



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 05:54 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 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/ValidationPDFNotes.html>

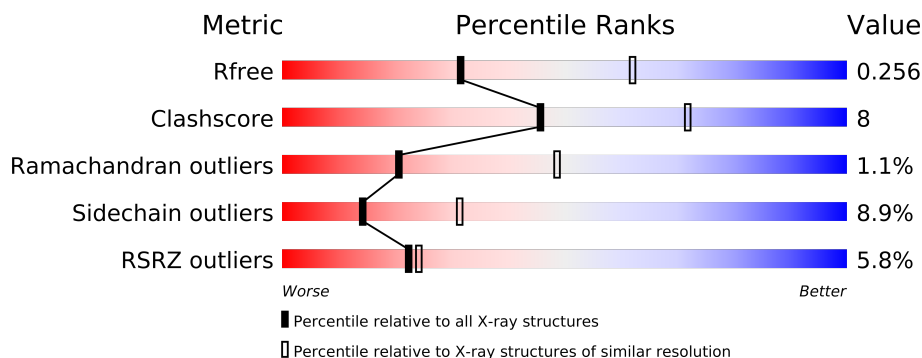
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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

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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	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.

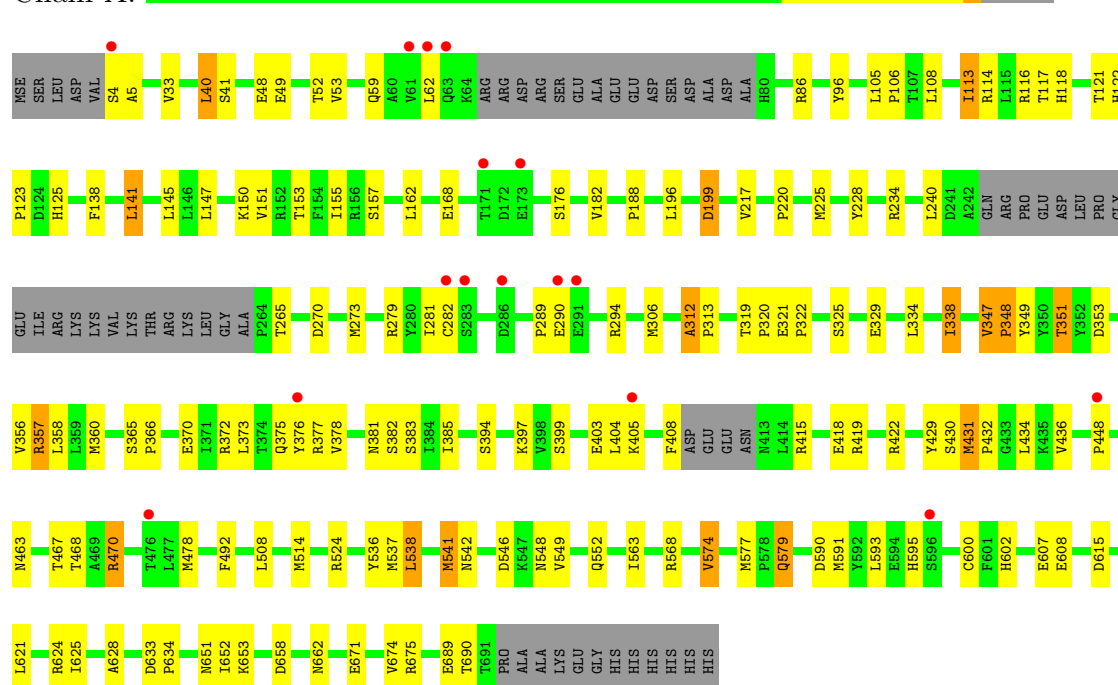
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total 38	O 38	0	0
3	B	18	Total 18	O 18	0	0

3 Residue-property plots

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.

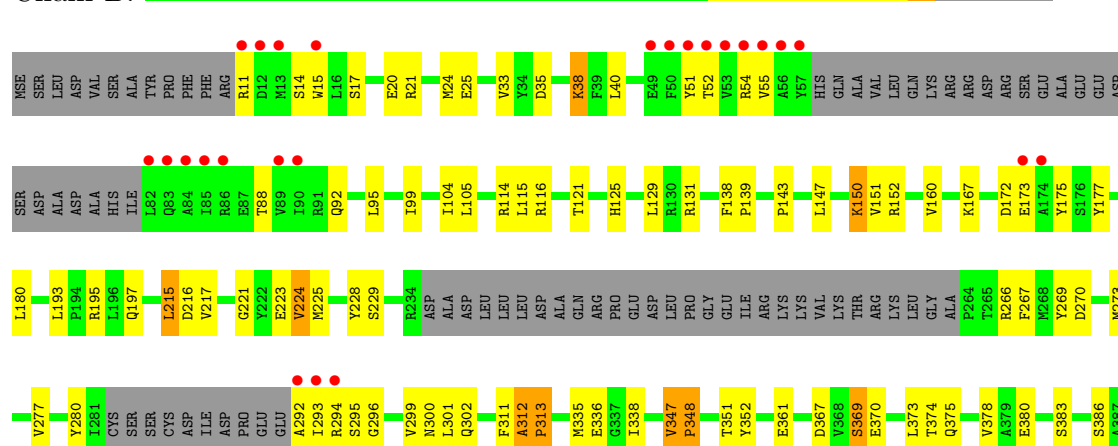
• Molecule 1: Polyphosphate kinase

Chain A:



• Molecule 1: Polyphosphate kinase

Chain B:





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 0.191 , 0.256	Depositor DCC
R_{free} test set	1583 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)	0.30 , 52.0	EDS
Estimated twinning fraction	0.067 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 50844 reflections	Xtriage
F_o, F_c correlation	0.94	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (172) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:86:ARG:NH1	1:A:290:GLU:O	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	644/705 (91%)	612 (95%)	26 (4%)	6 (1%)	25	55
1	B	596/705 (84%)	553 (93%)	36 (6%)	7 (1%)	19	45
All	All	1240/1410 (88%)	1165 (94%)	62 (5%)	13 (1%)	21	51

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%)	17	36
1	B	547/612 (89%)	493 (90%)	54 (10%)	11	26
All	All	1134/1224 (93%)	1032 (91%)	102 (9%)	14	31

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0.16	0	6,6,6	0.23	0
2	SO4	A	705	-	4,4,4	0.17	0	6,6,6	0.21	0
2	SO4	A	706	-	4,4,4	0.15	0	6,6,6	0.22	0
2	SO4	A	707	-	4,4,4	0.19	0	6,6,6	0.26	0
2	SO4	A	708	-	4,4,4	0.28	0	6,6,6	0.12	0
2	SO4	A	709	-	4,4,4	0.19	0	6,6,6	0.10	0
2	SO4	A	710	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	A	711	-	4,4,4	0.26	0	6,6,6	0.18	0
2	SO4	B	704	-	4,4,4	0.21	0	6,6,6	0.08	0
2	SO4	B	705	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	B	706	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	B	707	-	4,4,4	0.20	0	6,6,6	0.07	0
2	SO4	B	708	-	4,4,4	0.16	0	6,6,6	0.11	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	648/705 (91%)	-0.15	16 (2%) 54 61	39, 62, 107, 168	0
1	B	605/705 (85%)	0.16	58 (9%) 8 8	41, 72, 114, 163	0
All	All	1253/1410 (88%)	0.00	74 (5%) 22 23	39, 67, 110, 168	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	ILE	9.7
1	B	571	CYS	8.2
1	B	573	LEU	7.4
1	B	669	SER	6.4
1	B	82	LEU	5.9
1	B	578	PRO	5.3
1	B	668	ASN	5.1
1	B	572	CYS	4.8
1	B	53	VAL	4.7
1	B	574	VAL	4.7
1	B	575	PRO	4.6
1	B	13	MSE	4.6
1	B	570	ILE	4.5
1	A	405	LYS	4.4
1	B	670	ASP	4.3
1	A	286	ASP	4.2
1	B	173	GLU	4.2
1	B	547	LYS	4.1
1	B	54	ARG	4.1
1	B	57	TYR	4.0
1	B	622	TYR	3.9
1	A	283	SER	3.9
1	B	56	ALA	3.8
1	B	466	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	84	ALA	3.8
1	B	544	LEU	3.7
1	B	15	TRP	3.7
1	B	86	ARG	3.7
1	A	171	THR	3.7
1	A	62	LEU	3.6
1	B	549	VAL	3.6
1	B	553	LEU	3.6
1	B	52	THR	3.5
1	B	89	VAL	3.5
1	B	501	PRO	3.5
1	B	690	THR	3.4
1	A	290	GLU	3.4
1	B	90	ILE	3.3
1	B	545	GLN	3.3
1	B	83	GLN	3.2
1	B	55	VAL	3.1
1	B	667	HIS	2.9
1	B	292	ALA	2.8
1	A	596	SER	2.8
1	A	4	SER	2.8
1	B	467	THR	2.8
1	B	449	ALA	2.8
1	B	12	ASP	2.7
1	B	51	TYR	2.7
1	B	450	GLY	2.7
1	B	621	LEU	2.6
1	A	61	VAL	2.6
1	B	546	ASP	2.6
1	B	11	ARG	2.6
1	B	293	ILE	2.6
1	B	294	ARG	2.5
1	A	476	THR	2.5
1	B	468	THR	2.5
1	B	548	ASN	2.5
1	A	291	GLU	2.4
1	B	50	PHE	2.4
1	B	576	ASP	2.4
1	A	448	PRO	2.4
1	B	465	ASN	2.3
1	A	63	GLN	2.3
1	A	173	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	376	TYR	2.3
1	B	671	GLU	2.2
1	B	577	MSE	2.2
1	B	554	TYR	2.2
1	B	49	GLU	2.1
1	B	500	GLU	2.1
1	A	282	CYS	2.1
1	B	174	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	B	707	5/5	0.19	1.74	138,140,146,150	0
2	SO4	A	708	5/5	0.20	1.58	114,123,127,134	0
2	SO4	A	705	5/5	0.15	0.40	89,114,127,132	0
2	SO4	A	710	5/5	0.15	0.24	103,116,127,134	0
2	SO4	A	707	5/5	0.21	0.16	68,68,92,102	0
2	SO4	A	706	5/5	0.20	0.04	101,117,123,127	0
2	SO4	B	706	5/5	0.15	-0.21	116,122,128,133	0
2	SO4	A	709	5/5	0.12	-0.76	66,77,96,99	0
2	SO4	A	711	5/5	0.12	-0.93	131,132,134,135	0
2	SO4	B	704	5/5	0.08	-1.56	88,96,109,111	0
2	SO4	B	708	5/5	0.15	-1.75	123,145,145,147	0
2	SO4	B	705	5/5	0.14	-1.81	108,109,122,138	0
2	SO4	A	704	5/5	0.08	-2.27	79,84,104,105	0

6.5 Other polymers ⓘ

There are no such residues in this entry.