



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:58 PM UTC

PDB ID : 4YNG / pdb_00004yng
Title : Twinned pyruvate kinase from E. coli in the T-state
Authors : Donovan, K.A.; Dobson, R.C.J.
Deposited on : 2015-03-10
Resolution : 2.28 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

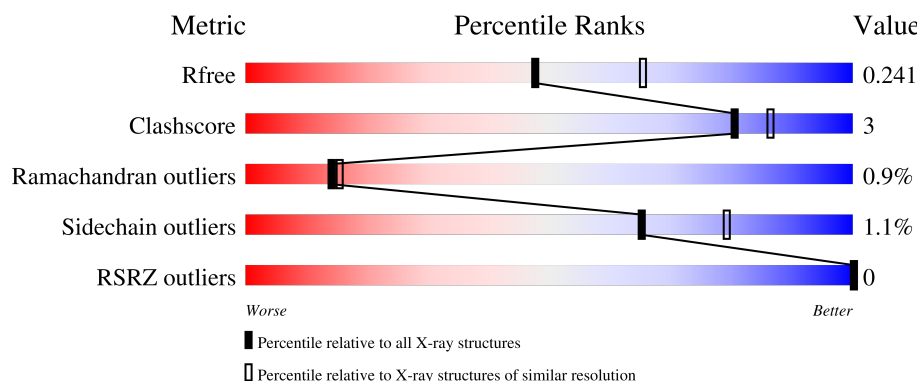
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

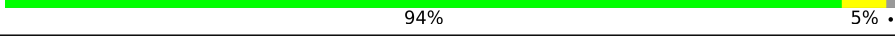
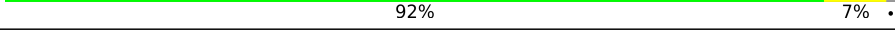
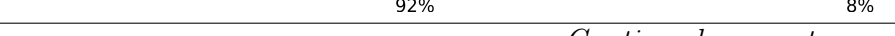
The reported resolution of this entry is 2.28 Å.

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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	470	
1	B	470	
1	C	470	
1	D	470	
1	E	470	

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Mol	Chain	Length	Quality of chain
1	F	470	 91% 7% •
1	G	470	 92% 5% ••
1	H	470	 88% 11% •

2 Entry composition

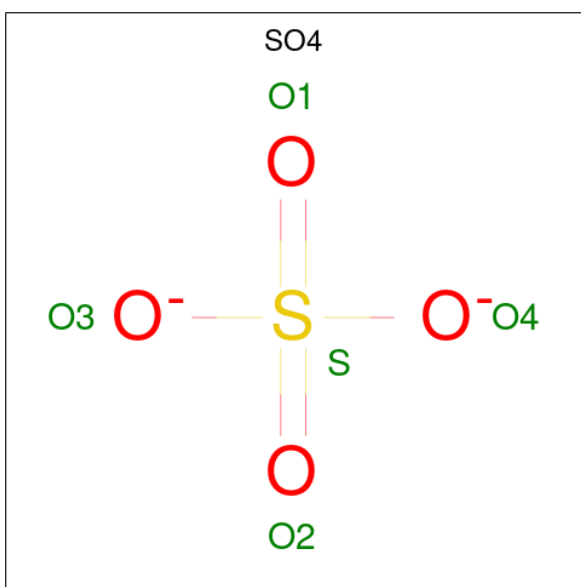
There are 3 unique types of molecules in this entry. The entry contains 59246 atoms, of which 28738 are hydrogens and 0 are deuteriums.

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 kinase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	465	Total	C	H	N	O	S	0	2	0
			7095	2184	3593	608	686	24			
1	B	464	Total	C	H	N	O	S	0	2	0
			7060	2173	3572	607	684	24			
1	C	467	Total	C	H	N	O	S	0	0	0
			7145	2195	3625	614	687	24			
1	D	463	Total	C	H	N	O	S	0	0	0
			7057	2168	3580	605	680	24			
1	E	470	Total	C	H	N	O	S	0	0	0
			7171	2204	3631	618	694	24			
1	F	465	Total	C	H	N	O	S	0	0	0
			7092	2182	3595	607	684	24			
1	G	463	Total	C	H	N	O	S	0	2	0
			7061	2173	3574	607	683	24			
1	H	463	Total	C	H	N	O	S	0	0	0
			7044	2167	3568	603	682	24			

- 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	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

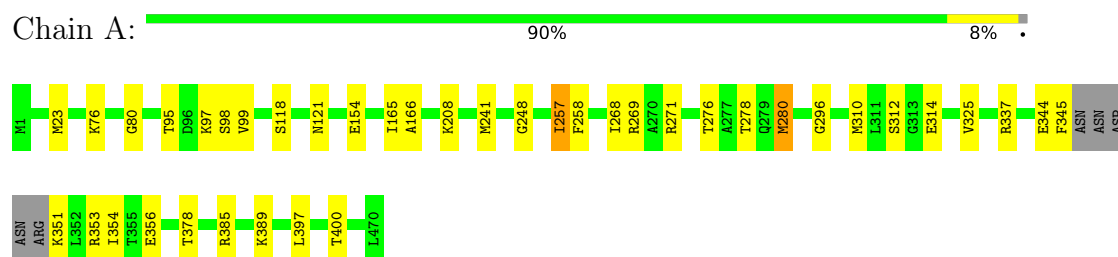
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	303	Total 303	O 303	0	0
3	B	299	Total 299	O 299	0	0
3	C	396	Total 396	O 396	0	0
3	D	425	Total 425	O 425	0	0
3	E	218	Total 218	O 218	0	0
3	F	250	Total 250	O 250	0	0
3	G	288	Total 288	O 288	0	0
3	H	282	Total 282	O 282	0	0

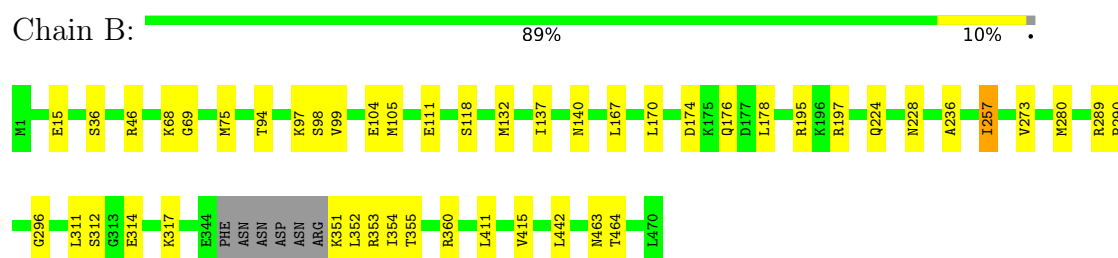
3 Residue-property plots

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.

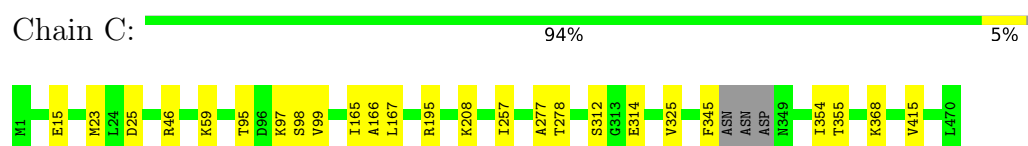
• Molecule 1: Pyruvate kinase I



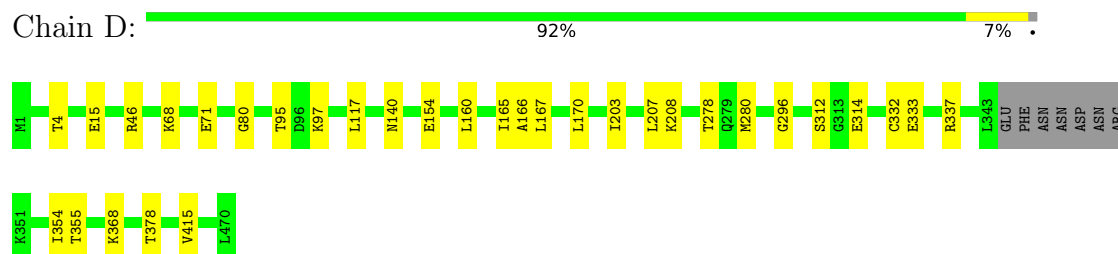
• Molecule 1: Pyruvate kinase I



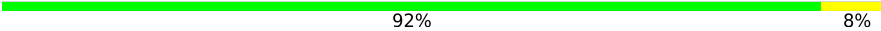
• Molecule 1: Pyruvate kinase I

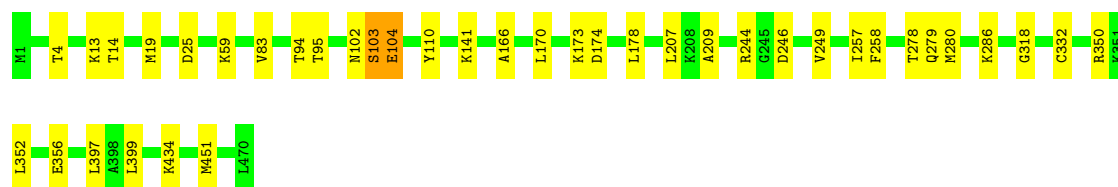


• Molecule 1: Pyruvate kinase I



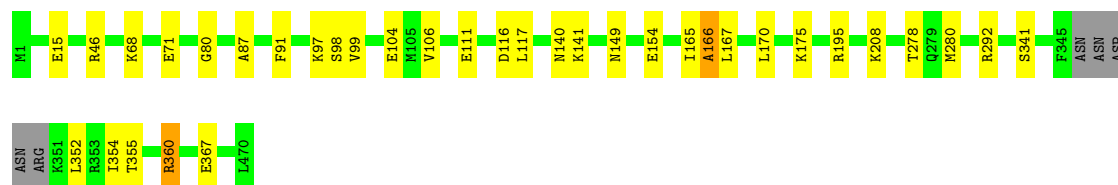
• Molecule 1: Pyruvate kinase I

Chain E:  92% 8%

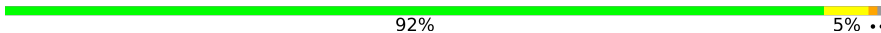


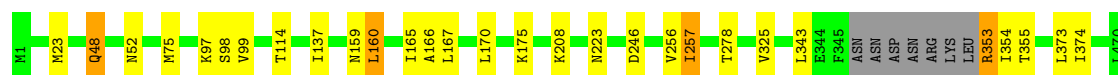
• Molecule 1: Pyruvate kinase I

Chain F:  91% 7%



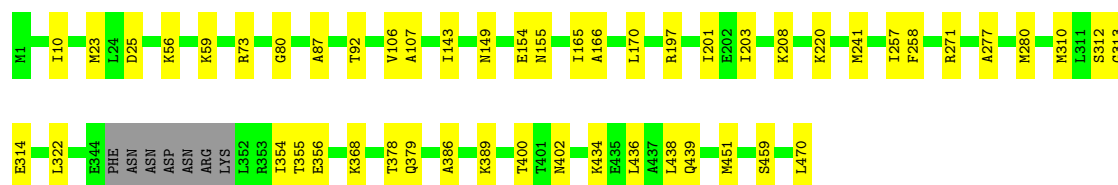
• Molecule 1: Pyruvate kinase I

Chain G:  92% 5%



• Molecule 1: Pyruvate kinase I

Chain H:  88% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.09Å 74.60Å 241.63Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	44.13 – 2.28 44.13 – 2.28	Depositor EDS
% Data completeness (in resolution range)	95.2 (44.13-2.28) 92.1 (44.13-2.28)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 2.22Å)	Xtriage
Refinement program	PHENIX, REFMAC	Depositor
R, R_{free}	0.217 , 0.244 0.215 , 0.241	Depositor DCC
R_{free} test set	2329 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 24.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.450 for h,-k,-l	Xtriage
Reported twinning fraction	0.480 for h,-k,-l	Depositor
Outliers	8 of 213569 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	59246	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3394e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.31	0/3545	0.73	1/4780 (0.0%)
1	B	0.33	0/3531	0.75	3/4763 (0.1%)
1	C	0.31	0/3555	0.72	0/4790
1	D	0.31	0/3511	0.71	0/4733
1	E	0.33	0/3576	0.76	0/4822
1	F	0.32	0/3532	0.73	1/4761 (0.0%)
1	G	0.31	0/3531	0.73	1/4760 (0.0%)
1	H	0.32	0/3510	0.74	1/4733 (0.0%)
All	All	0.32	0/28291	0.73	7/38142 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	ILE	CB-CA-C	-5.87	104.45	111.97
1	G	256	VAL	N-CA-C	5.62	115.81	110.42
1	H	165	ILE	N-CA-C	5.61	114.68	106.55
1	A	165	ILE	N-CA-C	5.60	114.68	106.55
1	B	69	GLY	CA-C-N	5.30	125.51	120.31
1	B	69	GLY	C-N-CA	5.30	125.51	120.31
1	F	104	GLU	N-CA-C	5.03	117.49	111.71

There are no chirality outliers.

There are no planarity outliers.

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	3502	3593	3588	22	0
1	B	3488	3572	3560	24	0
1	C	3520	3625	3625	12	0
1	D	3477	3580	3580	15	0
1	E	3540	3631	3631	23	0
1	F	3497	3595	3595	17	0
1	G	3487	3574	3560	14	0
1	H	3476	3568	3568	27	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	1	0
3	A	303	0	0	4	0
3	B	299	0	0	0	0
3	C	396	0	0	0	0
3	D	425	0	0	1	0
3	E	218	0	0	1	0
3	F	250	0	0	0	0
3	G	288	0	0	4	0
3	H	282	0	0	1	0
All	All	30508	28738	28707	145	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 3.

All (145) 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:F:97:LYS:NZ	1:F:111:GLU:OE1	2.11	0.83
1:C:25:ASP:OD1	1:C:59:LYS:NZ	2.12	0.83
1:E:25:ASP:OD1	1:E:59:LYS:NZ	2.23	0.72
1:E:13:LYS:NZ	1:E:318:GLY:O	2.23	0.70
1:F:68:LYS:NZ	1:F:71:GLU:OE2	2.25	0.70
1:F:87:ALA:N	1:F:149:ASN:OD1	2.26	0.68
1:H:400:THR:HG22	1:H:402:ASN:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:GLU:OE2	1:F:46:ARG:NH1	2.27	0.67
1:C:165:ILE:O	1:C:195:ARG:NH2	2.30	0.65
1:A:351:LYS:N	3:A:757:HOH:O	2.31	0.63
1:B:167:LEU:O	1:B:195:ARG:NH1	2.32	0.62
1:E:102:ASN:O	1:E:104:GLU:N	2.32	0.61
1:G:343:LEU:O	3:G:713:HOH:O	2.16	0.60
1:D:68:LYS:NZ	1:D:71:GLU:OE2	2.33	0.60
1:B:97:LYS:NZ	1:B:111:GLU:OE2	2.27	0.60
1:G:175:LYS:NZ	3:G:604:HOH:O	2.34	0.59
1:H:434:LYS:HG3	1:H:451:MET:HE1	1.86	0.58
1:B:224:GLN:NE2	1:B:228:ASN:OD1	2.37	0.57
1:C:257:ILE:H	1:C:257:ILE:HD12	1.70	0.57
1:E:173:LYS:NZ	3:E:802:HOH:O	2.38	0.56
1:A:97:LYS:O	1:A:99:VAL:N	2.39	0.56
1:H:73:ARG:NE	1:H:155:ASN:OD1	2.34	0.56
1:E:94:THR:HA	1:E:141:LYS:HD2	1.87	0.56
1:A:312:SER:N	1:A:314:GLU:OE1	2.39	0.55
1:D:97:LYS:NZ	3:D:773:HOH:O	2.38	0.55
1:E:397:LEU:HD21	1:E:399:LEU:HD21	1.89	0.55
1:H:197:ARG:NH1	1:H:201:ILE:HD11	2.22	0.55
1:H:87:ALA:N	1:H:149:ASN:OD1	2.40	0.54
1:B:257:ILE:H	1:B:257:ILE:HD12	1.73	0.54
1:C:97:LYS:O	1:C:99:VAL:N	2.41	0.54
1:B:118:SER:HA	1:B:137:ILE:HD11	1.91	0.53
1:D:170:LEU:HD11	1:D:203:ILE:CD1	2.39	0.53
1:D:312:SER:N	1:D:314:GLU:OE1	2.42	0.53
1:B:351:LYS:NZ	1:B:353:ARG:HG2	2.24	0.53
1:G:97:LYS:O	1:G:99:VAL:N	2.42	0.52
1:E:95:THR:H	1:E:141:LYS:HE3	1.74	0.52
1:C:15:GLU:OE1	1:C:46:ARG:NH1	2.43	0.52
1:E:83:VAL:HG11	1:E:102:ASN:HB3	1.91	0.51
1:F:97:LYS:O	1:F:99:VAL:N	2.44	0.51
1:C:95:THR:HG22	1:C:95:THR:O	2.10	0.51
1:A:385:ARG:NH2	3:A:898:HOH:O	2.44	0.51
1:A:276:THR:HG22	1:A:280:MET:HE1	1.91	0.51
1:H:25:ASP:OD1	1:H:59:LYS:NZ	2.43	0.51
1:E:434:LYS:HG3	1:E:451:MET:HE1	1.94	0.50
1:C:257:ILE:HG12	1:D:296:GLY:HA2	1.93	0.50
1:H:354:ILE:HG22	1:H:355:THR:N	2.27	0.50
1:E:4:THR:HG23	1:E:332:CYS:SG	2.52	0.49
1:D:170:LEU:HD21	1:D:203:ILE:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:THR:OG1	1:B:140:ASN:OD1	2.29	0.49
1:E:110:TYR:OH	1:E:166:ALA:HB3	2.12	0.49
1:E:352:LEU:HD21	1:E:356:GLU:HG2	1.94	0.49
1:A:271:ARG:NH1	1:A:356:GLU:OE2	2.46	0.49
1:G:373:LEU:HD23	1:G:374:ILE:N	2.28	0.48
1:G:246:ASP:OD2	3:G:735:HOH:O	2.20	0.48
1:G:114:THR:HG23	1:G:137:ILE:CG2	2.43	0.48
1:G:165:ILE:O	1:G:167:LEU:N	2.40	0.48
1:C:165:ILE:O	1:C:167:LEU:N	2.42	0.48
1:E:95:THR:HG22	1:E:95:THR:O	2.13	0.48
1:H:378:THR:O	1:H:400:THR:HG23	2.14	0.47
1:H:459:SER:OG	2:H:501:SO4:O2	2.31	0.47
1:A:337:ARG:NH2	3:A:689:HOH:O	2.47	0.47
1:A:345:PHE:HZ	1:C:368:LYS:HZ3	1.54	0.47
1:D:165:ILE:O	1:D:167:LEU:N	2.43	0.47
1:E:244:ARG:HB3	1:F:292:ARG:HD2	1.96	0.47
1:H:277:ALA:HA	1:H:310:MET:HB3	1.95	0.47
1:B:75:MET:SD	1:B:97:LYS:HA	2.54	0.47
1:B:170:LEU:HD22	1:B:174:ASP:HB3	1.96	0.46
1:B:273:VAL:HG11	1:B:411:LEU:HG	1.96	0.46
1:D:4:THR:HG23	1:D:332:CYS:SG	2.55	0.46
1:G:170:LEU:HD23	1:G:175:LYS:HG2	1.96	0.46
1:A:389:LYS:NZ	3:A:883:HOH:O	2.49	0.46
1:B:312:SER:N	1:B:314:GLU:OE1	2.49	0.46
1:E:14:THR:HG22	1:E:19:MET:HE2	1.97	0.46
1:G:48:GLN:O	1:G:52:ASN:ND2	2.48	0.46
1:D:80:GLY:HA2	1:D:154:GLU:OE2	2.16	0.46
1:E:102:ASN:C	1:E:103:SER:HG	2.18	0.46
1:A:97:LYS:C	1:A:99:VAL:H	2.24	0.46
1:D:333:GLU:OE2	1:D:337:ARG:NE	2.39	0.46
1:H:400:THR:HG22	1:H:402:ASN:N	2.30	0.46
1:C:23:MET:SD	1:C:325:VAL:HG21	2.56	0.45
1:E:246:ASP:O	1:E:249:VAL:HG22	2.16	0.45
1:A:296:GLY:HA2	1:B:257:ILE:HG12	1.99	0.45
1:E:103:SER:HG	1:E:104:GLU:H	1.64	0.45
1:H:312:SER:N	1:H:314:GLU:OE1	2.49	0.45
1:C:312:SER:N	1:C:314:GLU:OE1	2.49	0.45
1:E:279:GLN:OE1	1:F:292:ARG:NE	2.42	0.45
1:D:15:GLU:HB2	1:D:46:ARG:HG2	1.99	0.45
1:E:170:LEU:HD12	1:E:174:ASP:HB3	1.99	0.44
1:B:36:SER:HA	1:B:68:LYS:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ARG:HG2	1:B:290:PRO:HD2	1.99	0.44
1:B:463:ASN:OD1	1:B:464:THR:HG23	2.17	0.44
1:F:91:PHE:CE2	1:F:106:VAL:HG12	2.53	0.44
1:H:356:GLU:OE1	1:H:389:LYS:NZ	2.43	0.44
1:B:75:MET:HE1	1:B:97:LYS:HB3	1.99	0.44
1:H:257:ILE:HD12	1:H:258:PHE:N	2.32	0.44
1:F:80:GLY:HA2	1:F:154:GLU:OE2	2.18	0.43
1:F:165:ILE:O	1:F:167:LEU:N	2.40	0.43
1:B:97:LYS:O	1:B:99:VAL:N	2.51	0.43
1:B:104:GLU:C	1:B:105:MET:HG3	2.43	0.43
1:D:170:LEU:HD11	1:D:203:ILE:HD13	2.01	0.43
1:E:207:LEU:C	1:E:209:ALA:H	2.27	0.43
1:D:117:LEU:HD21	1:D:160:LEU:HD22	2.01	0.43
1:E:257:ILE:HD12	1:E:258:PHE:N	2.34	0.43
1:G:353:ARG:O	1:G:355:THR:N	2.52	0.43
1:B:352:LEU:HD21	1:D:368:LYS:HZ3	1.84	0.42
1:H:56:LYS:NZ	3:H:604:HOH:O	2.51	0.42
1:H:80:GLY:HA2	1:H:154:GLU:OE2	2.18	0.42
1:A:248:GLY:O	1:B:289:ARG:NH2	2.47	0.42
1:A:257:ILE:HG12	1:B:296:GLY:HA2	2.00	0.42
1:B:197:ARG:HG3	1:B:236:ALA:HB2	2.01	0.42
1:A:378:THR:HG23	1:A:400:THR:HG22	2.01	0.42
1:G:23:MET:SD	1:G:325:VAL:HG21	2.59	0.42
1:A:23:MET:SD	1:A:325:VAL:HG21	2.60	0.42
1:H:436:LEU:HA	1:H:439:GLN:HG2	2.01	0.42
1:E:170:LEU:HD21	1:E:178:LEU:HD12	2.02	0.42
1:F:165:ILE:O	1:F:195:ARG:NH2	2.53	0.42
1:A:241:MET:HE2	1:A:310:MET:HE1	2.02	0.41
1:B:15:GLU:OE1	1:B:46:ARG:NH1	2.53	0.41
1:F:116:ASP:OD2	1:F:166:ALA:HB3	2.20	0.41
1:F:341:SER:OG	1:F:367:GLU:OE1	2.19	0.41
1:H:106:VAL:HG12	1:H:107:ALA:N	2.35	0.41
1:A:97:LYS:C	1:A:99:VAL:N	2.77	0.41
1:C:277:ALA:O	1:C:278:THR:OG1	2.30	0.41
1:F:352:LEU:HD23	1:H:368:LYS:HB3	2.02	0.41
1:H:10:ILE:CD1	1:H:23:MET:HE1	2.51	0.41
1:H:271:ARG:HD3	1:H:386:ALA:HA	2.02	0.41
1:H:354:ILE:HG22	1:H:355:THR:H	1.85	0.41
1:A:80:GLY:HA2	1:A:154:GLU:OE2	2.21	0.41
1:H:92:THR:HG23	1:H:143:ILE:HD13	2.02	0.41
1:H:170:LEU:HD13	1:H:203:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LYS:HA	1:A:154:GLU:HG2	2.03	0.41
1:F:360:ARG:HH11	1:F:360:ARG:HB3	1.84	0.41
1:H:23:MET:HG2	1:H:322:LEU:HD23	2.03	0.41
1:A:257:ILE:HD12	1:A:258:PHE:N	2.36	0.41
1:G:223:ASN:ND2	3:G:761:HOH:O	2.54	0.41
1:F:140:ASN:C	1:F:141:LYS:HD2	2.46	0.40
1:F:170:LEU:HD23	1:F:175:LYS:HG2	2.02	0.40
1:G:159:ASN:C	1:G:160:LEU:HD13	2.46	0.40
1:G:257:ILE:H	1:G:257:ILE:HG13	1.75	0.40
1:A:118:SER:N	1:A:121:ASN:OD1	2.47	0.40
1:A:95:THR:O	1:A:95:THR:HG22	2.21	0.40
1:D:95:THR:HG22	1:D:140:ASN:HB2	2.04	0.40
1:H:220:LYS:HG2	1:H:241:MET:HB3	2.04	0.40
1:H:438:LEU:HD21	1:H:470:LEU:HB3	2.03	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	463/470 (98%)	444 (96%)	14 (3%)	5 (1%)	11	11
1	B	462/470 (98%)	439 (95%)	20 (4%)	3 (1%)	21	25
1	C	463/470 (98%)	445 (96%)	13 (3%)	5 (1%)	11	11
1	D	459/470 (98%)	441 (96%)	12 (3%)	6 (1%)	9	9
1	E	468/470 (100%)	446 (95%)	20 (4%)	2 (0%)	30	36
1	F	461/470 (98%)	441 (96%)	14 (3%)	6 (1%)	9	9
1	G	461/470 (98%)	442 (96%)	14 (3%)	5 (1%)	11	11
1	H	459/470 (98%)	441 (96%)	15 (3%)	3 (1%)	18	21
All	All	3696/3760 (98%)	3539 (96%)	122 (3%)	35 (1%)	14	15

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	SER
1	A	166	ALA
1	B	98	SER
1	C	98	SER
1	C	166	ALA
1	D	166	ALA
1	D	208	LYS
1	F	98	SER
1	F	166	ALA
1	G	98	SER
1	G	166	ALA
1	H	166	ALA
1	B	354	ILE
1	C	354	ILE
1	D	354	ILE
1	F	354	ILE
1	G	208	LYS
1	A	344	GLU
1	A	354	ILE
1	F	208	LYS
1	F	355	THR
1	G	354	ILE
1	H	208	LYS
1	A	278	THR
1	B	355	THR
1	C	208	LYS
1	C	355	THR
1	E	278	THR
1	G	278	THR
1	D	207	LEU
1	D	278	THR
1	D	355	THR
1	F	278	THR
1	E	103	SER
1	H	313	GLY

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	384/389 (99%)	377 (98%)	7 (2%)	51	68
1	B	382/389 (98%)	374 (98%)	8 (2%)	47	63
1	C	386/389 (99%)	384 (100%)	2 (0%)	81	89
1	D	381/389 (98%)	378 (99%)	3 (1%)	73	84
1	E	388/389 (100%)	384 (99%)	4 (1%)	68	81
1	F	383/389 (98%)	380 (99%)	3 (1%)	73	84
1	G	382/389 (98%)	377 (99%)	5 (1%)	61	76
1	H	380/389 (98%)	378 (100%)	2 (0%)	81	89
All	All	3066/3112 (98%)	3032 (99%)	34 (1%)	65	79

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	LYS
1	A	257	ILE
1	A	268	ILE
1	A	269	ARG
1	A	280	MET
1	A	353	ARG
1	A	397	LEU
1	B	132	MET
1	B	176	GLN
1	B	280	MET
1	B	311	LEU
1	B	317	LYS
1	B	360	ARG
1	B	415	VAL
1	B	442	LEU
1	C	345	PHE
1	C	415	VAL
1	D	280	MET
1	D	378	THR
1	D	415	VAL
1	E	104	GLU
1	E	280	MET
1	E	286	LYS
1	E	350	ARG

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Mol	Chain	Res	Type
1	F	117	LEU
1	F	280	MET
1	F	360	ARG
1	G	48	GLN
1	G	75	MET
1	G	160	LEU
1	G	257	ILE
1	G	353	ARG
1	H	280	MET
1	H	379	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	45	GLN
1	A	214	ASN
1	A	300	ASN
1	A	407	HIS
1	B	287	ASN
1	C	37	HIS
1	C	444	HIS
1	D	216	HIS
1	D	224	GLN
1	D	418	GLN
1	D	444	HIS
1	E	45	GLN
1	E	210	HIS
1	E	228	ASN
1	E	347	ASN
1	F	159	ASN
1	G	37	HIS
1	G	45	GLN
1	G	176	GLN
1	G	287	ASN
1	G	444	HIS
1	H	37	HIS
1	H	45	GLN
1	H	300	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	D	501	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	B	501	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	B	502	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	501	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	H	502	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	E	501	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	D	502	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	F	501	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	F	502	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	H	501	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	G	501	-	4,4,4	0.24	0	6,6,6	0.08	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	H	501	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	465/470 (98%)	-1.38	0 100 100	13, 26, 38, 57	1 (0%)
1	B	464/470 (98%)	-1.26	0 100 100	17, 27, 67, 90	1 (0%)
1	C	467/470 (99%)	-1.40	0 100 100	15, 23, 37, 74	0
1	D	463/470 (98%)	-1.43	0 100 100	14, 22, 33, 59	0
1	E	470/470 (100%)	-1.16	0 100 100	24, 34, 77, 90	0
1	F	465/470 (98%)	-1.26	0 100 100	23, 36, 52, 64	0
1	G	463/470 (98%)	-1.31	0 100 100	14, 31, 39, 65	1 (0%)
1	H	463/470 (98%)	-1.27	0 100 100	23, 34, 46, 57	0
All	All	3720/3760 (98%)	-1.31	0 100 100	13, 30, 53, 90	3 (0%)

There are no RSRZ outliers to report.

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	H	502	5/5	0.97	0.05	36,37,47,59	0
2	SO4	F	502	5/5	0.98	0.05	50,54,57,59	0
2	SO4	D	502	5/5	0.99	0.04	22,22,32,36	0
2	SO4	E	501	5/5	0.99	0.03	25,25,26,27	0
2	SO4	F	501	5/5	0.99	0.03	29,30,31,31	0
2	SO4	B	502	5/5	0.99	0.05	30,33,42,45	0
2	SO4	H	501	5/5	0.99	0.03	35,36,36,36	0
2	SO4	D	501	5/5	0.99	0.03	21,23,24,24	0
2	SO4	A	501	5/5	1.00	0.03	23,24,27,27	0
2	SO4	G	501	5/5	1.00	0.03	30,30,32,34	0
2	SO4	C	501	5/5	1.00	0.03	19,20,20,23	0
2	SO4	B	501	5/5	1.00	0.04	21,23,26,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.