Full wwPDB X-ray Structure Validation Report (i)

Apr 4, 2016 – 09:00 PM EDT

PDB ID	:	4YNG
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

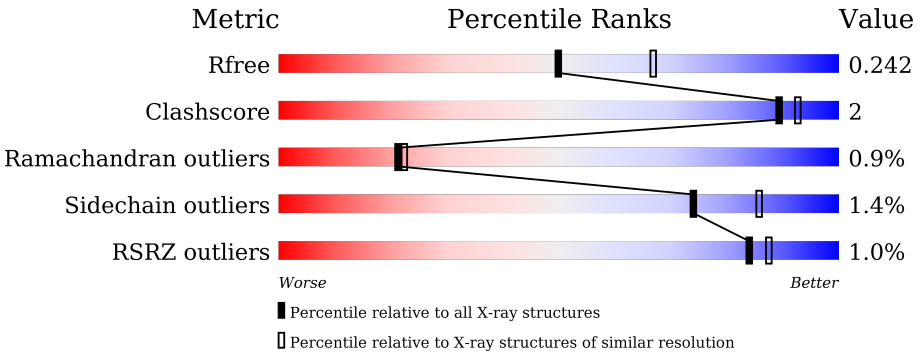
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.28 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}	91344	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	470	90% 8% •
1	B	470	3% 90% 9% •
1	C	470	94% 6% •
1	D	470	92% 7% •
1	E	470	3% 93% 7% •
1	F	470	92% 7% ••

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Mol	Chain	Length	Quality of chain
1	G	470	91% 6%
1	H	470	88% 10%

2 Entry composition

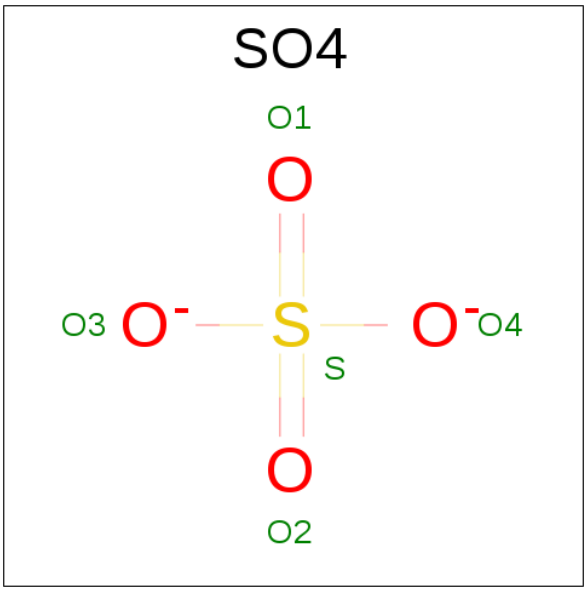
There are 3 unique types of molecules in this entry. The entry contains 59246 atoms, of which 28738 are hydrogens and 0 are deuteriums.

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 (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

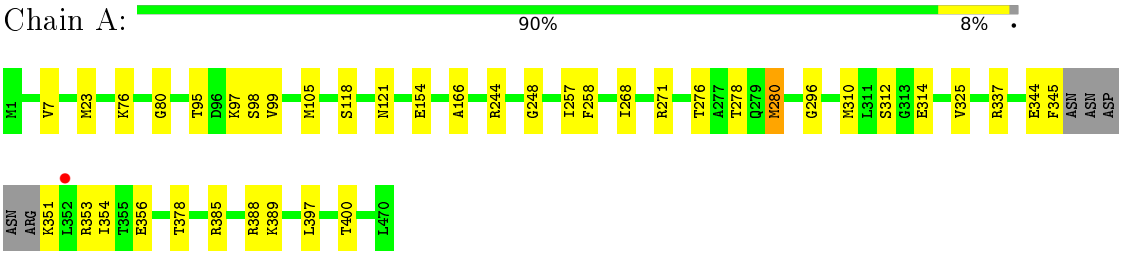
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	303	Total O 303 303	0	0
3	B	299	Total O 299 299	0	0
3	C	396	Total O 396 396	0	0
3	D	425	Total O 425 425	0	0
3	E	218	Total O 218 218	0	0
3	F	250	Total O 250 250	0	0
3	G	288	Total O 288 288	0	0
3	H	282	Total O 282 282	0	0

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

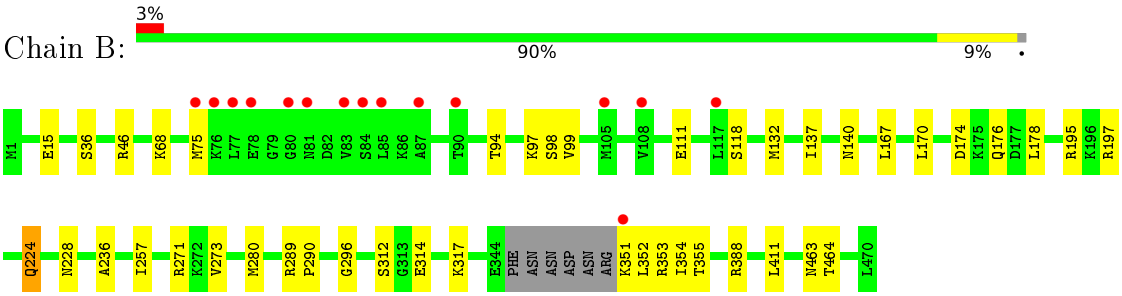
- Molecule 1: Pyruvate kinase I

Chain A:



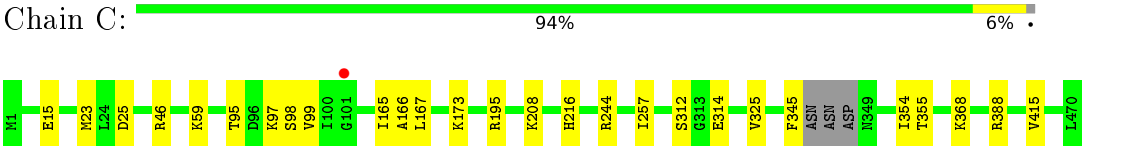
- Molecule 1: Pyruvate kinase I

Chain B:



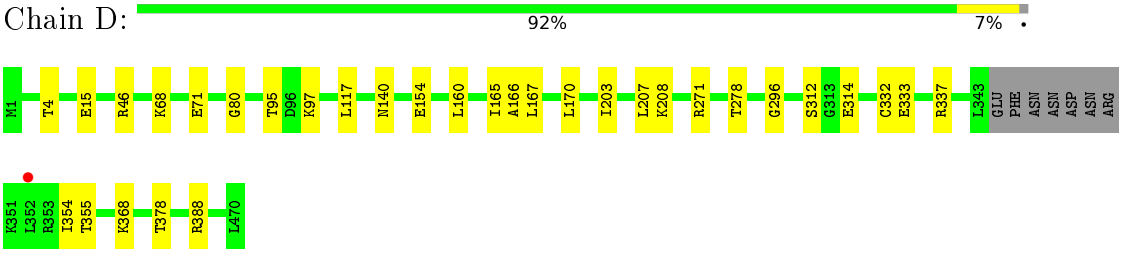
- Molecule 1: Pyruvate kinase I

Chain C:

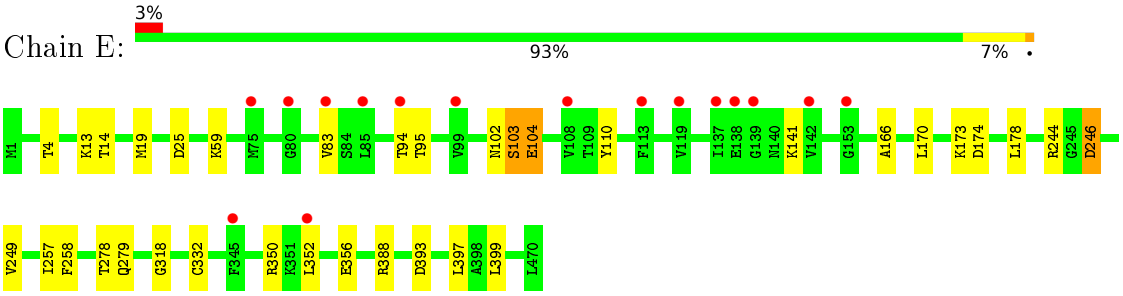


- Molecule 1: Pyruvate kinase I

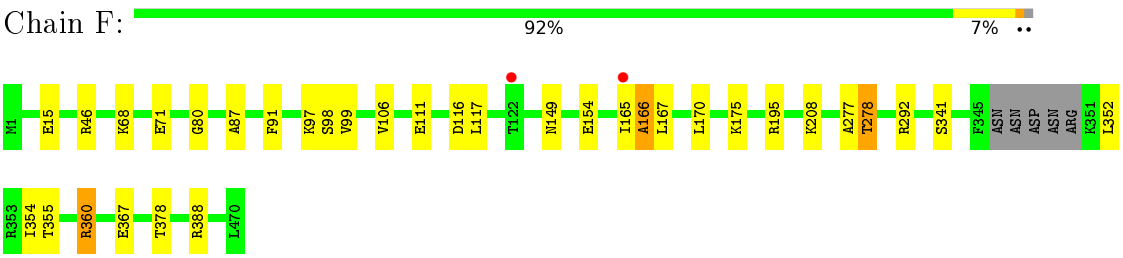
Chain D:



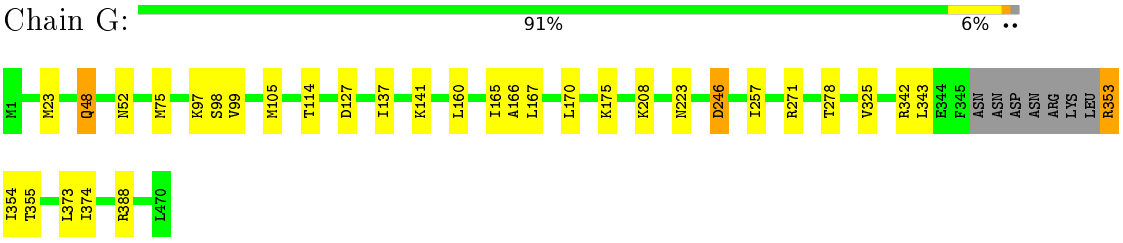
- Molecule 1: Pyruvate kinase I



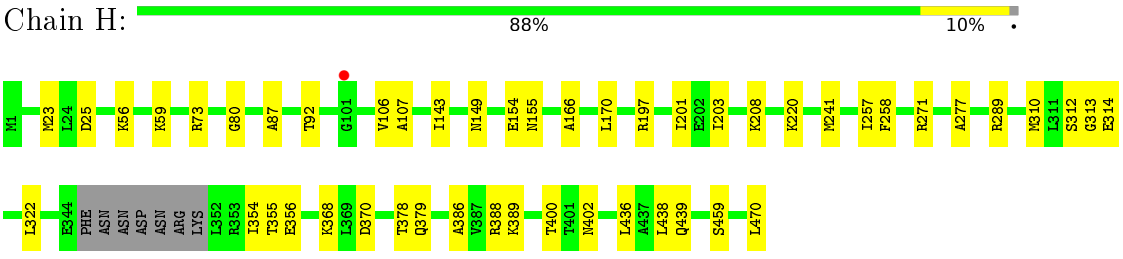
• Molecule 1: Pyruvate kinase I



• Molecule 1: Pyruvate kinase I



• Molecule 1: Pyruvate kinase I



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 – 2.22	Depositor EDS
% Data completeness (in resolution range)	95.2 (44.13-2.28) 88.6 (44.13-2.22)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.22Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.217 , 0.244 0.215 , 0.242	Depositor DCC
R_{free} test set	2101 reflections (1.07%)	DCC
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 25.3	EDS
Estimated twinning fraction	0.480 for h,-k,-l 0.448 for h,-k,-l	Xtriage
Reported twinning fraction	0.480 for h,-k,-l	Depositor
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	9 of 213139 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.92	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 41.42 % 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 2.3655e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.23	0/3545	0.45	0/4780
1	B	0.24	0/3531	0.47	0/4763
1	C	0.23	0/3555	0.44	0/4790
1	D	0.23	0/3511	0.45	0/4733
1	E	0.24	0/3576	0.47	0/4822
1	F	0.23	0/3532	0.46	0/4761
1	G	0.23	0/3531	0.46	0/4760
1	H	0.23	0/3510	0.47	0/4733
All	All	0.23	0/28291	0.46	0/38142

There are no bond length outliers.

There are no bond angle outliers.

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	3502	3593	3588	21	0
1	B	3488	3572	3560	22	0
1	C	3520	3625	3625	12	0
1	D	3477	3580	3580	15	0
1	E	3540	3631	3631	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3497	3595	3595	18	0
1	G	3487	3574	3560	14	0
1	H	3476	3568	3568	25	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	1	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	1	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	138	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 2.

All (138) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD12	1:B:257:ILE:H	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:O	1:C:95:THR:HG22	2.10	0.51
1:A:385:ARG:NH2	3:A:898:HOH:O	2.44	0.51
1:H:25:ASP:OD1	1:H:59:LYS:NZ	2.43	0.51
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
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:E:103:SER:HG	1:E:104:GLU:H	1.61	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:459:SER:OG	2:H:501:SO4:O2	2.31	0.48
1:E:95:THR:HG22	1:E:95:THR:O	2.13	0.48
1:A:276:THR:HG22	1:A:280:MET:HE1	1.95	0.47
1:H:378:THR:O	1:H:400:THR:HG23	2.14	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:C:173:LYS:NZ	3:C:659:HOH:O	2.38	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: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: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:289:ARG:HG2	1:B:290:PRO:HD2	1.99	0.44
1:B:36:SER:HA	1:B:68:LYS: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: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:D:170:LEU:HD11	1:D:203:ILE:HD13	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:353:ARG:O	1:G:355:THR:N	2.52	0.43
1:H:80:GLY:HA2	1:H:154:GLU:OE2	2.18	0.42
1:H:56:LYS:NZ	3:H:604:HOH:O	2.51	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:B:352:LEU:HD21	1:D:368:LYS:HZ3	1.85	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:F:277:ALA:O	1:F:278:THR:OG1	2.31	0.41
1:F:352:LEU:HD23	1:H:368:LYS:HB3	2.02	0.41
1:A:7:VAL:HG11	1:A:310:MET:HE2	2.01	0.41
1:H:354:ILE:HG22	1:H:355:THR:H	1.85	0.41
1:H:271:ARG:HD3	1:H:386:ALA:HA	2.02	0.41
1:A:80:GLY:HA2	1:A:154:GLU:OE2	2.21	0.41
1:H:170:LEU:HD13	1:H:203:ILE:CD1	2.51	0.41
1:H:92:THR:HG23	1:H:143:ILE:HD13	2.02	0.41
1:E:14:THR:HG22	1:E:19:MET:HE2	2.03	0.41
1:F:360:ARG:HH11	1:F:360:ARG:HB3	1.84	0.41
1:A:76:LYS:HA	1:A:154:GLU:HG2	2.03	0.41
1:A:97:LYS:C	1:A:99:VAL:H	2.24	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:105:MET:HE1	1:G:141:LYS:HE3	2.03	0.41
1:G:223:ASN:ND2	3:G:761:HOH:O	2.54	0.41
1:F:170:LEU:HD23	1:F:175:LYS:HG2	2.02	0.40
1:F:378:THR:OG1	2:F:501:SO4:O4	2.34	0.40
1:G:257:ILE:HG13	1:G:257:ILE:H	1.75	0.40
1:A:118:SER:N	1:A:121:ASN:OD1	2.47	0.40
1:A:95:THR:HG22	1:A:95:THR:O	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%)	17	17
1	B	462/470 (98%)	439 (95%)	20 (4%)	3 (1%)	30	34
1	C	463/470 (98%)	445 (96%)	13 (3%)	5 (1%)	17	17
1	D	459/470 (98%)	441 (96%)	12 (3%)	6 (1%)	15	14
1	E	468/470 (100%)	446 (95%)	20 (4%)	2 (0%)	39	47
1	F	461/470 (98%)	441 (96%)	14 (3%)	6 (1%)	15	14
1	G	461/470 (98%)	442 (96%)	14 (3%)	5 (1%)	17	17
1	H	459/470 (98%)	441 (96%)	15 (3%)	3 (1%)	26	30
All	All	3696/3760 (98%)	3539 (96%)	122 (3%)	35 (1%)	21	22

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

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Mol	Chain	Res	Type
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 (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	384/389 (99%)	377 (98%)	7 (2%)	66	80
1	B	382/389 (98%)	375 (98%)	7 (2%)	66	80
1	C	386/389 (99%)	381 (99%)	5 (1%)	76	87
1	D	381/389 (98%)	378 (99%)	3 (1%)	86	93
1	E	388/389 (100%)	383 (99%)	5 (1%)	76	87
1	F	383/389 (98%)	380 (99%)	3 (1%)	86	93
1	G	382/389 (98%)	372 (97%)	10 (3%)	54	69
1	H	380/389 (98%)	376 (99%)	4 (1%)	80	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3066/3112 (98%)	3022 (99%)	44 (1%)	74 86

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	MET
1	A	244	ARG
1	A	268	ILE
1	A	280	MET
1	A	353	ARG
1	A	388	ARG
1	A	397	LEU
1	B	132	MET
1	B	176	GLN
1	B	224	GLN
1	B	271	ARG
1	B	280	MET
1	B	317	LYS
1	B	388	ARG
1	C	216	HIS
1	C	244	ARG
1	C	345	PHE
1	C	388	ARG
1	C	415	VAL
1	D	271	ARG
1	D	378	THR
1	D	388	ARG
1	E	104	GLU
1	E	246	ASP
1	E	350	ARG
1	E	388	ARG
1	E	393	ASP
1	F	117	LEU
1	F	360	ARG
1	F	388	ARG
1	G	48	GLN
1	G	75	MET
1	G	127	ASP
1	G	160	LEU
1	G	246	ASP
1	G	271[A]	ARG
1	G	271[B]	ARG

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Mol	Chain	Res	Type
1	G	342	ARG
1	G	353	ARG
1	G	388	ARG
1	H	289	ARG
1	H	370	ASP
1	H	379	GLN
1	H	388	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	52	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 carbohydrates in this entry.

5.6 Ligand geometry

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	A	501	-	4,4,4	0.25	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	501	-	4,4,4	0.27	0	6,6,6	0.09	0
2	SO4	B	502	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	C	501	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	D	501	-	4,4,4	0.27	0	6,6,6	0.05	0
2	SO4	D	502	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	E	501	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	F	501	-	4,4,4	0.28	0	6,6,6	0.06	0
2	SO4	F	502	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	G	501	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	H	501	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	H	502	-	4,4,4	0.24	0	6,6,6	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0
2	SO4	C	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	502	-	-	0/0/0/0	0/0/0/0
2	SO4	E	501	-	-	0/0/0/0	0/0/0/0
2	SO4	F	501	-	-	0/0/0/0	0/0/0/0
2	SO4	F	502	-	-	0/0/0/0	0/0/0/0
2	SO4	G	501	-	-	0/0/0/0	0/0/0/0
2	SO4	H	501	-	-	0/0/0/0	0/0/0/0
2	SO4	H	502	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.30	1 (0%) 95 97	15, 24, 35, 50	0
1	B	464/470 (98%)	-0.08	15 (3%) 51 59	15, 24, 62, 83	0
1	C	467/470 (99%)	-0.34	1 (0%) 95 97	14, 21, 33, 66	0
1	D	463/470 (98%)	-0.35	1 (0%) 95 97	13, 20, 30, 52	0
1	E	470/470 (100%)	0.07	16 (3%) 49 57	21, 31, 69, 81	0
1	F	465/470 (98%)	-0.13	2 (0%) 93 95	21, 33, 48, 58	0
1	G	463/470 (98%)	-0.24	0 100 100	21, 28, 36, 60	0
1	H	463/470 (98%)	-0.18	1 (0%) 95 97	22, 31, 42, 52	0
All	All	3720/3760 (98%)	-0.19	37 (0%) 84 87	13, 27, 49, 83	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	137	ILE	7.8
1	E	139	GLY	7.0
1	B	80	GLY	5.1
1	E	75	MET	3.9
1	H	101	GLY	3.7
1	E	108	VAL	3.7
1	D	352	LEU	3.4
1	E	119	VAL	3.1
1	B	77	LEU	3.1
1	B	76	LYS	3.0
1	E	80	GLY	2.9
1	E	345	PHE	2.8
1	E	83	VAL	2.7
1	B	85	LEU	2.7
1	E	94	THR	2.7
1	E	138	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	81	ASN	2.6
1	B	78	GLU	2.6
1	B	117	LEU	2.6
1	E	153	GLY	2.4
1	A	352	LEU	2.4
1	B	75	MET	2.4
1	B	87	ALA	2.4
1	B	90	THR	2.4
1	B	108	VAL	2.3
1	E	352	LEU	2.3
1	B	83	VAL	2.3
1	E	99	VAL	2.2
1	B	105	MET	2.2
1	E	85	LEU	2.1
1	F	122	THR	2.1
1	B	84	SER	2.1
1	C	101	GLY	2.1
1	F	165	ILE	2.1
1	B	351	LYS	2.1
1	E	142	VAL	2.1
1	E	113	PHE	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	D	501	5/5	0.98	0.14	0.43	21,23,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	G	501	5/5	0.98	0.13	0.22	30,30,32,34	0
2	SO4	B	501	5/5	0.97	0.12	-0.27	21,23,26,27	0
2	SO4	A	501	5/5	0.99	0.12	-0.40	23,24,27,27	0
2	SO4	C	501	5/5	0.99	0.11	-0.53	19,20,20,23	0
2	SO4	E	501	5/5	0.99	0.11	-0.83	25,25,26,27	0
2	SO4	F	501	5/5	0.99	0.11	-1.32	29,30,31,31	0
2	SO4	H	502	5/5	0.97	0.09	-1.80	36,37,47,59	0
2	SO4	D	502	5/5	0.97	0.09	-1.81	22,22,32,36	0
2	SO4	F	502	5/5	0.97	0.08	-2.27	50,54,57,59	0
2	SO4	H	501	5/5	0.98	0.09	-2.47	35,36,36,36	0
2	SO4	B	502	5/5	0.98	0.09	-3.54	30,33,42,45	0

6.5 Other polymers

There are no such residues in this entry.