701	HIS	-	EXPRESSION TAG	UNP Q7MTR1
A	702	HIS	-	EXPRESSION TAG	UNP Q7MTR1
A	703	HIS	-	EXPRESSION TAG	UNP Q7MTR1
B	-1	MSE	-	CLONING ARTIFACT	UNP Q7MTR1
B	0	SER	-	CLONING ARTIFACT	UNP Q7MTR1
B	1	LEU	MET	ENGINEERED	UNP Q7MTR1
B	13	MSE	MET	ENGINEERED	UNP Q7MTR1
B	24	MSE	MET	ENGINEERED	UNP Q7MTR1
B	144	MSE	MET	ENGINEERED	UNP Q7MTR1
B	225	MSE	MET	ENGINEERED	UNP Q7MTR1
B	268	MSE	MET	ENGINEERED	UNP Q7MTR1
B	273	MSE	MET	ENGINEERED	UNP Q7MTR1
B	306	MSE	MET	ENGINEERED	UNP Q7MTR1
B	335	MSE	MET	ENGINEERED	UNP Q7MTR1
B	360	MSE	MET	ENGINEERED	UNP Q7MTR1
B	420	MSE	MET	ENGINEERED	UNP Q7MTR1
B	431	MSE	MET	ENGINEERED	UNP Q7MTR1
B	478	MSE	MET	ENGINEERED	UNP Q7MTR1
B	514	MSE	MET	ENGINEERED	UNP Q7MTR1
B	537	MSE	MET	ENGINEERED	UNP Q7MTR1
B	541	MSE	MET	ENGINEERED	UNP Q7MTR1
B	577	MSE	MET	ENGINEERED	UNP Q7MTR1
B	591	MSE	MET	ENGINEERED	UNP Q7MTR1
B	617	MSE	MET	ENGINEERED	UNP Q7MTR1
B	635	THR	ALA	ENGINEERED	UNP Q7MTR1
B	690	THR	ALA	ENGINEERED	UNP Q7MTR1
B	696	GLU	-	CLONING ARTIFACT	UNP Q7MTR1
B	697	GLY	-	CLONING ARTIFACT	UNP Q7MTR1
B	698	HIS	-	EXPRESSION TAG	UNP Q7MTR1
B	699	HIS	-	EXPRESSION TAG	UNP Q7MTR1
B	700	HIS	-	EXPRESSION TAG	UNP Q7MTR1
B	701	HIS	-	EXPRESSION TAG	UNP Q7MTR1
B	702	HIS	-	EXPRESSION TAG	UNP Q7MTR1
B	703	HIS	-	EXPRESSION TAG	UNP Q7MTR1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total 38	O 38	0	0
3	B	18	Total 18	O 18	0	0

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Chain A:

Chain B:

Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.25). The x-axis lists amino acids. The logo is divided into four segments: 9% (red), 62% (green), 22% (yellow), and 14% (grey).

Position	Amino Acid	Information Content (bits)
1	L180	0.05
2	L193	0.05
3	L194	0.05
4	K195	0.05
5	L196	0.05
6	Q197	0.05
7	L215	0.05
8	D216	0.05
9	V217	0.05
10	G221	0.05
11	Y222	0.05
12	E223	0.05
13	Y224	0.05
14	M225	0.05
15	Y228	0.05
16	S229	0.05
17	R234	0.05
18	ASP	0.05
19	ASP	0.05
20	ASP	0.05
21	ASP	0.05
22	LEU	0.05
23	LEU	0.05
24	ASP	0.05
25	GLN	0.05
26	GLN	0.05
27	ARG	0.05
28	PRO	0.05
29	GLU	0.05
30	ASP	0.05
31	LEU	0.05
32	PRO	0.05
33	GLY	0.05
34	GLU	0.05
35	ILE	0.05
36	ARG	0.05
37	LYS	0.05
38	LYS	0.05
39	VAL	0.05
40	L151	0.05
41	K152	0.05
42	ARG	0.05
43	LYS	0.05
44	GLY	0.05
45	GLY	0.05
46	K167	0.05
47	E168	0.05
48	K169	0.05
49	D172	0.05
50	E173	0.05
51	A174	0.05
52	Y175	0.05
53	S176	0.05
54	Y177	0.05



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	99.33Å 99.33Å 335.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70 37.11 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.70) 99.4 (37.11-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.255 0.186 , 0.252	Depositor DCC
R_{free} test set	1577 reflections (3.21%)	DCC
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.1	EDS
Estimated twinning fraction	0.067 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 50844 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10452	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.42	0/5452	0.65	2/7348 (0.0%)
1	B	0.41	0/5083	0.61	2/6849 (0.0%)
All	All	0.42	0/10535	0.63	4/14197 (0.0%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	VAL	C-N-CD	-10.48	97.55	120.60
1	A	347	VAL	C-N-CD	-10.34	97.85	120.60
1	B	347	VAL	C-N-CA	6.35	148.68	122.00
1	A	347	VAL	C-N-CA	5.97	147.09	122.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347	VAL	Peptide
1	B	347	VAL	Peptide

5.2 Too-close contacts ⓘ

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	5344	0	5385	92	0
1	B	4987	0	5028	86	0
2	A	40	0	0	3	0
2	B	25	0	0	0	0
3	A	38	0	0	0	0
3	B	18	0	0	1	0
All	All	10452	0	10413	172	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (172) 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:357:ARG:HG2	1:A:357:ARG:HH21	1.26	0.97
1:A:312:ALA:HB3	1:A:313:PRO:HD3	1.49	0.92
1:B:312:ALA:HB1	1:B:313:PRO:HD3	1.51	0.92
1:A:312:ALA:CB	1:A:313:PRO:HD3	2.00	0.91
1:A:579:GLN:H	1:A:579:GLN:HE21	1.14	0.89
1:A:348:PRO:HD2	1:A:349:TYR:H	1.38	0.88
1:B:20:GLU:HG2	1:B:92:GLN:HE21	1.43	0.83
1:B:312:ALA:CB	1:B:313:PRO:HD3	2.09	0.82
1:A:188:PRO:HD3	1:B:408:PHE:HB3	1.61	0.81
1:B:172:ASP:O	1:B:173:GLU:HB2	1.81	0.80
1:B:38:LYS:HB2	1:B:591:MSE:HE3	1.67	0.76
1:B:312:ALA:CB	1:B:313:PRO:CD	2.63	0.76
1:A:542:ASN:HD22	1:A:568:ARG:HE	1.33	0.76
1:A:279:ARG:HA	1:A:282:CYS:HB3	1.68	0.76
1:B:522:ILE:HG23	1:B:537:MSE:HE1	1.70	0.73
1:B:20:GLU:HG2	1:B:92:GLN:NE2	2.03	0.73
1:A:357:ARG:NH2	1:A:357:ARG:HG2	1.96	0.68
1:A:312:ALA:CB	1:A:313:PRO:CD	2.71	0.67
1:A:579:GLN:N	1:A:579:GLN:HE21	1.90	0.67
1:A:370:GLU:HB3	1:A:397:LYS:HB2	1.77	0.67
1:A:225:MSE:HA	1:A:225:MSE:HE2	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HA	1:A:360:MSE:HE3	1.75	0.66
1:A:514:MSE:HE3	1:A:621:LEU:HD23	1.79	0.65
1:B:195:ARG:HH12	1:B:197:GLN:HA	1.61	0.65
1:A:403:GLU:HB3	1:A:436:VAL:O	1.97	0.64
1:A:348:PRO:CD	1:A:349:TYR:H	2.01	0.64
1:B:147:LEU:HD23	1:B:150:LYS:HE2	1.80	0.62
1:B:541:MSE:HB3	1:B:567:VAL:HG12	1.81	0.62
1:A:579:GLN:H	1:A:579:GLN:NE2	1.94	0.61
1:B:273:MSE:CE	1:B:277:VAL:HG22	2.30	0.61
1:A:312:ALA:HB3	1:A:313:PRO:CD	2.25	0.61
1:A:418:GLU:HG3	1:A:422:ARG:HH22	1.65	0.60
1:B:348:PRO:HD3	1:B:352:TYR:OH	2.01	0.60
1:B:549:VAL:HA	1:B:552:GLN:HB2	1.84	0.60
1:A:351:THR:HB	1:A:353:ASP:H	1.67	0.59
1:B:510:ALA:HB2	1:B:626:GLU:H	1.68	0.59
1:B:335:MSE:HG3	1:B:361:GLU:OE1	2.02	0.59
1:A:138:PHE:HA	1:A:141:LEU:HD22	1.84	0.59
1:A:542:ASN:ND2	1:A:568:ARG:HE	2.02	0.58
1:B:129:LEU:HD21	1:B:193:LEU:HD11	1.86	0.57
1:B:312:ALA:HB3	1:B:313:PRO:CD	2.34	0.57
1:B:380:GLU:HG3	1:B:467:THR:HG21	1.86	0.56
1:A:542:ASN:HD21	1:A:595:HIS:HA	1.70	0.56
1:B:369:SER:HB2	1:B:446:HIS:CD2	2.41	0.56
1:A:40:LEU:HG	1:A:96:TYR:CZ	2.41	0.56
1:A:312:ALA:HB1	1:A:313:PRO:HD3	1.86	0.55
1:A:593:LEU:HD23	1:A:595:HIS:HB2	1.89	0.55
1:A:228:TYR:CG	1:A:273:MSE:HG3	2.42	0.55
1:A:651:ASN:HD22	1:A:671:GLU:HG3	1.71	0.55
1:A:108:LEU:HB3	1:A:113:ILE:HB	1.88	0.54
1:B:578:PRO:HA	1:B:581:ARG:CZ	2.37	0.54
1:A:356:VAL:HG22	1:A:360:MSE:HE2	1.89	0.53
1:B:21:ARG:HH12	1:B:25:GLU:HG2	1.73	0.53
1:A:372:ARG:HE	1:A:492:PHE:HB3	1.74	0.53
1:B:228:TYR:HB3	1:B:270:ASP:HB3	1.91	0.53
1:A:348:PRO:HD2	1:A:349:TYR:N	2.15	0.53
1:B:639:GLU:OE2	1:B:687:LYS:NZ	2.39	0.53
1:A:381:ASN:OD1	1:A:419:ARG:NH1	2.41	0.53
1:A:404:LEU:HG	1:A:405:LYS:HG2	1.91	0.53
1:A:118:HIS:ND1	2:A:711:SO4:O2	2.42	0.52
1:B:51:TYR:HD2	1:B:266:ARG:HH11	1.58	0.52
1:B:437:HIS:HB2	1:B:624:ARG:HD3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:NH1	1:A:290:GLU:O	2.42	0.52
1:A:334:LEU:HD11	1:A:357:ARG:NH2	2.25	0.52
1:B:177:TYR:CE1	1:B:277:VAL:HB	2.45	0.51
1:B:542:ASN:OD1	1:B:597:ARG:NE	2.44	0.51
1:A:658:ASP:OD2	1:A:662:ASN:HB2	2.10	0.51
1:B:175:TYR:HE1	1:B:225:MSE:HG3	1.75	0.51
1:A:147:LEU:HD23	1:A:150:LYS:HD2	1.91	0.51
1:A:358:LEU:HD22	1:A:478:MSE:CE	2.40	0.51
1:B:541:MSE:O	1:B:567:VAL:HA	2.10	0.51
1:B:603:ASN:HB3	1:B:606:LYS:O	2.11	0.50
1:B:269:TYR:CZ	1:B:294:ARG:HB3	2.47	0.50
1:A:415:ARG:O	1:A:418:GLU:HG2	2.12	0.50
1:A:538:LEU:HB3	1:A:600:CYS:HB2	1.93	0.50
1:A:356:VAL:HG21	1:A:383:SER:HB3	1.94	0.49
1:A:548:ASN:O	1:A:552:GLN:HG3	2.12	0.49
1:B:649:ARG:HG3	1:B:652:ILE:HG13	1.94	0.49
1:A:153:THR:HG22	1:B:143:PRO:HD2	1.95	0.49
1:B:370:GLU:HB3	1:B:397:LYS:HB2	1.94	0.48
1:A:220:PRO:HB3	1:B:152:ARG:HH21	1.78	0.48
1:B:21:ARG:NH1	1:B:25:GLU:HG2	2.28	0.48
1:B:95:LEU:O	1:B:99:ILE:HG12	2.14	0.47
1:A:48:GLU:O	1:A:52:THR:HG23	2.14	0.47
1:B:267:PHE:HB3	1:B:292:ALA:HA	1.95	0.47
1:A:196:LEU:O	1:A:199:ASP:HB2	2.14	0.47
1:A:372:ARG:HE	1:A:492:PHE:CB	2.28	0.47
1:A:116:ARG:NH2	1:A:125:HIS:ND1	2.59	0.47
1:A:382:SER:OG	1:A:385:ILE:HG12	2.14	0.47
1:B:195:ARG:NH1	1:B:197:GLN:HA	2.27	0.47
1:B:549:VAL:HG11	1:B:616:TRP:HB3	1.97	0.47
1:B:510:ALA:CB	1:B:626:GLU:H	2.27	0.47
1:A:348:PRO:CD	1:A:349:TYR:N	2.68	0.47
1:B:599:TRP:HB2	1:B:610:PHE:HB2	1.97	0.47
1:A:306:MSE:SE	1:B:411:GLU:HB3	2.65	0.47
1:B:470:ARG:HE	1:B:593:LEU:HD12	1.79	0.46
1:B:273:MSE:HE3	1:B:277:VAL:HG22	1.97	0.46
1:A:116:ARG:NH1	2:A:709:SO4:O4	2.47	0.46
1:A:49:GLU:O	1:A:53:VAL:HG13	2.14	0.46
1:A:357:ARG:HH21	1:A:357:ARG:CG	2.10	0.46
1:A:651:ASN:ND2	1:A:671:GLU:HG3	2.30	0.46
1:A:633:ASP:HA	1:A:634:PRO:HD3	1.81	0.46
1:B:470:ARG:NH1	1:B:591:MSE:O	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ARG:HH22	1:A:608:GLU:CD	2.19	0.46
1:B:54:ARG:HD2	1:B:54:ARG:HA	1.71	0.46
1:B:631:VAL:O	1:B:637:ARG:HG3	2.16	0.46
1:A:228:TYR:HB2	1:A:273:MSE:HE3	1.97	0.46
1:B:493:ARG:NH2	1:B:498[B]:ASP:OD1	2.49	0.46
1:A:546:ASP:OD2	1:A:549:VAL:HG23	2.16	0.46
1:B:273:MSE:HE2	1:B:277:VAL:HG22	1.96	0.45
1:B:215:LEU:HB3	1:B:224:VAL:HG11	1.97	0.45
1:A:150:LYS:HA	1:B:221:GLY:HA3	1.97	0.45
1:A:59:GLN:HE22	1:A:265:THR:HA	1.82	0.45
1:A:325:SER:O	1:A:329:GLU:HG2	2.16	0.45
1:A:155:ILE:O	1:A:234:ARG:NH1	2.49	0.45
1:A:541:MSE:HE2	1:A:615:ASP:HA	1.98	0.45
1:B:375:GLN:O	1:B:402:VAL:HA	2.17	0.45
1:B:138:PHE:HB3	1:B:139:PRO:HD3	1.98	0.44
1:B:374:THR:OG1	1:B:439:LYS:HA	2.17	0.44
1:A:365:SER:HA	1:A:366:PRO:HD2	1.75	0.44
1:B:338:ILE:HG21	1:B:456:ILE:HG23	1.99	0.44
1:B:373:LEU:HD22	1:B:388:LEU:HD11	2.00	0.44
1:A:377:ARG:HG2	1:A:404:LEU:HD22	2.00	0.44
1:B:311:PHE:O	1:B:312:ALA:C	2.56	0.44
1:B:35:ASP:HA	1:B:591:MSE:CE	2.47	0.43
1:A:157:SER:HB3	1:A:234:ARG:HG2	2.00	0.43
1:B:295:SER:HB2	1:B:296:GLY:H	1.71	0.43
1:B:502:ALA:HB1	1:B:512:TYR:CE1	2.53	0.43
1:A:338:ILE:H	1:A:338:ILE:HG12	1.63	0.43
1:B:40:LEU:HD11	1:B:104:ILE:HG13	2.01	0.43
1:B:529:VAL:HG11	1:B:559:ALA:O	2.19	0.43
1:B:180:LEU:HD12	1:B:180:LEU:HA	1.80	0.43
1:B:415:ARG:HG3	3:B:721:HOH:O	2.18	0.43
1:B:514:MSE:HE2	1:B:628:ALA:HB2	2.00	0.43
1:B:11:ARG:HH12	1:B:572:CYS:HA	1.83	0.43
1:A:372:ARG:HH21	1:A:492:PHE:HB3	1.84	0.43
1:B:105:LEU:HD21	1:B:115:LEU:HD23	2.00	0.42
1:B:131:ARG:HH11	1:B:131:ARG:HB3	1.83	0.42
1:A:574:VAL:HG22	1:A:577:MSE:HG3	2.00	0.42
1:B:266:ARG:HG2	1:B:267:PHE:H	1.84	0.42
1:B:373:LEU:HD12	1:B:441:ALA:HB2	2.00	0.42
1:A:536:TYR:HB3	1:A:602:HIS:HB2	2.01	0.42
1:A:537:MSE:HE3	1:A:563:ILE:HG12	2.01	0.42
1:A:470:ARG:NH1	1:A:591:MSE:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:NE	2:A:710:SO4:O4	2.49	0.42
1:A:431:MSE:H	1:A:431:MSE:HE3	1.85	0.42
1:B:577:MSE:HB2	1:B:577:MSE:HE3	1.89	0.41
1:A:376:TYR:HB2	1:A:463:ASN:HD21	1.85	0.41
1:B:125:HIS:CG	1:B:193:LEU:HD23	2.55	0.41
1:B:550:ILE:HG12	1:B:573:LEU:HD12	2.02	0.41
1:A:105:LEU:HB2	1:A:106:PRO:HD3	2.03	0.41
1:B:266:ARG:HD2	1:B:293:ILE:HD12	2.02	0.41
1:B:167:LYS:HG3	1:B:175:TYR:CE1	2.56	0.41
1:A:508:LEU:HB2	1:A:628:ALA:HB3	2.01	0.41
1:A:353:ASP:O	1:A:357:ARG:HB2	2.21	0.41
1:B:639:GLU:O	1:B:643:ILE:HG12	2.21	0.41
1:B:646:ILE:O	1:B:649:ARG:HG2	2.21	0.41
1:A:321:GLU:HA	1:A:322:PRO:HD3	1.91	0.41
1:A:653:LYS:HA	1:A:653:LYS:HD3	1.86	0.41
1:A:590:ASP:CG	1:A:653:LYS:HG3	2.42	0.41
1:B:405:LYS:HG2	1:B:429:TYR:CE1	2.55	0.41
1:B:116:ARG:NH2	1:B:125:HIS:ND1	2.69	0.41
1:B:160:VAL:HG22	1:B:299:VAL:HG23	2.03	0.41
1:B:538:LEU:HB3	1:B:600:CYS:HB3	2.02	0.41
1:A:370:GLU:CB	1:A:397:LYS:HB2	2.49	0.40
1:A:434:LEU:HD13	1:A:625:ILE:HD12	2.03	0.40
1:A:4:SER:OG	1:A:5:ALA:N	2.53	0.40
1:A:225:MSE:HA	1:A:225:MSE:CE	2.50	0.40
1:A:122:HIS:HA	1:A:123:PRO:HD3	1.90	0.40
1:A:381:ASN:HB3	1:B:386:SER:OG	2.21	0.40
1:B:431[A]:MSE:HE2	1:B:434:LEU:HD11	2.04	0.40
1:A:319:THR:HA	1:A:320:PRO:HD3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	644/705 (91%)	612 (95%)	26 (4%)	6 (1%)	21	49
1	B	596/705 (84%)	553 (93%)	36 (6%)	7 (1%)	16	39
All	All	1240/1410 (88%)	1165 (94%)	62 (5%)	13 (1%)	17	45

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	ALA
1	A	348	PRO
1	A	448	PRO
1	B	312	ALA
1	B	348	PRO
1	B	448	PRO
1	A	432	PRO
1	B	432	PRO
1	B	501	PRO
1	A	168	GLU
1	B	578	PRO
1	A	289	PRO
1	B	313	PRO

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	587/612 (96%)	539 (92%)	48 (8%)	14	32
1	B	547/612 (89%)	493 (90%)	54 (10%)	10	22
All	All	1134/1224 (93%)	1032 (91%)	102 (9%)	12	27

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	40	LEU
1	A	41	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	62	LEU
1	A	113	ILE
1	A	114	ARG
1	A	117	THR
1	A	121	THR
1	A	141	LEU
1	A	145	LEU
1	A	151	VAL
1	A	162	LEU
1	A	176	SER
1	A	182	VAL
1	A	199	ASP
1	A	217	VAL
1	A	240	LEU
1	A	270	ASP
1	A	281	ILE
1	A	294	ARG
1	A	338	ILE
1	A	351	THR
1	A	357	ARG
1	A	373	LEU
1	A	375	GLN
1	A	378	VAL
1	A	394	SER
1	A	399	SER
1	A	408	PHE
1	A	429[A]	TYR
1	A	429[B]	TYR
1	A	430	SER
1	A	431	MSE
1	A	467	THR
1	A	468	THR
1	A	470	ARG
1	A	538	LEU
1	A	541	MSE
1	A	574	VAL
1	A	579	GLN
1	A	607[A]	GLU
1	A	607[B]	GLU
1	A	624	ARG
1	A	652	ILE
1	A	674	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	675	ARG
1	A	689	GLU
1	A	690	THR
1	B	14	SER
1	B	15	TRP
1	B	17	SER
1	B	24	MSE
1	B	33	VAL
1	B	38	LYS
1	B	52	THR
1	B	55	VAL
1	B	88	THR
1	B	114	ARG
1	B	121	THR
1	B	150	LYS
1	B	151	VAL
1	B	215	LEU
1	B	216	ASP
1	B	217	VAL
1	B	223	GLU
1	B	224	VAL
1	B	229	SER
1	B	280	TYR
1	B	300	ASN
1	B	301	LEU
1	B	302	GLN
1	B	336	GLU
1	B	351	THR
1	B	367	ASP
1	B	369	SER
1	B	378	VAL
1	B	383	SER
1	B	394	SER
1	B	402	VAL
1	B	405	LYS
1	B	407	ARG
1	B	428	VAL
1	B	434	LEU
1	B	444	LEU
1	B	452	ARG
1	B	463	ASN
1	B	506	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	514	MSE
1	B	541	MSE
1	B	544	LEU
1	B	545	GLN
1	B	547	LYS
1	B	577	MSE
1	B	584	ARG
1	B	588	LEU
1	B	590	ASP
1	B	591	MSE
1	B	593	LEU
1	B	621	LEU
1	B	666	LYS
1	B	671	GLU
1	B	672	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	375	GLN
1	A	446	HIS
1	A	486	HIS
1	A	528	ASN
1	A	542	ASN
1	A	579	GLN
1	A	662	ASN
1	B	92	GLN
1	B	393	GLN
1	B	446	HIS
1	B	463	ASN
1	B	528	ASN
1	B	545	GLN
1	B	651	ASN
1	B	668	ASN

5.3.3 RNA ⓘ

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](#)

13 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	SO4	A	704	-	4,4,4	0.17	0	6,6,6	0.24	0
2	SO4	A	705	-	4,4,4	0.18	0	6,6,6	0.23	0
2	SO4	A	706	-	4,4,4	0.16	0	6,6,6	0.23	0
2	SO4	A	707	-	4,4,4	0.20	0	6,6,6	0.26	0
2	SO4	A	708	-	4,4,4	0.29	0	6,6,6	0.12	0
2	SO4	A	709	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	A	710	-	4,4,4	0.29	0	6,6,6	0.15	0
2	SO4	A	711	-	4,4,4	0.27	0	6,6,6	0.19	0
2	SO4	B	704	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	705	-	4,4,4	0.19	0	6,6,6	0.16	0
2	SO4	B	706	-	4,4,4	0.17	0	6,6,6	0.06	0
2	SO4	B	707	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	B	708	-	4,4,4	0.18	0	6,6,6	0.12	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
2	SO4	A	704	-	-	0/0/0/0	0/0/0/0
2	SO4	A	705	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	706	-	-	0/0/0/0	0/0/0/0
2	SO4	A	707	-	-	0/0/0/0	0/0/0/0
2	SO4	A	708	-	-	0/0/0/0	0/0/0/0
2	SO4	A	709	-	-	0/0/0/0	0/0/0/0
2	SO4	A	710	-	-	0/0/0/0	0/0/0/0
2	SO4	A	711	-	-	0/0/0/0	0/0/0/0
2	SO4	B	704	-	-	0/0/0/0	0/0/0/0
2	SO4	B	705	-	-	0/0/0/0	0/0/0/0
2	SO4	B	706	-	-	0/0/0/0	0/0/0/0
2	SO4	B	707	-	-	0/0/0/0	0/0/0/0
2	SO4	B	708	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	709	SO4	1	0
2	A	710	SO4	1	0
2	A	711	SO4	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	630/705 (89%)	-0.11	15 (2%) 62 62	39, 62, 107, 168	0
1	B	588/705 (83%)	0.26	63 (10%) 8 6	41, 72, 112, 163	0
All	All	1218/1410 (86%)	0.07	78 (6%) 23 21	39, 67, 109, 168	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	ILE	10.3
1	B	669	SER	8.5
1	B	571	CYS	7.6
1	B	573	LEU	7.2
1	B	578	PRO	6.9
1	B	82	LEU	5.9
1	B	670	ASP	5.6
1	B	668	ASN	5.5
1	B	575	PRO	5.1
1	B	574	VAL	5.0
1	B	56	ALA	4.6
1	A	286	ASP	4.6
1	B	15	TRP	4.6
1	B	54	ARG	4.5
1	B	173	GLU	4.3
1	A	283	SER	4.3
1	B	547	LYS	4.2
1	B	53	VAL	4.1
1	B	572	CYS	4.0
1	B	57	TYR	3.9
1	B	622	TYR	3.9
1	B	553	LEU	3.8
1	B	89	VAL	3.8
1	B	55	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	62	LEU	3.8
1	B	86	ARG	3.7
1	B	466	GLU	3.7
1	A	405	LYS	3.7
1	A	171	THR	3.6
1	B	549	VAL	3.6
1	B	84	ALA	3.6
1	B	52	THR	3.5
1	B	690	THR	3.5
1	B	621	LEU	3.3
1	B	293	ILE	3.3
1	B	544	LEU	3.2
1	A	290	GLU	3.2
1	B	294	ARG	3.1
1	B	545	GLN	3.1
1	B	570	ILE	3.1
1	B	292	ALA	3.1
1	B	576	ASP	3.0
1	B	14	SER	2.9
1	A	448	PRO	2.9
1	B	467	THR	2.8
1	B	16	LEU	2.8
1	B	51	TYR	2.8
1	B	667	HIS	2.8
1	B	90	ILE	2.7
1	B	449	ALA	2.7
1	B	50	PHE	2.7
1	B	554	TYR	2.7
1	B	12	ASP	2.6
1	A	63	GLN	2.6
1	B	450	GLY	2.6
1	A	61	VAL	2.5
1	B	579	GLN	2.5
1	A	291	GLU	2.5
1	B	11	ARG	2.5
1	B	83	GLN	2.5
1	B	671	GLU	2.4
1	B	548	ASN	2.4
1	B	404	LEU	2.3
1	B	546	ASP	2.3
1	B	17	SER	2.2
1	B	501	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	279	ARG	2.2
1	A	376	TYR	2.1
1	B	174	ALA	2.1
1	B	465	ASN	2.1
1	A	282	CYS	2.1
1	A	4	SER	2.1
1	B	468	THR	2.1
1	B	266	ARG	2.1
1	A	170	GLU	2.0
1	A	476	THR	2.0
1	B	172	ASP	2.0
1	B	169	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	710	5/5	0.93	0.17	1.32	103,116,127,134	0
2	SO4	A	705	5/5	0.91	0.16	0.68	89,114,127,132	0
2	SO4	A	707	5/5	0.96	0.20	0.58	68,68,92,102	0
2	SO4	A	711	5/5	0.97	0.18	0.52	131,132,134,135	0
2	SO4	B	706	5/5	0.95	0.15	-0.96	116,122,128,133	0
2	SO4	A	709	5/5	0.99	0.09	-1.47	66,77,96,99	0
2	SO4	B	704	5/5	0.97	0.09	-1.63	88,96,109,111	0
2	SO4	B	705	5/5	0.92	0.14	-1.80	108,109,122,138	0
2	SO4	A	704	5/5	0.97	0.09	-1.91	79,84,104,105	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	708	5/5	0.98	0.13	-	114,123,127,134	0
2	SO4	B	708	5/5	0.83	0.15	-	123,145,145,147	0
2	SO4	A	706	5/5	0.93	0.21	-	101,117,123,127	0
2	SO4	B	707	5/5	0.84	0.19	-	138,140,146,150	0

6.5 Other polymers [i](#)

There are no such residues in this entry.