



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:09 PM UTC

PDB ID : 1KZH / pdb_00001kzh
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)

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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

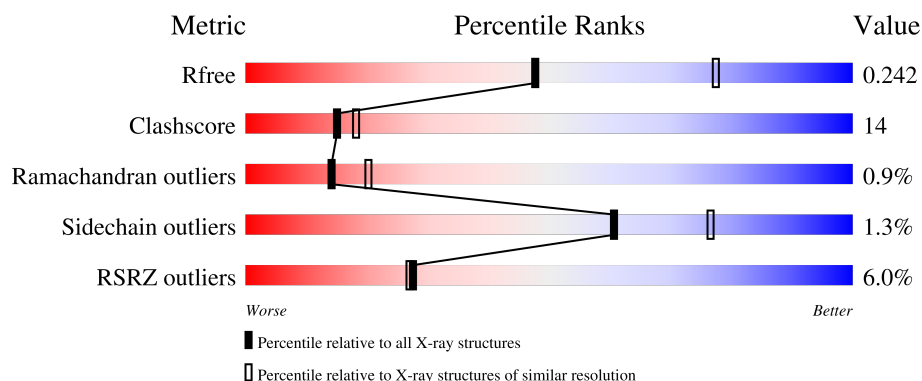
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	555	4% 76% 22% ..
1	B	555	8% 71% 23% 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	C	N	O	S	0	0	0
			4291	2765	703	805	18			
1	B	530	Total	C	N	O	S	0	0	0
			4045	2607	659	761	18			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

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

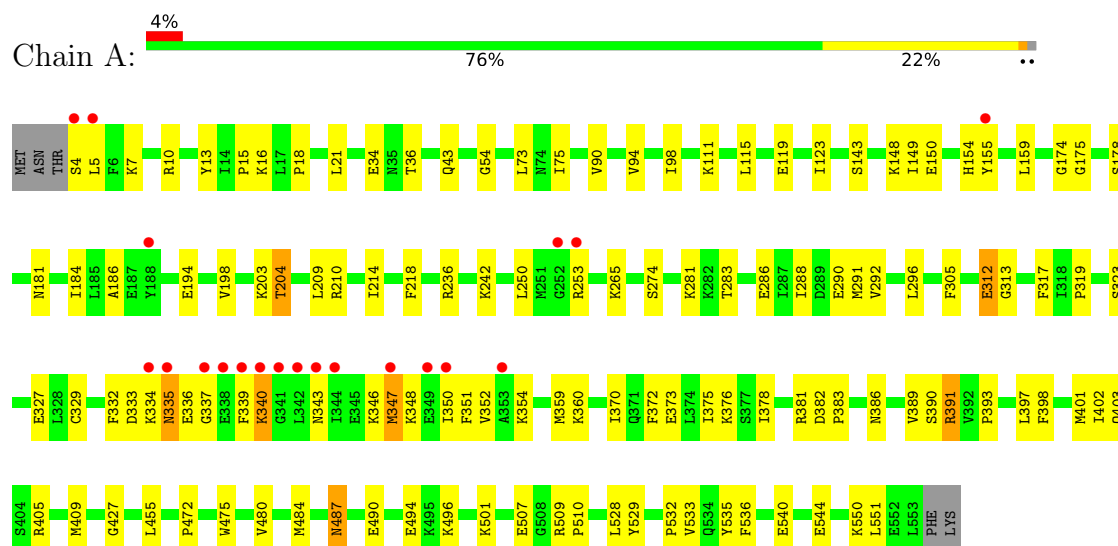
- Molecule 3 is water.

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

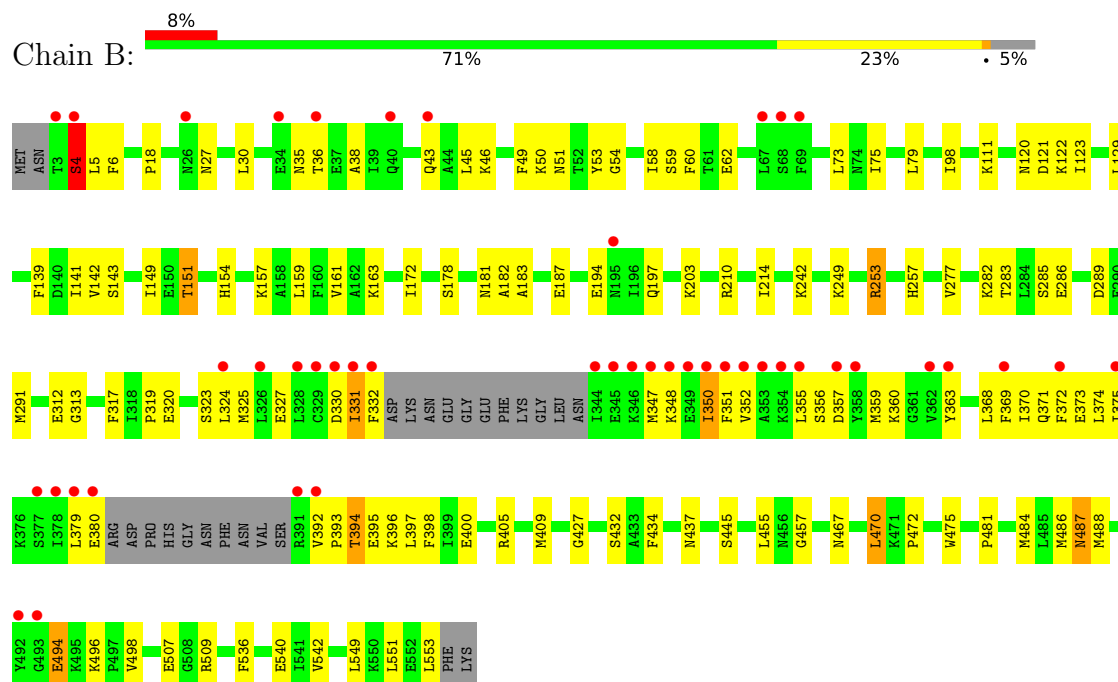
3 Residue-property plots [i](#)

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: phosphofructokinase



• Molecule 1: phosphofructokinase



4 Data and refinement statistics

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 81.70 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.8 (100.00-2.55) 96.8 (81.70-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.36 , 47.5	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	0.94	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.*

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

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	0.33	0/4379	0.69	0/5917
1	B	0.38	0/4125	0.73	2/5586 (0.0%)
All	All	0.35	0/8504	0.71	2/11503 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	VAL	N-CA-C	7.24	117.33	110.74
1	B	4	SER	N-CA-C	5.89	123.34	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	253	ARG	Mainchain
1	B	331	ILE	Peptide
1	B	4	SER	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	4291	0	4263	114	0
1	B	4045	0	3945	120	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	227	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 (227) 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:323:SER:HB3	1:A:359:MET:HE1	1.24	1.12
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:B:4:SER:HB2	1:B:6:PHE:H	1.34	0.91
1:A:323:SER:CB	1:A:359:MET:HE1	2.06	0.84
1:A:292:VAL:HG11	1:A:405:ARG:HD2	1.59	0.83
1:A:291:MET:HE3	1:A:402:ILE:HD11	1.60	0.82
1:A:291:MET:HE1	1:A:398:PHE:CD1	2.17	0.79
1:A:291:MET:HE1	1:A:398:PHE:HD1	1.47	0.78
1:B:285:SER:HB2	1:B:405:ARG:NH2	1.96	0.77
1:A:34:GLU:H	1:A:34:GLU:CD	1.92	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:45:LEU:HD23	1:B:488:MET:HE2	1.68	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:B:43:GLN:CD	1:B:43:GLN:H	1.98	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: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:H	1:B:487:ASN:HD22	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:288:ILE:HG13	1:A:401:MET:HE2	1.78	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:B:324:LEU:CA	1:B:359:MET:HE2	2.29	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:B:320:GLU:O	1:B:359:MET:HE1	2.01	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:34:GLU:CD	1:A:34:GLU:N	2.59	0.59
1:A:283:THR:OG1	1:A:286:GLU:HG3	2.03	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:B:330:ASP:C	1:B:332:PHE:H	2.11	0.57
1:A:43:GLN:H	1:A:43:GLN:CD	2.12	0.57
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:335:ASN:CG	1:A:354:LYS:HE3	2.31	0.55
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:A:487:ASN:C	1:A:487:ASN:HD22	2.14	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:324:LEU:HA	1:B:359:MET:HE2	1.87	0.55
1:B:370:ILE:HG13	1:B:397:LEU:HD13	1.88	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:B:203:LYS:HD2	1:B:203:LYS:C	2.33	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:203:LYS:HD2	1:A:203:LYS:C	2.33	0.53
1:A:540:GLU:CD	1:B:5:LEU:HD22	2.34	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:B:324:LEU:N	1:B:359:MET:HE2	2.24	0.53
1:B:120:ASN:C	1:B:120:ASN:HD22	2.17	0.53
1:A:472:PRO:HA	1:A:475:TRP:CD2	2.45	0.52
1:B:327:GLU:OE1	1:B:355:LEU:HD23	2.08	0.52
1:B:487:ASN:H	1:B:487:ASN:ND2	2.08	0.51
1:A:346:LYS:C	1:A:348:LYS:H	2.16	0.51
1:B:437:ASN:ND2	1:B:542:VAL:HG12	2.25	0.51
1:B:347:MET:O	1:B:347:MET:HG2	2.11	0.51
1:B:4:SER:CB	1:B:6:PHE:H	2.14	0.51
1:B:123:ILE:HD11	1:B:142:VAL:HG12	1.92	0.51
1:A:335:ASN:HB2	1:A:339:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:335:ASN:OD1	1:A:354:LYS:HE3	2.12	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: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:291:MET:CE	1:A:398:PHE:CD1	2.92	0.48
1:A:382:ASP:HB2	1:A:383:PRO:HD2	1.95	0.48
1:B:330:ASP:C	1:B:332:PHE:N	2.71	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: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:B:129:LEU:CD2	1:B:141:ILE:HD11	2.43	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:O	1:B:154:HIS:N	2.47	0.47
1:B:151:THR:HG23	1:B:154:HIS:CE1	2.49	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:A:544:GLU:OE2	1:A:550:LYS:NZ	2.47	0.47
1:B:51:ASN:N	1:B:187:GLU:OE2	2.40	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:N	2.72	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
1:B:36:THR:HB	1:B:484:MET:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:HB2	1:A:529:TYR:CE2	2.51	0.46
1:A:405:ARG:O	1:A:409:MET:HG3	2.15	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:ND2	1:B:487:ASN:N	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:B:291:MET:HE1	1:B:398:PHE:CG	2.51	0.45
1:A:73:LEU:HD11	1:A:455:LEU:HD21	1.98	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: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:HG3	1:A:391:ARG:HH11	1.81	0.45
1:B:320:GLU:O	1:B:323:SER:HB2	2.17	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:A:291:MET:CE	1:A:398:PHE:HD1	2.23	0.44
1:B:277:VAL:HG13	1:B:282:LYS:HB2	1.97	0.44
1:B:36:THR:HG21	1:B:481:PRO:HG3	1.99	0.44
1:B:172:ILE:HD12	1:B:182:ALA:HB2	1.99	0.44
1:B:27:ASN:ND2	1:B:62:GLU:HG3	2.33	0.44
1:A:339:PHE:O	1:A:340:LYS:C	2.59	0.44
1:B:370:ILE:HG13	1:B:397:LEU:CD1	2.48	0.44
1:B:487:ASN:HD22	1:B:487:ASN:C	2.24	0.44
1:A:480:VAL:HG13	1:A:484:MET:SD	2.57	0.44
1:A:348:LYS:HD3	1:A:372:PHE:CE2	2.52	0.44
1:A:350:ILE:HG23	1:A:354:LYS:HE2	2.00	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:B:5:LEU:O	1:B:5:LEU:HG	2.17	0.44
1:A:150:GLU:HA	1:A:155:TYR:OH	2.18	0.43
1:A:334:LYS:C	1:A:336:GLU:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:327:GLU:C	1:B:330:ASP:H	2.26	0.43
1:B:183:ALA:CB	1:B:486:MET:HE1	2.48	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:A:487:ASN:C	1:A:487:ASN:ND2	2.76	0.43
1:B:487:ASN:HD21	1:B:498:VAL:HG13	1.84	0.43
1:A:389:VAL:C	1:A:391:ARG:N	2.73	0.43
1:B:111:LYS:HE3	1:B:121:ASP:CG	2.44	0.43
1:A:36:THR:O	1:A:54:GLY:HA2	2.18	0.43
1:A:335:ASN:O	1:A:336:GLU:C	2.60	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:487:ASN:ND2	1:B:487:ASN:C	2.77	0.42
1:B:325:MET:SD	1:B:374:LEU:HD22	2.59	0.42
1:B:393:PRO:O	1:B:394:THR:C	2.62	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:B:163:LYS:HE3	1:B:194:GLU:CD	2.44	0.42
1:B:379:LEU:O	1:B:380:GLU:C	2.61	0.42
1:A:389:VAL:C	1:A:391:ARG:H	2.28	0.41
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:253:ARG:HG3	1:A:389:VAL:CG2	2.51	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:B:50:LYS:N	1:B:187:GLU:OE2	2.54	0.41
1:B:331:ILE:HD12	1:B:351:PHE:HA	2.03	0.41
1:A:16:LYS:HE2	3:A:749:HOH:O	2.21	0.40
1:B:73:LEU:HD11	1:B:455:LEU:CD2	2.51	0.40
1:B:79:LEU:HB3	1:B:139:PHE:CD1	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	11	15
1	B	524/555 (94%)	495 (94%)	25 (5%)	4 (1%)	16	22
All	All	1072/1110 (97%)	1011 (94%)	51 (5%)	10 (1%)	14	20

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%)	460 (99%)	5 (1%)	65	79
1	B	426/488 (87%)	419 (98%)	7 (2%)	55	73
All	All	891/976 (91%)	879 (99%)	12 (1%)	61	76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	GLU
1	A	391	ARG
1	A	403	GLN
1	A	487	ASN
1	A	507	GLU
1	B	151	THR
1	B	181	ASN
1	B	350	ILE
1	B	470	LEU
1	B	487	ASN
1	B	494	GLU
1	B	507	GLU

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

Mol	Chain	Res	Type
1	A	27	ASN
1	A	120	ASN
1	A	166	ASN
1	A	195	ASN
1	A	384	HIS
1	A	403	GLN
1	A	487	ASN
1	B	8	GLN
1	B	26	ASN
1	B	27	ASN
1	B	120	ASN
1	B	166	ASN
1	B	197	GLN
1	B	304	ASN
1	B	371	GLN
1	B	487	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	1604	-	4,4,4	0.37	0	6,6,6	0.06	0
2	SO4	A	601	-	4,4,4	0.37	0	6,6,6	0.07	0
2	SO4	B	1601	-	4,4,4	0.35	0	6,6,6	0.07	0
2	SO4	B	1602	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	A	600	-	4,4,4	0.35	0	6,6,6	0.07	0
2	SO4	B	1600	-	4,4,4	0.35	0	6,6,6	0.13	0
2	SO4	A	602	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SO4	B	1603	-	4,4,4	0.39	0	6,6,6	0.12	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 ⓘ

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	550/555 (99%)	-0.07	20 (3%)	46 47	13, 28, 53, 79	0
1	B	530/555 (95%)	0.33	45 (8%)	16 16	11, 33, 76, 87	0
All	All	1080/1110 (97%)	0.13	65 (6%)	27 27	11, 30, 69, 87	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	THR	5.5
1	B	345	GLU	5.4
1	B	358	TYR	5.0
1	B	379	LEU	5.0
1	B	348	LYS	4.8
1	B	349	GLU	4.8
1	B	351	PHE	4.7
1	A	350	ILE	4.2
1	B	69	PHE	4.2
1	B	353	ALA	4.2
1	A	155	TYR	4.1
1	B	4	SER	4.1
1	B	346	LYS	4.0
1	A	335	ASN	4.0
1	B	355	LEU	3.9
1	B	344	ILE	3.8
1	B	362	VAL	3.7
1	B	363	TYR	3.6
1	A	4	SER	3.5
1	B	493	GLY	3.5
1	B	332	PHE	3.4
1	B	392	VAL	3.4
1	B	67	LEU	3.4
1	B	350	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	330	ASP	3.4
1	B	352	VAL	3.3
1	B	354	LYS	3.3
1	A	334	LYS	3.2
1	B	378	ILE	3.2
1	B	347	MET	3.0
1	B	372	PHE	2.9
1	B	326	LEU	2.8
1	B	328	LEU	2.7
1	B	34	GLU	2.7
1	A	339	PHE	2.7
1	A	344	ILE	2.7
1	A	349	GLU	2.6
1	B	380	GLU	2.6
1	A	340	LYS	2.6
1	B	377	SER	2.6
1	A	343	ASN	2.5
1	A	188	TYR	2.5
1	B	331	ILE	2.5
1	B	26	ASN	2.5
1	B	375	ILE	2.5
1	A	353	ALA	2.5
1	B	324	LEU	2.4
1	B	195	ASN	2.4
1	B	40	GLN	2.4
1	A	338	GLU	2.4
1	A	342	LEU	2.4
1	B	68	SER	2.4
1	A	337	GLY	2.4
1	B	36	THR	2.3
1	B	43	GLN	2.3
1	B	391	ARG	2.3
1	A	252	GLY	2.2
1	B	329	CYS	2.2
1	B	492	TYR	2.2
1	A	347	MET	2.2
1	A	5	LEU	2.2
1	B	357	ASP	2.1
1	B	369	PHE	2.1
1	A	341	GLY	2.1
1	A	253	ARG	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	SO4	B	1602	5/5	0.88	0.15	76,77,79,79	0
2	SO4	B	1601	5/5	0.91	0.14	70,71,74,75	0
2	SO4	B	1603	5/5	0.92	0.23	67,67,67,69	0
2	SO4	B	1604	5/5	0.93	0.09	34,34,35,35	5
2	SO4	A	602	5/5	0.95	0.09	45,48,48,50	0
2	SO4	A	600	5/5	0.96	0.10	38,39,42,45	0
2	SO4	B	1600	5/5	0.96	0.11	36,36,39,41	0
2	SO4	A	601	5/5	0.98	0.06	31,36,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.