WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 12:13 pm BST

PDB ID	:	1KZH
Title	:	Structure of a pyrophosphate-dependent phosphofructokinase from the Lyme disease spirochete Borrelia burgdorferi
Authors	:	Moore, S.A.; Ronimus, R.S.; Roberson, R.S.; Morgan, H.W.
Deposited on	:	2002-02-06
Resolution	:	2.55 Å(reported)

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

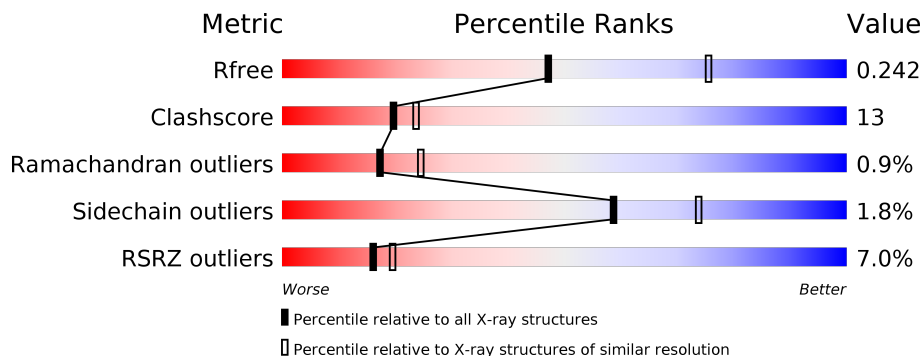|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.55 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	Percentile Ranks	Value
Rfree		0.242
Clashscore		13
Ramachandran outliers		0.9%
Sidechain outliers		1.8%
RSRZ outliers		7.0%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 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 <=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	555	3% / 76% / 21% / ••
1	B	555	11% / 73% / 21% / • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8512 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 phosphofructokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total 4291	C 2765	N 703	O 805	S 18	0	0	0
1	B	530	Total 4045	C 2607	N 659	O 761	S 18	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total 90	O 90	0	0
3	B	46	Total 46	O 46	0	0

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: phosphofructokinase

Chain A:

• Molecule 1: phosphofructokinase

Chain B:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.10Å 97.93Å 148.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.55 48.96 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.8 (100.00-2.55) 96.8 (48.96-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.34 (at 2.54Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.243 0.202 , 0.242	Depositor DCC
R_{free} test set	3995 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8512	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.35	0/4379	0.42	0/5917
1	B	0.41	1/4125 (0.0%)	0.47	3/5586 (0.1%)
All	All	0.38	1/8504 (0.0%)	0.44	3/11503 (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	B	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	PHE	CD2-CE2	7.10	1.53	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	332	PHE	CB-CG-CD2	6.29	125.20	120.80
1	B	253	ARG	NE-CZ-NH2	-6.22	117.19	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	253	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	B	331	ILE	Peptide
1	B	4	SER	Peptide

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	4291	0	4263	111	0
1	B	4045	0	3945	107	0
2	A	15	0	0	0	0
2	B	25	0	0	1	0
3	A	90	0	0	9	0
3	B	46	0	0	2	0
All	All	8512	0	8208	211	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 13.

All (211) 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:285:SER:HB2	1:B:405:ARG:HH22	1.20	1.05
1:A:323:SER:HB3	1:A:359:MET:CE	1.96	0.96
1:A:323:SER:HB3	1:A:359:MET:HE1	1.47	0.96
1:B:4:SER:HB2	1:B:6:PHE:H	1.34	0.91
1:A:292:VAL:HG11	1:A:405:ARG:HD2	1.59	0.83
1:B:285:SER:HB2	1:B:405:ARG:NH2	1.96	0.77
1:B:369:PHE:O	1:B:373:GLU:HB2	1.83	0.77
1:B:49:PHE:HA	1:B:187:GLU:OE1	1.85	0.77
1:B:331:ILE:HD12	1:B:351:PHE:CD2	2.20	0.76
1:A:329:CYS:SG	1:A:378:ILE:HD12	2.26	0.76
1:A:148:LYS:HE3	1:A:150:GLU:HB3	1.67	0.75
1:B:249:LYS:HD3	1:B:395:GLU:OE1	1.87	0.74
1:B:320:GLU:HG3	3:B:814:HOH:O	1.89	0.72
1:A:34:GLU:CD	1:A:34:GLU:H	1.92	0.72
1:A:4:SER:HB3	1:A:7:LYS:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ARG:HD2	1:B:312:GLU:HG2	1.72	0.72
1:B:372:PHE:HA	1:B:375:ILE:HD12	1.72	0.71
1:B:393:PRO:HB2	1:B:396:LYS:H	1.56	0.71
1:A:327:GLU:OE1	1:A:359:MET:HG3	1.91	0.70
1:A:343:ASN:O	1:A:347:MET:HB2	1.91	0.70
1:A:111:LYS:HE2	1:A:123:ILE:HG23	1.75	0.69
1:B:43:GLN:H	1:B:43:GLN:CD	1.98	0.68
1:A:494:GLU:HB2	1:A:496:LYS:HE3	1.75	0.67
1:A:382:ASP:OD2	1:A:386:ASN:HB2	1.95	0.66
1:B:487:ASN:HD22	1:B:487:ASN:H	1.43	0.66
1:B:324:LEU:HD21	1:B:363:TYR:HD1	1.59	0.66
1:B:405:ARG:O	1:B:409:MET:HG3	1.96	0.66
1:B:331:ILE:HD12	1:B:351:PHE:HD2	1.61	0.65
1:A:501:LYS:HE3	3:A:795:HOH:O	1.95	0.65
1:A:149:ILE:HG23	1:A:154:HIS:HB3	1.78	0.65
1:A:323:SER:HB3	1:A:359:MET:HE3	1.77	0.65
1:A:174:GLY:HA2	1:A:203:LYS:HE3	1.78	0.65
1:A:21:LEU:O	3:A:821:HOH:O	2.15	0.64
1:B:210:ARG:HH21	1:B:257:HIS:CE1	2.16	0.64
1:B:178:SER:HB2	2:B:1601:SO4:O1	1.97	0.63
1:B:509:ARG:HD2	1:B:551:LEU:O	1.99	0.63
1:A:286:GLU:O	1:A:290:GLU:HG3	1.99	0.63
1:A:149:ILE:HG22	1:A:155:TYR:CE2	2.33	0.62
1:B:348:LYS:CB	1:B:375:ILE:HD11	2.30	0.62
1:A:253:ARG:O	1:A:313:GLY:HA3	1.99	0.61
1:A:323:SER:CB	1:A:359:MET:HE1	2.27	0.61
1:B:348:LYS:O	1:B:351:PHE:HB2	2.01	0.61
1:B:120:ASN:ND2	1:B:122:LYS:HD2	2.16	0.61
1:B:283:THR:OG1	1:B:286:GLU:HG3	2.01	0.61
1:B:36:THR:HG21	1:B:481:PRO:CG	2.31	0.61
1:B:289:ASP:OD1	1:B:405:ARG:NH1	2.34	0.60
1:A:319:PRO:HG2	3:A:735:HOH:O	2.00	0.60
1:B:393:PRO:HB3	1:B:395:GLU:HG2	1.83	0.60
1:A:155:TYR:OH	1:A:184:ILE:HG21	2.01	0.60
1:A:333:ASP:O	1:A:336:GLU:HG3	2.02	0.59
1:B:163:LYS:HE3	1:B:194:GLU:OE1	2.03	0.59
1:A:283:THR:OG1	1:A:286:GLU:HG3	2.03	0.59
1:B:324:LEU:N	1:B:359:MET:HE1	2.18	0.59
1:A:370:ILE:HG13	1:A:397:LEU:HD13	1.85	0.59
1:B:36:THR:HG21	1:B:481:PRO:HG2	1.85	0.59
1:A:372:PHE:O	1:A:375:ILE:HB	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:TYR:OH	1:B:371:GLN:HB3	2.03	0.58
1:A:178:SER:O	1:A:181:ASN:HB2	2.05	0.57
1:A:291:MET:CE	1:A:402:ILE:HD11	2.34	0.57
1:B:253:ARG:O	1:B:313:GLY:HA3	2.04	0.57
1:A:5:LEU:HD21	1:B:540:GLU:HG2	1.88	0.56
1:A:75:ILE:HD12	1:A:98:ILE:HG21	1.88	0.56
1:A:174:GLY:HA3	1:A:178:SER:HB2	1.88	0.55
1:B:4:SER:OG	1:B:6:PHE:HB3	2.06	0.55
1:B:324:LEU:HB2	1:B:359:MET:CE	2.37	0.55
1:A:376:LYS:HD3	1:A:391:ARG:NH2	2.21	0.55
1:B:370:ILE:HD12	1:B:392:VAL:CG2	2.37	0.55
1:A:352:VAL:O	1:A:360:LYS:HD3	2.06	0.55
1:B:370:ILE:HG13	1:B:397:LEU:HD13	1.88	0.55
1:A:34:GLU:CD	1:A:34:GLU:N	2.59	0.55
1:B:472:PRO:HA	1:B:475:TRP:CD2	2.43	0.54
1:B:368:LEU:HD23	1:B:371:GLN:NE2	2.23	0.54
1:A:210:ARG:HB2	1:A:214:ILE:O	2.08	0.54
1:B:369:PHE:HE2	1:B:400:GLU:HG3	1.72	0.54
1:A:253:ARG:HG3	1:A:389:VAL:HG22	1.89	0.53
1:A:291:MET:HE3	1:A:402:ILE:HD11	1.89	0.53
1:B:347:MET:O	1:B:350:ILE:CG2	2.56	0.53
1:A:5:LEU:CD2	1:B:540:GLU:HG2	2.39	0.53
1:B:38:ALA:CB	1:B:45:LEU:HD12	2.39	0.53
1:A:509:ARG:HD2	1:A:551:LEU:O	2.07	0.53
1:A:291:MET:CE	1:A:398:PHE:CD1	2.92	0.53
1:A:43:GLN:H	1:A:43:GLN:CD	2.12	0.53
1:A:472:PRO:HA	1:A:475:TRP:CD2	2.45	0.52
1:A:291:MET:CE	1:A:398:PHE:HD1	2.23	0.52
1:B:330:ASP:C	1:B:332:PHE:H	2.11	0.52
1:B:327:GLU:OE1	1:B:355:LEU:HD23	2.08	0.52
1:A:291:MET:HE1	1:A:398:PHE:CD1	2.45	0.51
1:B:487:ASN:H	1:B:487:ASN:ND2	2.08	0.51
1:B:437:ASN:ND2	1:B:542:VAL:HG12	2.25	0.51
1:A:291:MET:HE1	1:A:398:PHE:HD1	1.76	0.51
1:B:347:MET:O	1:B:347:MET:HG2	2.11	0.51
1:B:123:ILE:HD11	1:B:142:VAL:HG12	1.92	0.51
1:B:4:SER:CB	1:B:6:PHE:H	2.14	0.51
1:A:335:ASN:HB2	1:A:339:PHE:CE1	2.46	0.51
1:B:151:THR:O	1:B:154:HIS:HB2	2.10	0.50
1:B:487:ASN:HD22	1:B:487:ASN:N	2.04	0.50
1:A:487:ASN:HD22	1:A:487:ASN:C	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ASN:OD1	1:A:354:LYS:HE3	2.12	0.50
1:A:335:ASN:CG	1:A:354:LYS:HE3	2.31	0.50
1:A:73:LEU:HD11	1:A:455:LEU:CD2	2.42	0.50
1:A:159:LEU:CD1	1:A:194:GLU:HG3	2.42	0.49
1:B:494:GLU:CG	1:B:496:LYS:HE3	2.42	0.49
1:B:149:ILE:HG23	1:B:154:HIS:HB3	1.95	0.49
1:A:242:LYS:HE2	1:B:143:SER:OG	2.13	0.49
1:A:274:SER:HB3	1:A:317:PHE:CG	2.48	0.49
1:B:203:LYS:HD2	1:B:203:LYS:C	2.33	0.49
1:A:203:LYS:HD2	1:A:203:LYS:C	2.33	0.49
1:B:331:ILE:CD1	1:B:351:PHE:HA	2.43	0.49
1:B:357:ASP:O	1:B:360:LYS:N	2.45	0.49
1:A:18:PRO:HD2	1:A:21:LEU:HD12	1.95	0.48
1:B:432:SER:HA	3:B:764:HOH:O	2.12	0.48
1:A:382:ASP:HB2	1:A:383:PRO:HD2	1.95	0.48
1:A:540:GLU:CD	1:B:5:LEU:HD22	2.34	0.48
1:B:494:GLU:HG3	1:B:496:LYS:HE3	1.96	0.48
1:A:174:GLY:HA3	1:A:178:SER:CB	2.43	0.48
1:B:120:ASN:HD22	1:B:120:ASN:C	2.17	0.48
1:B:129:LEU:CD2	1:B:141:ILE:HD11	2.43	0.48
1:B:18:PRO:HD3	1:B:445:SER:OG	2.13	0.48
1:B:58:ILE:HG22	1:B:59:SER:N	2.28	0.48
1:A:381:ARG:HA	1:A:386:ASN:O	2.14	0.47
1:B:30:LEU:CD2	1:B:60:PHE:HE2	2.27	0.47
1:A:533:VAL:HG13	3:A:804:HOH:O	2.14	0.47
1:A:373:GLU:HG3	1:A:393:PRO:HD2	1.97	0.47
1:B:157:LYS:O	1:B:161:VAL:HG23	2.14	0.47
1:B:151:THR:HG23	1:B:154:HIS:CE1	2.49	0.47
1:B:151:THR:O	1:B:154:HIS:N	2.47	0.47
1:A:143:SER:OG	1:B:242:LYS:HE2	2.14	0.47
1:A:203:LYS:HB2	1:A:218:PHE:CE1	2.50	0.47
1:A:490:GLU:HA	1:A:494:GLU:O	2.14	0.47
1:B:51:ASN:N	1:B:187:GLU:OE2	2.40	0.47
1:A:544:GLU:OE2	1:A:550:LYS:NZ	2.47	0.47
1:A:382:ASP:HB2	1:A:383:PRO:CD	2.44	0.47
1:A:346:LYS:C	1:A:348:LYS:H	2.16	0.46
1:B:120:ASN:HD22	1:B:122:LYS:HD2	1.80	0.46
1:B:351:PHE:O	1:B:355:LEU:HG	2.15	0.46
1:A:203:LYS:O	1:A:204:THR:HB	2.14	0.46
1:A:376:LYS:CD	1:A:391:ARG:NH2	2.78	0.46
1:B:317:PHE:O	1:B:319:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:THR:HB	1:B:484:MET:HB3	1.96	0.46
1:A:405:ARG:O	1:A:409:MET:HG3	2.15	0.46
1:A:236:ARG:HB2	1:A:529:TYR:CE2	2.51	0.46
1:A:90:VAL:O	1:A:94:VAL:HG23	2.16	0.46
1:B:58:ILE:CG2	1:B:59:SER:N	2.78	0.46
1:A:174:GLY:HA2	1:A:203:LYS:CE	2.44	0.46
1:A:472:PRO:HA	1:A:475:TRP:CE2	2.50	0.46
1:B:487:ASN:N	1:B:487:ASN:ND2	2.64	0.46
1:A:351:PHE:CD1	1:A:375:ILE:HD12	2.50	0.45
1:A:332:PHE:HA	1:A:339:PHE:CE1	2.51	0.45
1:A:296:LEU:HD11	1:A:409:MET:SD	2.57	0.45
1:A:312:GLU:OE2	1:A:390:SER:HA	2.15	0.45
1:A:73:LEU:HD11	1:A:455:LEU:HD21	1.98	0.45
1:A:148:LYS:HE3	1:A:150:GLU:CB	2.43	0.45
1:B:46:LYS:HA	1:B:53:TYR:CG	2.51	0.45
1:A:391:ARG:HH11	1:A:391:ARG:HG3	1.81	0.45
1:B:320:GLU:O	1:B:323:SER:HB2	2.17	0.45
1:A:291:MET:HB2	1:A:291:MET:HE3	1.84	0.45
1:B:159:LEU:HD11	1:B:194:GLU:HG3	1.99	0.44
1:B:467:ASN:HB3	1:B:470:LEU:HD22	1.99	0.44
1:B:277:VAL:HG13	1:B:282:LYS:HB2	1.97	0.44
1:B:172:ILE:HD12	1:B:182:ALA:HB2	1.99	0.44
1:B:330:ASP:C	1:B:332:PHE:N	2.71	0.44
1:B:36:THR:HG21	1:B:481:PRO:HG3	1.99	0.44
1:B:27:ASN:ND2	1:B:62:GLU:HG3	2.33	0.44
1:B:370:ILE:HG13	1:B:397:LEU:CD1	2.48	0.44
1:A:480:VAL:HG13	1:A:484:MET:SD	2.57	0.44
1:B:5:LEU:HG	1:B:5:LEU:O	2.17	0.44
1:A:350:ILE:HG23	1:A:354:LYS:HE2	2.00	0.44
1:A:348:LYS:HD3	1:A:372:PHE:CE2	2.52	0.44
1:A:536:PHE:O	1:B:536:PHE:HB2	2.17	0.44
1:A:242:LYS:HA	1:A:305:PHE:CD2	2.53	0.44
1:A:250:LEU:O	1:A:312:GLU:HB3	2.18	0.44
1:A:532:PRO:HG3	3:A:833:HOH:O	2.17	0.44
3:A:755:HOH:O	1:B:434:PHE:HD1	2.01	0.44
1:A:150:GLU:HA	1:A:155:TYR:OH	2.18	0.43
1:B:210:ARG:HB2	1:B:214:ILE:O	2.18	0.43
1:B:549:LEU:O	1:B:553:LEU:HB2	2.18	0.43
1:B:35:ASN:ND2	1:B:54:GLY:O	2.51	0.43
1:A:13:TYR:O	1:A:15:PRO:HD3	2.18	0.43
1:A:509:ARG:N	1:A:510:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LYS:C	1:A:348:LYS:N	2.72	0.43
1:B:197:GLN:NE2	1:B:457:GLY:HA2	2.33	0.43
1:A:175:GLY:HA2	1:A:209:LEU:HD22	1.99	0.43
1:A:265:LYS:O	1:A:528:LEU:HB2	2.18	0.43
1:B:487:ASN:HD21	1:B:498:VAL:HG13	1.84	0.43
1:A:36:THR:O	1:A:54:GLY:HA2	2.18	0.43
1:A:159:LEU:HD13	1:A:194:GLU:HG3	2.01	0.42
1:B:348:LYS:O	1:B:351:PHE:N	2.52	0.42
1:B:325:MET:SD	1:B:374:LEU:HD22	2.59	0.42
1:B:75:ILE:HD12	1:B:98:ILE:HG21	2.01	0.42
1:A:115:LEU:HD11	1:A:119:GLU:OE2	2.18	0.42
1:A:536:PHE:HB2	1:B:536:PHE:O	2.20	0.41
1:B:392:VAL:HA	1:B:393:PRO:HD3	1.94	0.41
1:A:10:ARG:CZ	1:A:535:TYR:HD2	2.33	0.41
1:A:186:ALA:HB2	1:A:198:VAL:HB	2.03	0.41
1:A:360:LYS:HE3	3:A:819:HOH:O	2.21	0.41
1:A:373:GLU:HG3	1:A:393:PRO:CD	2.51	0.41
1:A:163:LYS:HZ1	1:A:194:GLU:CD	2.25	0.41
1:A:360:LYS:CE	3:A:819:HOH:O	2.68	0.41
1:B:283:THR:HG23	1:B:286:GLU:OE1	2.21	0.41
1:B:348:LYS:HA	1:B:351:PHE:HD1	1.86	0.41
1:A:253:ARG:HG3	1:A:389:VAL:CG2	2.51	0.41
1:B:331:ILE:HD12	1:B:351:PHE:HA	2.03	0.41
1:B:50:LYS:N	1:B:187:GLU:OE2	2.54	0.41
1:A:16:LYS:HE2	3:A:749:HOH:O	2.21	0.40
1:B:79:LEU:HB3	1:B:139:PHE:CD1	2.56	0.40
1:B:73:LEU:HD11	1:B:455:LEU:CD2	2.51	0.40
1:A:335:ASN:O	1:A:337:GLY:N	2.54	0.40
1:A:350:ILE:CG2	1:A:354:LYS:HE2	2.51	0.40
1:B:120:ASN:ND2	1:B:120:ASN:O	2.54	0.40
1:A:389:VAL:C	1:A:391:ARG:N	2.73	0.40
1:B:4:SER:CB	1:B:6:PHE:HB3	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	548/555 (99%)	516 (94%)	26 (5%)	6 (1%)	14	19
1	B	524/555 (94%)	495 (94%)	25 (5%)	4 (1%)	19	27
All	All	1072/1110 (97%)	1011 (94%)	51 (5%)	10 (1%)	17	24

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	LYS
1	B	4	SER
1	A	281	LYS
1	B	394	THR
1	A	335	ASN
1	B	427	GLY
1	A	204	THR
1	A	347	MET
1	A	427	GLY
1	B	356	SER

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	465/488 (95%)	458 (98%)	7 (2%)	65	77
1	B	426/488 (87%)	417 (98%)	9 (2%)	53	68
All	All	891/976 (91%)	875 (98%)	16 (2%)	59	74

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	203	LYS

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Mol	Chain	Res	Type
1	A	312	GLU
1	A	391	ARG
1	A	405	ARG
1	A	487	ASN
1	A	507	GLU
1	B	120	ASN
1	B	122	LYS
1	B	181	ASN
1	B	203	LYS
1	B	267	HIS
1	B	350	ILE
1	B	487	ASN
1	B	494	GLU
1	B	507	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	166	ASN
1	A	195	ASN
1	A	371	GLN
1	A	384	HIS
1	A	403	GLN
1	A	487	ASN
1	B	8	GLN
1	B	26	ASN
1	B	120	ASN
1	B	166	ASN
1	B	371	GLN
1	B	487	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)

8 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	602	-	4,4,4	0.26	0	6,6,6	0.05	0
2	SO4	B	1601	-	4,4,4	0.24	0	6,6,6	0.04	0
2	SO4	A	601	-	4,4,4	0.26	0	6,6,6	0.04	0
2	SO4	B	1604	-	4,4,4	0.26	0	6,6,6	0.05	0
2	SO4	B	1600	-	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	A	600	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	B	1603	-	4,4,4	0.28	0	6,6,6	0.09	0
2	SO4	B	1602	-	4,4,4	0.25	0	6,6,6	0.05	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1601	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 (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	550/555 (99%)	0.03	15 (2%)	54	61	13, 28, 53, 79	0
1	B	530/555 (95%)	0.58	61 (11%)	4	6	11, 33, 76, 87	0
All	All	1080/1110 (97%)	0.30	76 (7%)	16	19	11, 30, 69, 87	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	PHE	8.6
1	B	355	LEU	7.7
1	B	353	ALA	7.4
1	B	358	TYR	7.4
1	A	342	LEU	7.4
1	B	379	LEU	7.3
1	B	347	MET	7.1
1	B	350	ILE	7.0
1	B	330	ASP	6.9
1	A	350	ILE	6.8
1	B	326	LEU	6.2
1	B	375	ILE	6.2
1	B	372	PHE	6.1
1	B	348	LYS	6.0
1	B	3	THR	5.7
1	B	344	ILE	5.4
1	B	352	VAL	5.4
1	A	339	PHE	5.2
1	B	378	ILE	5.2
1	B	374	LEU	5.1
1	B	377	SER	5.1
1	B	364	LEU	4.9
1	B	357	ASP	4.9
1	A	155	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	363	TYR	4.7
1	B	67	LEU	4.6
1	B	361	GLY	4.5
1	B	362	VAL	4.4
1	A	338	GLU	4.3
1	B	368	LEU	4.3
1	A	341	GLY	4.3
1	B	329	CYS	4.2
1	A	335	ASN	4.2
1	B	328	LEU	4.2
1	A	347	MET	3.9
1	B	346	LYS	3.8
1	B	370	ILE	3.8
1	B	371	GLN	3.8
1	B	160	PHE	3.6
1	B	360	LYS	3.5
1	B	354	LYS	3.4
1	B	345	GLU	3.3
1	B	69	PHE	3.3
1	B	331	ILE	3.3
1	B	332	PHE	3.2
1	B	349	GLU	3.1
1	B	68	SER	3.1
1	B	4	SER	3.1
1	B	325	MET	3.0
1	B	359	MET	3.0
1	B	380	GLU	2.8
1	B	153	GLU	2.7
1	A	353	ALA	2.7
1	B	356	SER	2.7
1	B	45	LEU	2.6
1	A	332	PHE	2.6
1	A	296	LEU	2.6
1	B	43	GLN	2.6
1	B	195	ASN	2.6
1	B	36	THR	2.6
1	A	344	ILE	2.6
1	A	343	ASN	2.5
1	B	492	TYR	2.4
1	B	188	TYR	2.4
1	B	366	LEU	2.4
1	B	493	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	151	THR	2.4
1	B	369	PHE	2.4
1	B	373	GLU	2.3
1	A	188	TYR	2.2
1	B	192	ASN	2.2
1	A	348	LYS	2.2
1	B	376	LYS	2.2
1	B	164	GLU	2.2
1	B	365	SER	2.0
1	B	411	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. 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(Å^2)	Q<0.9
2	SO4	B	1604	5/5	0.92	0.19	34,34,35,35	5
2	SO4	B	1602	5/5	0.92	0.22	76,77,79,79	0
2	SO4	B	1603	5/5	0.93	0.18	67,67,67,69	0
2	SO4	A	600	5/5	0.95	0.20	38,39,42,45	0
2	SO4	B	1601	5/5	0.95	0.14	70,71,74,75	0
2	SO4	A	602	5/5	0.95	0.12	45,48,48,50	0
2	SO4	B	1600	5/5	0.96	0.14	36,36,39,41	0
2	SO4	A	601	5/5	0.98	0.13	31,36,38,38	0

6.5   Other polymers (i)

There are no such residues in this entry.