



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 08:01 AM EDT

PDB ID : 1KBL / pdb_00001kbl
Title : PYRUVATE PHOSPHATE DIKINASE
Authors : Herzberg, O.; Chen, C.C.; Liu, S.
Deposited on : 2001-11-06
Resolution : 1.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

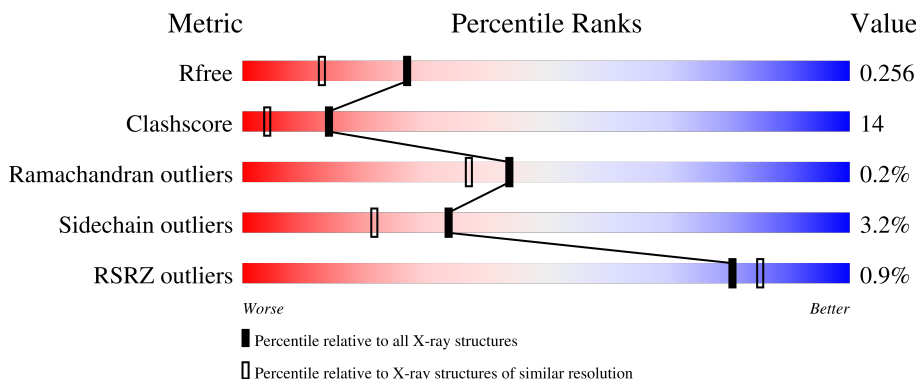
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1306 (1.94-1.94)
Clashscore	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	873	

2 Entry composition [i](#)

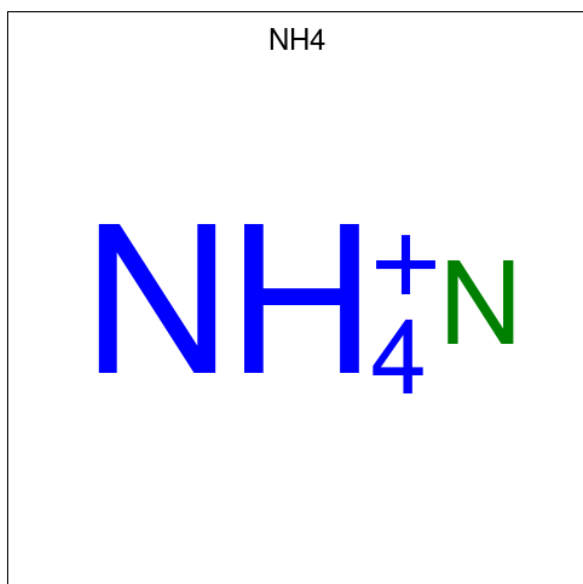
There are 4 unique types of molecules in this entry. The entry contains 7657 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PYRUVATE PHOSPHATE DIKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	872	Total	C	N	O	S	25	0	0
			6752	4250	1143	1308	51			

- Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

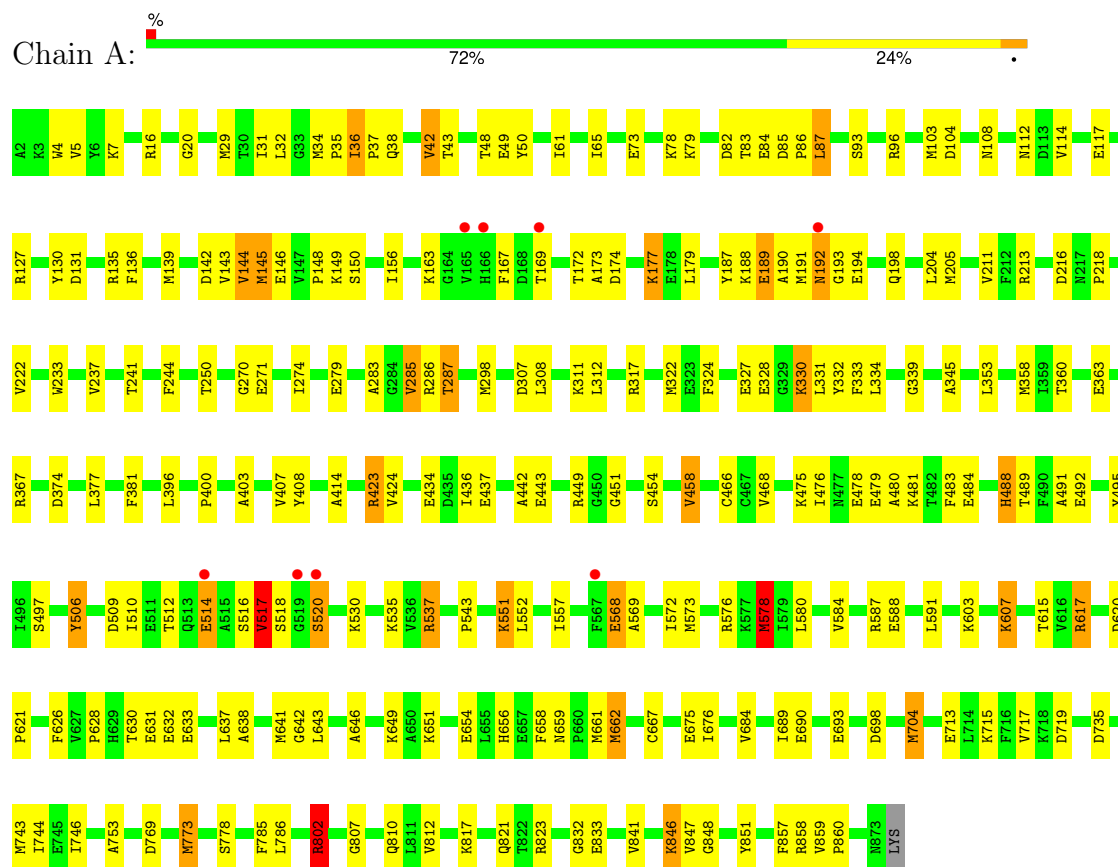
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	879	Total	O	0	0
			879	879		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PYRUVATE PHOSPHATE DIKINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.84Å 58.84Å 102.95Å 90.00° 94.84° 90.00°	Depositor
Resolution (Å)	20.00 – 1.94 20.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	90.9 (20.00-1.94) 94.7 (20.00-1.94)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.195 , 0.257 0.194 , 0.256	Depositor DCC
R_{free} test set	4598 reflections (6.09%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7657	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, NH4

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	1.15	20/6876 (0.3%)	1.27	62/9269 (0.7%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	773	MET	SD-CE	13.40	2.13	1.79
1	A	704	MET	SD-CE	10.28	2.05	1.79
1	A	667	CYS	CA-CB	8.34	1.66	1.53
1	A	322	MET	SD-CE	6.93	1.96	1.79
1	A	36	ILE	CA-CB	-6.80	1.46	1.54
1	A	573	MET	SD-CE	6.79	1.96	1.79
1	A	578	MET	SD-CE	-6.72	1.62	1.79
1	A	638	ALA	CA-CB	6.54	1.63	1.53
1	A	847	VAL	CA-CB	6.05	1.62	1.54
1	A	103	MET	SD-CE	6.00	1.94	1.79
1	A	746	ILE	CA-C	5.88	1.57	1.52
1	A	817	LYS	N-CA	5.62	1.53	1.46
1	A	250	THR	CA-CB	-5.62	1.45	1.53
1	A	802	ARG	N-CA	5.60	1.52	1.46
1	A	345	ALA	CA-CB	5.57	1.61	1.53
1	A	324	PHE	C-O	5.55	1.30	1.23
1	A	744	ILE	CA-C	-5.54	1.46	1.52
1	A	615	THR	CA-C	5.28	1.59	1.52
1	A	823	ARG	CA-CB	5.08	1.59	1.53
1	A	744	ILE	CA-CB	5.05	1.60	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ASP	CA-C-N	-9.26	111.23	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ASP	C-N-CA	-9.26	111.23	120.31
1	A	145	MET	N-CA-C	-8.83	96.47	109.63
1	A	517	VAL	N-CA-C	8.65	119.13	108.06
1	A	488	HIS	N-CA-C	8.02	120.31	108.60
1	A	520	SER	N-CA-C	-7.94	102.22	112.23
1	A	621	PRO	N-CA-C	7.79	120.21	110.70
1	A	537	ARG	NE-CZ-NH2	-7.66	112.30	119.20
1	A	43	THR	N-CA-C	7.66	120.64	110.53
1	A	537	ARG	NE-CZ-NH1	7.57	129.07	121.50
1	A	177	LYS	N-CA-C	-7.48	103.20	111.36
1	A	285	VAL	N-CA-C	-7.32	103.39	110.42
1	A	423	ARG	N-CA-C	-7.12	97.64	109.46
1	A	659	ASN	CA-C-N	6.98	127.57	119.47
1	A	659	ASN	C-N-CA	6.98	127.57	119.47
1	A	144	VAL	N-CA-C	6.78	116.91	110.53
1	A	753	ALA	N-CA-C	6.69	120.32	111.75
1	A	244	PHE	N-CA-C	6.69	119.82	107.99
1	A	7	LYS	N-CA-C	-6.65	101.58	110.55
1	A	286	ARG	N-CA-C	-6.51	99.02	109.96
1	A	143	VAL	N-CA-C	6.48	116.64	110.42
1	A	620	ASP	N-CA-C	6.42	123.99	109.81
1	A	42	VAL	N-CA-C	-6.38	98.47	108.23
1	A	86	PRO	N-CA-C	6.33	121.19	111.57
1	A	84	GLU	N-CA-C	6.32	120.87	111.96
1	A	443	GLU	N-CA-C	-6.29	104.31	112.23
1	A	339	GLY	N-CA-C	6.16	119.92	111.54
1	A	87	LEU	N-CA-C	-6.09	99.31	109.24
1	A	746	ILE	N-CA-C	-6.00	101.35	107.89
1	A	557	ILE	N-CA-C	5.96	116.46	107.75
1	A	812	VAL	N-CA-C	-5.82	105.06	110.53
1	A	832	GLY	CA-C-O	-5.67	115.55	122.75
1	A	832	GLY	N-CA-C	-5.64	102.82	112.30
1	A	407	VAL	N-CA-C	5.63	116.87	109.21
1	A	735	ASP	N-CA-C	-5.59	103.98	111.87
1	A	713	GLU	N-CA-C	-5.56	105.13	111.14
1	A	287	THR	CA-C-N	-5.52	114.24	119.76
1	A	287	THR	C-N-CA	-5.52	114.24	119.76
1	A	568	GLU	N-CA-C	5.51	118.23	110.23
1	A	36	ILE	CB-CA-C	-5.50	104.49	110.37
1	A	145	MET	CA-C-N	-5.47	113.70	122.62
1	A	145	MET	C-N-CA	-5.47	113.70	122.62
1	A	506	TYR	N-CA-C	5.47	118.48	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	LEU	N-CA-C	5.47	117.62	109.25
1	A	846	LYS	N-CA-C	5.47	118.00	111.71
1	A	400	PRO	N-CA-C	5.45	119.78	111.34
1	A	442	ALA	N-CA-C	5.42	118.94	110.32
1	A	821	GLN	N-CA-C	-5.41	105.46	111.36
1	A	131	ASP	N-CA-C	-5.24	105.48	111.14
1	A	283	ALA	N-CA-C	5.24	117.90	111.82
1	A	848	GLY	N-CA-C	5.16	122.71	115.43
1	A	717	VAL	N-CA-C	5.14	115.91	110.72
1	A	537	ARG	CB-CG-CD	5.14	123.12	111.30
1	A	374	ASP	N-CA-C	-5.11	105.89	111.82
1	A	48	THR	N-CA-C	-5.10	105.80	111.36
1	A	743	MET	N-CA-C	-5.10	102.93	110.48
1	A	476	ILE	CB-CA-C	-5.10	104.22	111.21
1	A	684	VAL	N-CA-C	5.09	115.31	110.42
1	A	468	VAL	N-CA-C	-5.07	101.02	108.11
1	A	841	VAL	N-CA-C	-5.06	105.46	110.62
1	A	20	GLY	N-CA-C	-5.01	106.14	112.65
1	A	744	ILE	N-CA-C	-5.01	98.75	106.72

There are no chirality outliers.

There are no planarity outliers.

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	6752	0	6668	187	0
2	A	1	0	0	0	0
3	A	25	0	0	0	0
4	A	879	0	0	26	0
All	All	7657	0	6668	187	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 14.

All (187) 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:704:MET:CE	1:A:704:MET:SD	2.05	1.44
1:A:773:MET:CE	1:A:773:MET:SD	2.13	1.36
1:A:172:THR:HG22	1:A:174:ASP:H	1.09	1.16
1:A:144:VAL:HG12	1:A:145:MET:HE3	1.30	1.07
1:A:514:GLU:HG2	4:A:1238:HOH:O	1.60	0.99
1:A:29:MET:CB	1:A:36:ILE:HD11	1.94	0.98
1:A:353:LEU:HD22	1:A:358:MET:HE2	1.48	0.93
1:A:29:MET:HB3	1:A:36:ILE:HD11	1.49	0.93
1:A:580:LEU:CB	1:A:641:MET:HE1	2.02	0.89
1:A:580:LEU:HG	1:A:641:MET:HE1	1.60	0.83
1:A:317:ARG:HA	1:A:358:MET:HE3	1.58	0.83
1:A:584:VAL:O	1:A:588:GLU:HG3	1.80	0.82
1:A:144:VAL:HG12	1:A:145:MET:CE	2.10	0.80
1:A:172:THR:HG22	1:A:174:ASP:N	1.93	0.79
1:A:190:ALA:C	1:A:191:MET:HE2	2.08	0.79
1:A:580:LEU:CG	1:A:641:MET:HE1	2.15	0.76
1:A:156:ILE:HG13	1:A:179:LEU:HD21	1.67	0.75
1:A:576:ARG:HD3	1:A:626:PHE:O	1.87	0.74
1:A:537:ARG:HD2	4:A:1047:HOH:O	1.86	0.74
1:A:654:GLU:HG3	4:A:1765:HOH:O	1.88	0.73
1:A:29:MET:HB2	1:A:36:ILE:HD11	1.70	0.73
1:A:65:ILE:HG21	1:A:205:MET:HE1	1.72	0.72
1:A:188:LYS:C	1:A:190:ALA:H	1.98	0.71
1:A:662:MET:CE	1:A:773:MET:HG2	2.21	0.71
1:A:144:VAL:O	1:A:145:MET:HE2	1.91	0.70
1:A:189:GLU:O	1:A:189:GLU:HG3	1.92	0.68
1:A:481:LYS:HD3	1:A:492:GLU:OE2	1.94	0.68
1:A:662:MET:HE1	1:A:773:MET:HG2	1.76	0.68
1:A:434:GLU:HG3	4:A:1507:HOH:O	1.93	0.67
1:A:578:MET:HG2	1:A:587:ARG:HG2	1.75	0.67
1:A:423:ARG:HH22	1:A:509:ASP:CG	2.02	0.66
1:A:630:THR:HG22	1:A:633:GLU:H	1.61	0.66
1:A:580:LEU:HB2	1:A:641:MET:HE1	1.78	0.66
1:A:37:PRO:HB3	1:A:241:THR:HG23	1.79	0.64
1:A:488:HIS:CD2	1:A:489:THR:H	2.14	0.64
1:A:551:LYS:NZ	1:A:551:LYS:HB2	2.10	0.64
1:A:675:GLU:HG3	4:A:1710:HOH:O	1.97	0.64
1:A:641:MET:HE3	1:A:643:LEU:HD12	1.80	0.63
1:A:506:TYR:CG	1:A:510:ILE:HD11	2.34	0.63
1:A:108:ASN:HB2	1:A:136:PHE:HB2	1.81	0.62
1:A:188:LYS:HG3	1:A:194:GLU:O	2.00	0.61
1:A:167:PHE:HB3	1:A:169:THR:HG22	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:ARG:HG3	1:A:802:ARG:NH1	2.14	0.61
1:A:580:LEU:HG	1:A:641:MET:CE	2.28	0.61
1:A:334:LEU:HD12	4:A:1234:HOH:O	2.00	0.60
1:A:858:ARG:HD2	4:A:1632:HOH:O	2.01	0.60
1:A:5:VAL:HG21	1:A:65:ILE:HD13	1.84	0.60
1:A:29:MET:HB2	1:A:36:ILE:CD1	2.31	0.60
1:A:190:ALA:O	1:A:191:MET:HE2	2.03	0.59
1:A:317:ARG:CA	1:A:358:MET:HE3	2.30	0.59
1:A:353:LEU:HD22	1:A:358:MET:CE	2.30	0.59
1:A:576:ARG:HD2	1:A:628:PRO:HD3	1.84	0.59
1:A:769:ASP:HB3	1:A:773:MET:HE3	1.85	0.58
1:A:4:TRP:CH2	1:A:49:GLU:HG2	2.37	0.58
1:A:423:ARG:NH2	1:A:509:ASP:OD2	2.35	0.58
1:A:630:THR:CG2	1:A:632:GLU:HB3	2.34	0.58
1:A:785:PHE:N	4:A:1156:HOH:O	2.36	0.58
1:A:34:MET:HE3	1:A:308:LEU:HD22	1.85	0.58
1:A:484:GLU:HG3	1:A:489:THR:OG1	2.04	0.58
1:A:150:SER:HA	4:A:1620:HOH:O	2.04	0.58
1:A:307:ASP:HB3	4:A:1441:HOH:O	2.04	0.57
1:A:846:LYS:HE2	4:A:1567:HOH:O	2.05	0.57
1:A:144:VAL:CG1	1:A:145:MET:HE3	2.21	0.56
1:A:82:ASP:OD2	1:A:83:THR:N	2.38	0.56
1:A:142:ASP:CG	1:A:149:LYS:HE3	2.31	0.56
1:A:112:ASN:HB2	1:A:198:GLN:OE1	2.06	0.56
1:A:377:LEU:HD12	1:A:857:PHE:O	2.06	0.56
1:A:83:THR:OG1	1:A:114:VAL:CG1	2.54	0.55
1:A:689:ILE:O	1:A:693:GLU:HG3	2.06	0.55
1:A:630:THR:HG22	1:A:632:GLU:N	2.23	0.54
1:A:454:SER:O	1:A:458:VAL:HG13	2.07	0.54
1:A:551:LYS:NZ	1:A:551:LYS:CB	2.70	0.54
1:A:187:TYR:CE1	1:A:191:MET:HG3	2.43	0.53
1:A:32:LEU:HD22	1:A:311:LYS:NZ	2.24	0.53
1:A:578:MET:HG2	1:A:587:ARG:CG	2.38	0.53
1:A:144:VAL:C	1:A:145:MET:HE2	2.34	0.52
1:A:117:GLU:OE2	1:A:130:TYR:OH	2.21	0.52
1:A:802:ARG:HH11	1:A:802:ARG:CG	2.23	0.52
1:A:50:TYR:OH	1:A:213:ARG:HG2	2.09	0.52
1:A:535:LYS:HE3	4:A:1256:HOH:O	2.10	0.52
1:A:617:ARG:HB2	1:A:704:MET:HE2	1.91	0.52
1:A:156:ILE:HG13	1:A:179:LEU:CD2	2.38	0.51
1:A:578:MET:CG	1:A:587:ARG:HG2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:SER:O	1:A:517:VAL:HG13	2.10	0.51
1:A:642:GLY:HA2	4:A:1169:HOH:O	2.10	0.51
1:A:42:VAL:HG22	1:A:65:ILE:CD1	2.41	0.51
1:A:188:LYS:C	1:A:190:ALA:N	2.65	0.51
1:A:317:ARG:C	1:A:358:MET:HE3	2.36	0.51
1:A:833:GLU:O	1:A:858:ARG:NH2	2.35	0.51
1:A:475:LYS:O	1:A:483:PHE:HA	2.11	0.51
1:A:285:VAL:N	4:A:1062:HOH:O	2.41	0.50
1:A:16:ARG:NE	1:A:96:ARG:O	2.34	0.50
1:A:530:LYS:HD2	4:A:1692:HOH:O	2.12	0.50
1:A:802:ARG:NH1	1:A:802:ARG:CG	2.75	0.50
1:A:396:LEU:HD12	1:A:451:GLY:HA2	1.92	0.50
1:A:646:ALA:O	4:A:1656:HOH:O	2.18	0.50
1:A:218:PRO:O	1:A:222:VAL:HG23	2.11	0.50
1:A:317:ARG:HH22	1:A:363:GLU:CD	2.20	0.50
1:A:578:MET:CE	1:A:591:LEU:HD21	2.42	0.49
1:A:551:LYS:HB2	1:A:551:LYS:HZ2	1.73	0.49
1:A:204:LEU:HG	1:A:205:MET:CE	2.42	0.49
1:A:480:ALA:O	1:A:481:LYS:HB2	2.13	0.49
1:A:73:GLU:HG2	1:A:78:LYS:O	2.13	0.49
1:A:360:THR:OG1	1:A:363:GLU:HG3	2.13	0.49
1:A:802:ARG:HG3	1:A:802:ARG:HH11	1.78	0.48
1:A:661:MET:HE1	1:A:778:SER:HB3	1.94	0.48
1:A:658:PHE:HA	4:A:1165:HOH:O	2.13	0.48
1:A:130:TYR:CD2	1:A:177:LYS:HG2	2.49	0.48
1:A:189:GLU:O	1:A:189:GLU:CG	2.61	0.48
1:A:16:ARG:HD3	1:A:96:ARG:HG3	1.96	0.47
1:A:96:ARG:HD2	1:A:233:TRP:CZ3	2.48	0.47
1:A:537:ARG:HD3	1:A:851:TYR:CD1	2.49	0.47
1:A:475:LYS:HD3	1:A:475:LYS:HA	1.61	0.47
1:A:330:LYS:HE2	4:A:1546:HOH:O	2.13	0.47
1:A:408:TYR:HD1	1:A:424:VAL:HG13	1.80	0.47
1:A:628:PRO:HB3	1:A:633:GLU:HB3	1.97	0.47
1:A:211:VAL:HG11	1:A:237:VAL:HG22	1.96	0.47
1:A:135:ARG:O	1:A:139:MET:HG3	2.15	0.47
1:A:578:MET:HE1	1:A:676:ILE:HG12	1.96	0.47
1:A:330:LYS:HD2	1:A:332:TYR:OH	2.14	0.47
1:A:637:LEU:HG	1:A:641:MET:HE2	1.97	0.47
1:A:769:ASP:HB3	1:A:773:MET:CE	2.44	0.46
1:A:38:GLN:O	1:A:241:THR:HG22	2.15	0.46
1:A:617:ARG:HB2	1:A:704:MET:CE	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:TYR:CZ	1:A:191:MET:HG3	2.50	0.46
1:A:607:LYS:HB3	1:A:607:LYS:HE3	1.67	0.46
1:A:4:TRP:CG	1:A:61:ILE:HG12	2.50	0.46
1:A:785:PHE:CA	4:A:1156:HOH:O	2.64	0.46
1:A:130:TYR:CG	1:A:177:LYS:HG2	2.51	0.46
1:A:403:ALA:HB2	1:A:466:CYS:HB3	1.98	0.46
1:A:204:LEU:HG	1:A:205:MET:HE2	1.97	0.46
1:A:603:LYS:NZ	1:A:690:GLU:OE1	2.40	0.46
1:A:436:ILE:HG23	1:A:437:GLU:N	2.31	0.46
1:A:576:ARG:CD	1:A:628:PRO:HD3	2.45	0.46
1:A:334:LEU:CD1	4:A:1234:HOH:O	2.61	0.45
1:A:172:THR:HG22	1:A:173:ALA:N	2.32	0.45
1:A:858:ARG:CD	4:A:1632:HOH:O	2.61	0.45
1:A:191:MET:HB3	1:A:194:GLU:HB3	1.99	0.45
1:A:551:LYS:CB	1:A:551:LYS:HZ3	2.30	0.45
1:A:715:LYS:HZ2	1:A:719:ASP:CG	2.25	0.45
1:A:807:GLY:O	1:A:810:GLN:HB2	2.17	0.44
1:A:414:ALA:HB1	1:A:424:VAL:HG11	1.99	0.44
1:A:145:MET:O	1:A:146:GLU:HG2	2.17	0.44
1:A:381:PHE:HA	1:A:512:THR:HA	2.00	0.44
1:A:580:LEU:HD13	1:A:651:LYS:HG2	2.00	0.44
1:A:630:THR:HG22	1:A:632:GLU:H	1.82	0.44
1:A:148:PRO:O	1:A:149:LYS:C	2.60	0.43
1:A:491:ALA:O	1:A:492:GLU:C	2.61	0.43
1:A:488:HIS:CG	1:A:489:THR:H	2.36	0.43
1:A:506:TYR:CB	1:A:510:ILE:HD11	2.48	0.43
1:A:188:LYS:HE3	1:A:193:GLY:O	2.18	0.43
1:A:628:PRO:CB	1:A:633:GLU:HB3	2.47	0.43
1:A:172:THR:CG2	1:A:173:ALA:N	2.82	0.43
1:A:34:MET:SD	1:A:312:LEU:HD21	2.59	0.43
1:A:163:LYS:HE2	1:A:163:LYS:HB3	1.82	0.43
1:A:535:LYS:HE2	4:A:946:HOH:O	2.18	0.43
1:A:572:ILE:O	1:A:576:ARG:HG3	2.18	0.43
1:A:188:LYS:O	1:A:190:ALA:N	2.52	0.43
1:A:478:GLU:O	1:A:481:LYS:N	2.48	0.42
1:A:578:MET:HE3	1:A:591:LEU:HD21	2.00	0.42
1:A:859:VAL:N	1:A:860:PRO:CD	2.82	0.42
1:A:142:ASP:OD2	1:A:149:LYS:HE3	2.19	0.42
1:A:192:ASN:HD22	1:A:192:ASN:HA	1.65	0.42
1:A:656:HIS:HE1	4:A:1650:HOH:O	2.03	0.42
1:A:495:TYR:CD2	1:A:509:ASP:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:MET:HB3	1:A:35:PRO:HD2	2.01	0.42
1:A:367:ARG:HD2	4:A:1283:HOH:O	2.19	0.42
1:A:588:GLU:HG2	1:A:675:GLU:HG2	2.02	0.41
1:A:649:LYS:HE3	1:A:649:LYS:HB2	1.85	0.41
1:A:333:PHE:C	1:A:334:LEU:HD23	2.45	0.41
1:A:497:SER:HB2	1:A:506:TYR:HB2	2.02	0.41
1:A:145:MET:HE2	1:A:145:MET:HA	2.01	0.41
1:A:73:GLU:HG2	1:A:79:LYS:HA	2.02	0.41
1:A:327:GLU:O	1:A:328:GLU:C	2.63	0.41
1:A:367:ARG:CD	4:A:1283:HOH:O	2.69	0.41
1:A:78:LYS:HB2	1:A:87:LEU:HB2	2.02	0.41
1:A:205:MET:HE2	1:A:205:MET:N	2.36	0.41
1:A:270:GLY:C	1:A:271:GLU:HG3	2.46	0.41
1:A:274:ILE:CD1	1:A:298:MET:HE1	2.51	0.41
1:A:552:LEU:HD23	1:A:552:LEU:HA	1.90	0.41
1:A:568:GLU:O	1:A:569:ALA:C	2.64	0.41
1:A:37:PRO:CB	1:A:241:THR:HG23	2.49	0.41
1:A:93:SER:HB3	1:A:211:VAL:HG13	2.03	0.40
1:A:317:ARG:NH2	1:A:363:GLU:OE2	2.54	0.40
1:A:104:ASP:HA	4:A:1049:HOH:O	2.21	0.40
1:A:661:MET:CE	1:A:778:SER:HB3	2.51	0.40
1:A:5:VAL:CG2	1:A:65:ILE:HD13	2.51	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	870/873 (100%)	837 (96%)	31 (4%)	2 (0%)	44	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	GLU
1	A	518	SER

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	713/714 (100%)	690 (97%)	23 (3%)	34	22

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

Mol	Chain	Res	Type
1	A	31	ILE
1	A	127	ARG
1	A	192	ASN
1	A	216	ASP
1	A	279	GLU
1	A	287	THR
1	A	330	LYS
1	A	449	ARG
1	A	458	VAL
1	A	479	GLU
1	A	514	GLU
1	A	517	VAL
1	A	520	SER
1	A	543	PRO
1	A	551	LYS
1	A	578	MET
1	A	607	LYS
1	A	617	ARG
1	A	631	GLU
1	A	662	MET
1	A	698	ASP
1	A	786	LEU
1	A	802	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	108	ASN
1	A	138	GLN
1	A	192	ASN
1	A	217	ASN
1	A	277	GLN
1	A	289	GLN
1	A	378	HIS
1	A	488	HIS
1	A	513	GLN
1	A	640	ASN
1	A	727	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is modelled with single atom - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	906	-	4,4,4	0.37	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	902	-	4,4,4	0.11	0	6,6,6	0.55	0
3	SO4	A	904	-	4,4,4	1.39	1 (25%)	6,6,6	1.37	2 (33%)
3	SO4	A	903	-	4,4,4	0.51	0	6,6,6	0.33	0
3	SO4	A	905	-	4,4,4	0.50	0	6,6,6	0.33	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	904	SO4	O2-S	-2.03	1.32	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	904	SO4	O4-S-O3	2.61	122.93	108.54
3	A	904	SO4	O3-S-O1	-2.01	99.08	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	872/873 (99%)	-0.06	8 (0%) 81 85	12, 34, 61, 82	7 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	HIS	2.9
1	A	165	VAL	2.6
1	A	519	GLY	2.2
1	A	514	GLU	2.2
1	A	192	ASN	2.1
1	A	567	PHE	2.1
1	A	169	THR	2.1
1	A	520	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	905	5/5	0.85	0.12	64,65,73,77	0
3	SO4	A	904	5/5	0.91	0.14	35,42,44,47	5
3	SO4	A	903	5/5	0.91	0.13	42,50,63,72	0
3	SO4	A	906	5/5	0.94	0.11	52,58,65,65	0
2	NH4	A	901	1/1	0.95	0.06	26,26,26,26	0
3	SO4	A	902	5/5	0.99	0.04	28,29,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.