



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:11 am GMT

PDB ID : 4QGC
Title : crystal structure of PKM2-K422R mutant
Authors : Wang, P.; Sun, C.; Zhu, T.; Xu, Y.
Deposited on : 2014-05-22
Resolution : 2.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

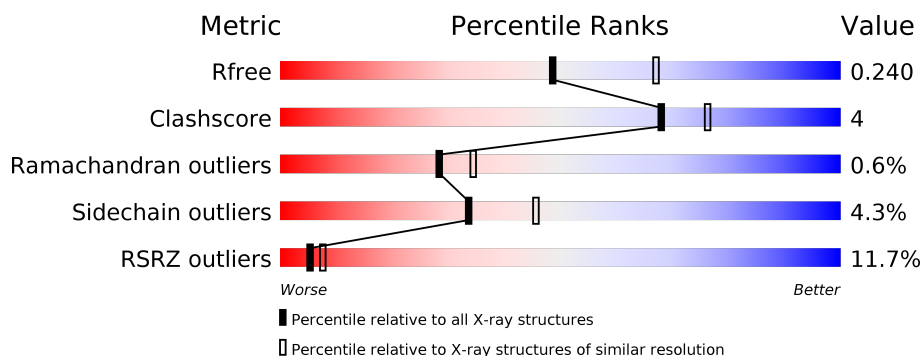
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 $\leq 5\%$. 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	535	<div> <div>3%</div> <div>83%</div> <div>10%</div> <div>6%</div> </div>
1	B	535	<div> <div>15%</div> <div>79%</div> <div>13%</div> <div>7%</div> </div>
1	C	535	<div> <div>14%</div> <div>80%</div> <div>12%</div> <div>7%</div> </div>
1	D	535	<div> <div>12%</div> <div>78%</div> <div>14%</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1004	-	-	X	-
4	GOL	B	1004	-	-	-	X
4	GOL	C	1004	-	-	-	X
4	GOL	D	1004	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16046 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			3861	2429	686	722	24			
1	B	499	Total	C	N	O	S	0	0	0
			3839	2415	682	718	24			
1	C	498	Total	C	N	O	S	0	0	0
			3834	2411	681	718	24			
1	D	500	Total	C	N	O	S	0	0	0
			3840	2416	683	717	24			

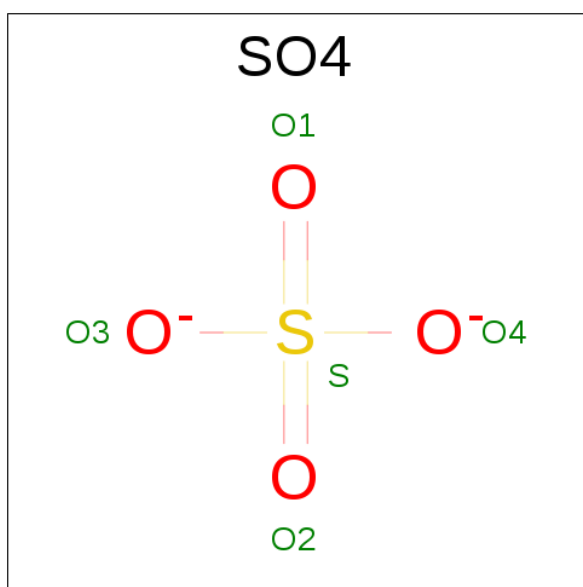
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P14618
A	-2	PRO	-	EXPRESSION TAG	UNP P14618
A	-1	GLY	-	EXPRESSION TAG	UNP P14618
A	0	SER	-	EXPRESSION TAG	UNP P14618
A	422	ARG	LYS	ENGINEERED MUTATION	UNP P14618
B	-3	GLY	-	EXPRESSION TAG	UNP P14618
B	-2	PRO	-	EXPRESSION TAG	UNP P14618
B	-1	GLY	-	EXPRESSION TAG	UNP P14618
B	0	SER	-	EXPRESSION TAG	UNP P14618
B	422	ARG	LYS	ENGINEERED MUTATION	UNP P14618
C	-3	GLY	-	EXPRESSION TAG	UNP P14618
C	-2	PRO	-	EXPRESSION TAG	UNP P14618
C	-1	GLY	-	EXPRESSION TAG	UNP P14618
C	0	SER	-	EXPRESSION TAG	UNP P14618
C	422	ARG	LYS	ENGINEERED MUTATION	UNP P14618
D	-3	GLY	-	EXPRESSION TAG	UNP P14618
D	-2	PRO	-	EXPRESSION TAG	UNP P14618
D	-1	GLY	-	EXPRESSION TAG	UNP P14618
D	0	SER	-	EXPRESSION TAG	UNP P14618
D	422	ARG	LYS	ENGINEERED MUTATION	UNP P14618

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	170	Total	O	0	0
			170	170		
5	B	161	Total	O	0	0
			161	161		
5	C	132	Total	O	0	0
			132	132		

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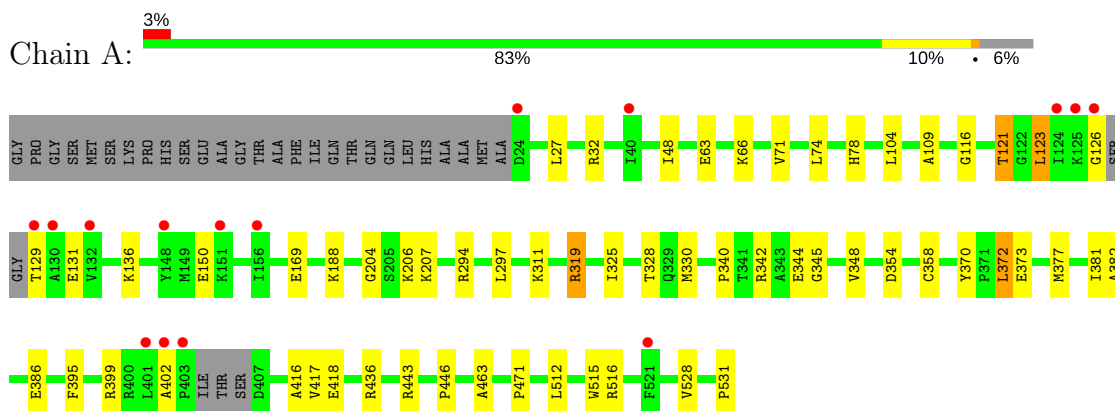
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	136	Total 136	O 136	0	0

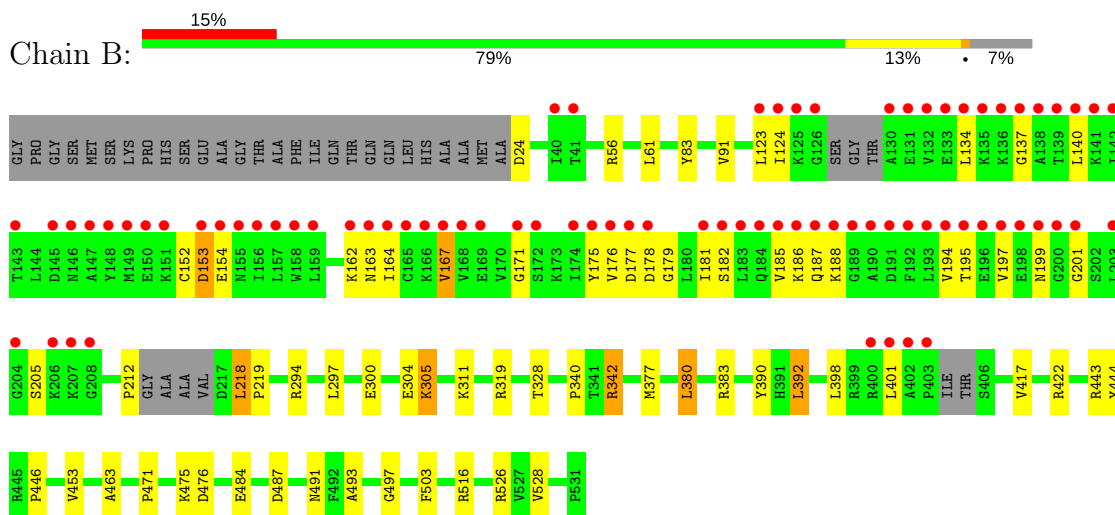
3 Residue-property plots [i](#)

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.

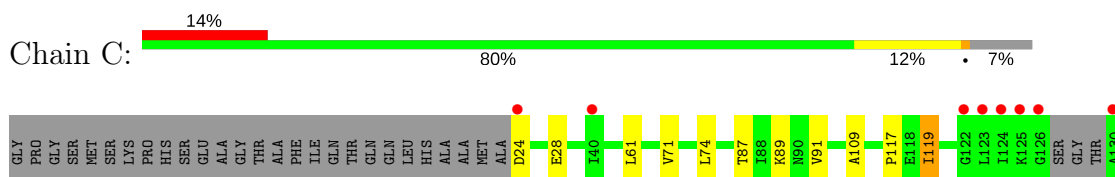
• Molecule 1: Pyruvate kinase PKM

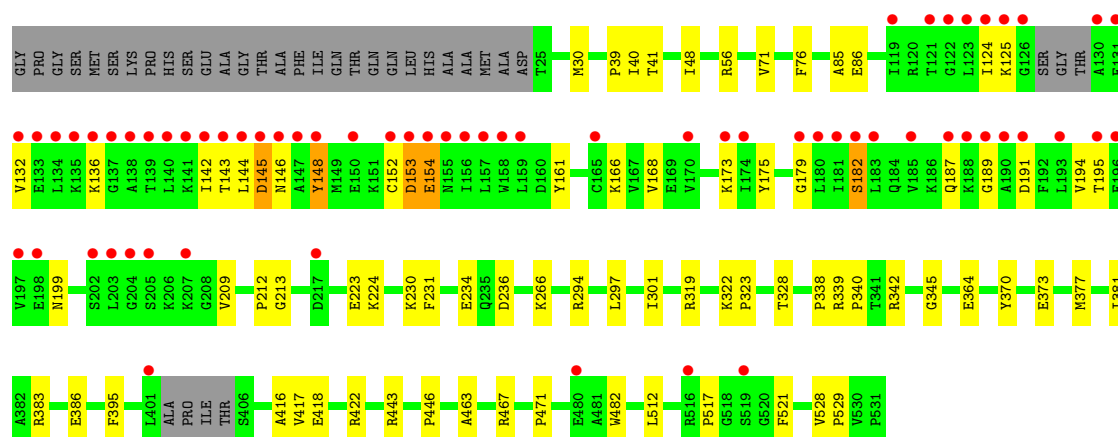


• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.09Å 70.92Å 169.54Å 90.00° 100.21° 90.00°	Depositor
Resolution (Å)	39.91 – 2.30 39.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.91-2.30) 96.7 (39.91-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.197 , 0.240 0.197 , 0.240	Depositor DCC
R_{free} test set	4929 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16046	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, K, 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	0.20	0/3922	0.40	0/5293
1	B	0.20	0/3899	0.41	2/5259 (0.0%)
1	C	0.20	0/3893	0.39	0/5250
1	D	0.21	0/3900	0.39	0/5261
All	All	0.21	0/15614	0.40	2/21063 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	422	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	422	ARG	NE-CZ-NH1	5.73	123.17	120.30

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	3861	0	3942	35	0
1	B	3839	0	3917	41	0
1	C	3834	0	3912	33	0
1	D	3840	0	3924	38	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	15	0	0	2	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	170	0	0	5	0
5	B	161	0	0	6	0
5	C	132	0	0	6	0
5	D	136	0	0	5	0
All	All	16046	0	15727	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 4.

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:B:305:LYS:NZ	5:B:1214:HOH:O	2.08	0.86
1:A:121:THR:HG22	1:A:207:LYS:H	1.44	0.83
3:A:1004:SO4:O4	5:A:1169:HOH:O	1.98	0.80
1:C:285:GLU:OE1	5:C:1129:HOH:O	2.01	0.77
1:A:399:ARG:NH1	1:A:418:GLU:OE2	2.20	0.73
1:D:124:ILE:HG12	1:D:152:CYS:HB2	1.71	0.73
1:D:236:ASP:OD1	5:D:1219:HOH:O	2.04	0.73
1:C:161:TYR:HH	1:C:217:ASP:N	1.87	0.72
1:B:487:ASP:OD1	5:B:1140:HOH:O	2.07	0.71
1:C:482:TRP:HB2	1:C:517:PRO:HG3	1.78	0.66
1:B:380:LEU:HD22	1:C:304:GLU:HG3	1.78	0.66
1:D:364:GLU:O	5:D:1108:HOH:O	2.14	0.65
1:C:161:TYR:OH	1:C:217:ASP:N	2.31	0.63
1:B:383:ARG:NE	5:B:1188:HOH:O	2.28	0.63
1:A:402:ALA:HB1	1:A:443:ARG:HH22	1.63	0.63
1:D:136:LYS:HG2	1:D:199:ASN:HA	1.83	0.61
1:C:516:ARG:NH1	5:C:1164:HOH:O	2.33	0.61
1:A:319:ARG:NH1	5:A:1137:HOH:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ASP:N	1:D:153:ASP:OD1	2.36	0.59
1:A:123:LEU:HB3	1:A:150:GLU:HA	1.84	0.59
1:A:126:GLY:O	1:A:129:THR:N	2.34	0.59
1:C:24:ASP:N	1:C:390:TYR:HH	2.00	0.59
1:B:319:ARG:O	1:B:443:ARG:NH2	2.35	0.58
1:A:531:PRO:OXT	5:A:1163:HOH:O	2.17	0.58
1:A:32:ARG:NH1	5:A:1252:HOH:O	2.36	0.58
1:D:340:PRO:HG3	1:D:377:MET:HG2	1.86	0.57
1:C:395:PHE:HZ	1:C:418:GLU:HG3	1.70	0.56
1:A:516:ARG:NH2	1:B:484:GLU:HG3	2.20	0.56
1:B:475:LYS:NZ	5:B:1241:HOH:O	2.38	0.56
1:D:175:TYR:HD1	1:D:179:GLY:HA2	1.70	0.56
1:D:187:GLN:HB2	1:D:194:VAL:HB	1.87	0.56
1:D:482:TRP:HB2	1:D:517:PRO:HG3	1.88	0.55
1:B:24:ASP:O	1:B:390:TYR:OH	2.24	0.55
1:D:182:SER:OG	1:D:199:ASN:OD1	2.25	0.54
1:B:123:LEU:HA	1:B:205:SER:HB2	1.89	0.54
1:A:121:THR:O	1:A:206:LYS:HA	2.07	0.54
1:A:340:PRO:HG3	1:A:377:MET:HG2	1.88	0.54
1:C:168:VAL:HG13	1:C:172:SER:HB2	1.88	0.54
1:A:71:VAL:HG22	1:A:109:ALA:HB3	1.90	0.53
1:D:383:ARG:NH1	5:D:1153:HOH:O	2.40	0.53
1:D:145:ASP:HB3	1:D:148:TYR:HB2	1.90	0.53
1:B:417:VAL:HG13	1:B:446:PRO:HB3	1.92	0.52
1:C:157:LEU:HD13	1:C:203:LEU:HD21	1.93	0.51
1:B:342:ARG:NH2	1:C:347:ASP:OD1	2.43	0.50
1:A:463:ALA:HB3	1:A:471:PRO:HB3	1.93	0.50
1:C:71:VAL:HG22	1:C:109:ALA:HB3	1.93	0.50
1:A:370:TYR:HB3	1:A:373:GLU:HB2	1.93	0.50
1:B:218:LEU:HD12	1:B:219:PRO:HD2	1.94	0.49
1:C:405:THR:HG21	1:C:410:GLU:HG2	1.95	0.49
1:A:63:GLU:OE2	1:A:66:LYS:NZ	2.46	0.48
1:B:182:SER:OG	1:B:199:ASN:OD1	2.32	0.48
1:B:187:GLN:HB3	1:B:194:VAL:HB	1.95	0.48
1:D:386:GLU:OE2	1:D:467:ARG:NH2	2.44	0.48
1:D:39:PRO:O	1:D:383:ARG:NH2	2.46	0.47
1:B:137:GLY:H	1:B:197:VAL:HB	1.80	0.47
1:D:48:ILE:HG12	1:D:71:VAL:HB	1.96	0.47
1:C:300:GLU:HB3	5:C:1120:HOH:O	2.13	0.47
1:A:516:ARG:HH22	1:B:484:GLU:HG3	1.77	0.47
1:D:417:VAL:HG13	1:D:446:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ALA:HB2	1:A:512:LEU:HD21	1.97	0.47
1:B:154:GLU:OE2	1:B:154:GLU:N	2.47	0.47
1:B:185:VAL:HA	1:B:195:THR:HG22	1.95	0.47
1:C:132:VAL:HG11	1:C:153:ASP:HA	1.96	0.47
1:D:124:ILE:HG21	1:D:132:VAL:HG22	1.96	0.47
1:B:61:LEU:HD13	1:B:91:VAL:HA	1.97	0.46
1:C:117:PRO:HD2	1:C:244:PHE:HB2	1.97	0.46
1:B:176:VAL:HB	1:B:181:ILE:HB	1.97	0.46
1:B:401:LEU:HD11	1:C:28:GLU:HG3	1.98	0.46
1:C:241:PHE:HE1	1:C:268:ILE:HD13	1.81	0.46
1:A:48:ILE:HG12	1:A:71:VAL:HB	1.97	0.46
1:B:162:LYS:O	1:B:164:ILE:N	2.45	0.46
1:C:410:GLU:OE2	1:C:444:TYR:OH	2.23	0.46
1:C:431:LEU:HD22	1:C:513:THR:HG22	1.98	0.46
1:C:340:PRO:HG3	1:C:377:MET:HG2	1.97	0.45
1:D:463:ALA:HB3	1:D:471:PRO:HB3	1.98	0.45
1:A:116:GLY:O	5:A:1170:HOH:O	2.21	0.45
1:B:463:ALA:HB3	1:B:471:PRO:HB3	1.99	0.45
1:C:443:ARG:NH1	5:C:1219:HOH:O	2.49	0.45
1:C:418:GLU:OE2	1:D:422:ARG:NH2	2.45	0.45
1:D:395:PHE:CZ	1:D:418:GLU:HG3	2.52	0.44
1:A:311:LYS:NZ	1:A:354:ASP:OD1	2.51	0.44
1:A:121:THR:HG22	1:A:207:LYS:N	2.22	0.44
1:D:319:ARG:HD2	5:D:1118:HOH:O	2.18	0.44
1:A:131:GLU:HG2	1:A:204:GLY:HA2	1.98	0.44
1:A:330:MET:HE3	1:A:348:VAL:HG22	1.99	0.44
1:B:56:ARG:HD2	1:B:83:TYR:OH	2.18	0.44
1:C:372:LEU:HB2	5:C:1162:HOH:O	2.17	0.43
1:A:515:TRP:HB2	1:B:526:ARG:HD3	1.99	0.43
1:D:143:THR:OG1	1:D:144:LEU:N	2.51	0.43
1:A:344:GLU:O	1:A:348:VAL:HG23	2.19	0.43
1:C:119:ILE:HG13	1:C:209:VAL:HB	1.99	0.43
1:B:392:LEU:HD13	1:B:392:LEU:HA	1.87	0.43
1:D:416:ALA:HB2	1:D:512:LEU:HD21	2.00	0.43
1:A:325:ILE:HG12	1:A:358:CYS:HB2	2.01	0.43
1:A:382:ALA:O	1:A:386:GLU:HG2	2.19	0.43
1:C:61:LEU:HD13	1:C:91:VAL:HA	2.00	0.43
1:D:76:PHE:O	1:D:224:LYS:NZ	2.52	0.43
1:B:188:LYS:HB3	1:B:188:LYS:HE2	1.70	0.43
1:D:85:ALA:HB2	1:D:231:PHE:HZ	1.84	0.43
1:B:175:TYR:HB3	1:B:179:GLY:HA2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:VAL:HG13	1:C:446:PRO:HB3	2.00	0.42
1:C:416:ALA:HB2	1:C:512:LEU:HD21	2.01	0.42
1:C:131:GLU:HG2	1:C:204:GLY:HA2	2.00	0.42
1:D:395:PHE:HZ	1:D:418:GLU:HG3	1.83	0.42
1:A:395:PHE:HZ	1:A:418:GLU:HG2	1.84	0.42
1:A:417:VAL:HG13	1:A:446:PRO:HB3	2.00	0.42
1:B:24:ASP:N	5:B:1106:HOH:O	2.52	0.42
1:D:322:LYS:HA	1:D:323:PRO:HD3	1.90	0.42
1:A:78:HIS:NE2	3:A:1004:SO4:O2	2.50	0.42
1:B:304:GLU:OE1	1:C:380:LEU:HB3	2.19	0.42
1:B:417:VAL:HG21	1:B:444:TYR:HB2	2.02	0.42
1:B:134:LEU:HG	1:B:140:LEU:HD11	2.01	0.42
1:D:212:PRO:HA	1:D:213:GLY:HA2	1.51	0.42
1:D:345:GLY:HA2	1:D:381:ILE:HD13	2.01	0.42
1:D:230:LYS:O	1:D:234:GLU:HG2	2.19	0.42
1:D:528:VAL:HA	1:D:529:PRO:HD3	1.90	0.42
1:B:153:ASP:HB2	1:B:154:GLU:H	1.65	0.42
1:D:338:PRO:HG3	1:D:370:TYR:CZ	2.55	0.41
1:A:136:LYS:HE2	1:A:136:LYS:HB3	1.84	0.41
1:B:340:PRO:HG3	1:B:377:MET:HG2	2.03	0.41
1:D:85:ALA:O	5:D:1115:HOH:O	2.21	0.41
1:B:398:LEU:HD13	1:B:443:ARG:O	2.21	0.41
1:A:169:GLU:HA	1:A:188:LYS:HD2	2.01	0.41
1:B:319:ARG:HD2	5:B:1145:HOH:O	2.19	0.41
1:D:56:ARG:NH2	1:D:86:GLU:OE1	2.53	0.41
1:B:311:LYS:HE2	1:C:353:LEU:HD13	2.01	0.41
1:A:345:GLY:HA2	1:A:381:ILE:HD13	2.03	0.41
1:D:370:TYR:HB3	1:D:373:GLU:HB2	2.03	0.41
1:D:132:VAL:HB	1:D:154:GLU:HG3	2.03	0.41
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.57	0.41
1:C:319:ARG:HD2	5:C:1116:HOH:O	2.20	0.41
1:A:372:LEU:HA	1:A:372:LEU:HD12	1.91	0.40
1:A:311:LYS:HB3	1:D:30:MET:HE3	2.02	0.40
1:B:124:ILE:HG23	1:B:152:CYS:O	2.21	0.40
1:B:453:VAL:HG21	1:B:493:ALA:HB2	2.04	0.40
1:D:166:LYS:HB3	1:D:166:LYS:HE2	1.83	0.40
1:B:212:PRO:HB3	1:B:300:GLU:HG2	2.04	0.40
1:C:74:LEU:HD11	1:C:87:THR:HG21	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	497/535 (93%)	485 (98%)	11 (2%)	1 (0%)	51	63
1	B	491/535 (92%)	466 (95%)	20 (4%)	5 (1%)	18	20
1	C	490/535 (92%)	476 (97%)	11 (2%)	3 (1%)	28	34
1	D	494/535 (92%)	470 (95%)	21 (4%)	3 (1%)	28	34
All	All	1972/2140 (92%)	1897 (96%)	63 (3%)	12 (1%)	28	34

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	ASN
1	D	328	THR
1	A	328	THR
1	B	328	THR
1	C	328	THR
1	D	125	LYS
1	B	171	GLY
1	C	190	ALA
1	C	518	GLY
1	B	167	VAL
1	B	201	GLY
1	D	189	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	415/438 (95%)	403 (97%)	12 (3%)	48	64
1	B	414/438 (94%)	398 (96%)	16 (4%)	37	51
1	C	414/438 (94%)	394 (95%)	20 (5%)	30	40
1	D	413/438 (94%)	389 (94%)	24 (6%)	23	31
All	All	1656/1752 (94%)	1584 (96%)	72 (4%)	33	45

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	74	LEU
1	A	104	LEU
1	A	121	THR
1	A	123	LEU
1	A	294	ARG
1	A	297	LEU
1	A	319	ARG
1	A	342	ARG
1	A	372	LEU
1	A	436	ARG
1	A	528	VAL
1	B	153	ASP
1	B	167	VAL
1	B	177	ASP
1	B	178	ASP
1	B	186	LYS
1	B	218	LEU
1	B	294	ARG
1	B	297	LEU
1	B	305	LYS
1	B	342	ARG
1	B	380	LEU
1	B	392	LEU
1	B	476	ASP
1	B	491	ASN
1	B	516	ARG
1	B	528	VAL
1	C	89	LYS
1	C	119	ILE
1	C	164	ILE
1	C	173	LYS
1	C	186	LYS

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Mol	Chain	Res	Type
1	C	187	GLN
1	C	217	ASP
1	C	221	VAL
1	C	246	ARG
1	C	266	LYS
1	C	294	ARG
1	C	297	LEU
1	C	332	GLU
1	C	372	LEU
1	C	393	GLN
1	C	436	ARG
1	C	467	ARG
1	C	480	GLU
1	C	516	ARG
1	C	528	VAL
1	D	40	ILE
1	D	41	THR
1	D	142	ILE
1	D	145	ASP
1	D	146	ASN
1	D	148	TYR
1	D	153	ASP
1	D	154	GLU
1	D	161	TYR
1	D	168	VAL
1	D	173	LYS
1	D	182	SER
1	D	191	ASP
1	D	195	THR
1	D	209	VAL
1	D	223	GLU
1	D	266	LYS
1	D	294	ARG
1	D	297	LEU
1	D	301	ILE
1	D	339	ARG
1	D	342	ARG
1	D	443	ARG
1	D	521	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	318	ASN
1	C	318	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](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	1002	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	A	1003	-	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	A	1004	-	4,4,4	0.13	0	6,6,6	0.14	0
4	GOL	A	1005	-	5,5,5	0.34	0	5,5,5	0.30	0
3	SO4	B	1002	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	1003	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	B	1004	-	5,5,5	0.32	0	5,5,5	0.31	0
3	SO4	C	1002	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	C	1003	-	4,4,4	0.14	0	6,6,6	0.06	0
4	GOL	C	1004	-	5,5,5	0.37	0	5,5,5	0.28	0
3	SO4	D	1002	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	D	1003	-	4,4,4	0.14	0	6,6,6	0.07	0
4	GOL	D	1004	-	5,5,5	0.34	0	5,5,5	0.31	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
3	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1005	-	-	0/4/4/4	0/0/0/0
3	SO4	B	1002	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
4	GOL	B	1004	-	-	0/4/4/4	0/0/0/0
3	SO4	C	1002	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1003	-	-	0/0/0/0	0/0/0/0
4	GOL	C	1004	-	-	0/4/4/4	0/0/0/0
3	SO4	D	1002	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1003	-	-	0/0/0/0	0/0/0/0
4	GOL	D	1004	-	-	0/4/4/4	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1004	SO4	2	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, 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	503/535 (94%)	0.14	15 (2%) 51 58	14, 27, 58, 82	0
1	B	499/535 (93%)	0.69	79 (15%) 2 3	12, 27, 100, 111	0
1	C	498/535 (93%)	0.70	75 (15%) 3 4	12, 30, 89, 106	0
1	D	500/535 (93%)	0.66	65 (13%) 4 5	14, 31, 91, 114	0
All	All	2000/2140 (93%)	0.55	234 (11%) 5 7	12, 29, 91, 114	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	GLY	9.9
1	D	203	LEU	9.7
1	B	181	ILE	9.6
1	C	168	VAL	9.5
1	B	140	LEU	9.5
1	D	152	CYS	9.3
1	B	168	VAL	8.9
1	C	190	ALA	8.5
1	B	134	LEU	8.5
1	D	123	LEU	8.4
1	D	189	GLY	8.1
1	C	193	LEU	7.6
1	C	123	LEU	7.6
1	D	190	ALA	7.5
1	C	167	VAL	7.4
1	D	153	ASP	7.4
1	D	147	ALA	7.4
1	C	165	CYS	7.3
1	C	166	LYS	7.2
1	C	192	PHE	7.2
1	B	197	VAL	7.0

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Mol	Chain	Res	Type	RSRZ
1	B	193	LEU	7.0
1	B	153	ASP	7.0
1	C	147	ALA	7.0
1	B	157	LEU	6.9
1	B	183	LEU	6.6
1	B	402	ALA	6.6
1	C	142	ILE	6.4
1	C	126	GLY	6.3
1	C	137	GLY	6.3
1	C	148	TYR	6.2
1	B	130	ALA	6.0
1	C	185	VAL	5.9
1	D	132	VAL	5.9
1	D	202	SER	5.8
1	D	139	THR	5.7
1	D	144	LEU	5.7
1	C	187	GLN	5.7
1	C	173	LYS	5.6
1	D	155	ASN	5.6
1	B	195	THR	5.6
1	C	164	ILE	5.6
1	B	164	ILE	5.6
1	D	179	GLY	5.5
1	C	138	ALA	5.4
1	B	154	GLU	5.4
1	B	148	TYR	5.4
1	D	187	GLN	5.4
1	B	137	GLY	5.3
1	D	156	ILE	5.3
1	B	201	GLY	5.2
1	B	185	VAL	5.2
1	B	177	ASP	5.2
1	D	143	THR	5.1
1	C	130	ALA	5.1
1	B	142	ILE	5.0
1	D	197	VAL	4.9
1	C	141	LYS	4.9
1	D	154	GLU	4.8
1	B	192	PHE	4.8
1	D	134	LEU	4.8
1	C	143	THR	4.7
1	C	194	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	125	LYS	4.7
1	D	188	LYS	4.7
1	D	122	GLY	4.7
1	D	142	ILE	4.6
1	A	403	PRO	4.6
1	B	200	GLY	4.6
1	D	130	ALA	4.6
1	C	189	GLY	4.6
1	B	131	GLU	4.5
1	D	205	SER	4.5
1	B	156	ILE	4.5
1	C	136	LYS	4.5
1	B	158	TRP	4.4
1	D	181	ILE	4.4
1	B	167	VAL	4.4
1	B	165	CYS	4.4
1	B	174	ILE	4.4
1	A	148	TYR	4.4
1	C	134	LEU	4.3
1	B	191	ASP	4.3
1	B	139	THR	4.3
1	B	138	ALA	4.3
1	B	132	VAL	4.3
1	B	135	LYS	4.3
1	D	157	LEU	4.3
1	B	123	LEU	4.3
1	C	169	GLU	4.3
1	B	136	LYS	4.3
1	C	195	THR	4.2
1	D	148	TYR	4.2
1	B	146	ASN	4.1
1	C	191	ASP	4.1
1	B	184	GLN	4.1
1	B	196	GLU	4.1
1	C	184	GLN	4.0
1	D	136	LYS	4.0
1	C	183	LEU	3.9
1	D	124	ILE	3.9
1	B	403	PRO	3.9
1	D	135	LYS	3.9
1	B	124	ILE	3.8
1	B	194	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	199	ASN	3.8
1	C	40	ILE	3.7
1	C	135	LYS	3.7
1	C	124	ILE	3.7
1	C	149	MET	3.7
1	C	174	ILE	3.7
1	C	521	PHE	3.6
1	D	207	LYS	3.6
1	A	401	LEU	3.5
1	C	217	ASP	3.5
1	B	175	TYR	3.4
1	C	171	GLY	3.4
1	C	520	GLY	3.4
1	C	199	ASN	3.4
1	D	198	GLU	3.3
1	D	191	ASP	3.3
1	C	157	LEU	3.3
1	B	204	GLY	3.3
1	C	170	VAL	3.3
1	D	133	GLU	3.2
1	C	139	THR	3.2
1	D	140	LEU	3.2
1	D	180	LEU	3.2
1	B	141	LYS	3.2
1	C	24	ASP	3.2
1	B	190	ALA	3.2
1	B	151	LYS	3.2
1	B	133	GLU	3.2
1	C	163	ASN	3.2
1	B	176	VAL	3.2
1	D	401	LEU	3.2
1	B	189	GLY	3.1
1	B	150	GLU	3.1
1	B	155	ASN	3.1
1	B	186	LYS	3.1
1	A	125	LYS	3.1
1	B	171	GLY	3.0
1	C	145	ASP	3.0
1	D	519	SER	3.0
1	B	125	LYS	3.0
1	A	132	VAL	3.0
1	B	172	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	198	GLU	3.0
1	C	131	GLU	3.0
1	B	178	ASP	3.0
1	C	140	LEU	3.0
1	C	186	LYS	3.0
1	C	122	GLY	2.9
1	B	206	LYS	2.9
1	A	40	ILE	2.9
1	D	182	SER	2.8
1	D	196	GLU	2.8
1	C	155	ASN	2.8
1	D	137	GLY	2.8
1	B	182	SER	2.8
1	C	156	ILE	2.8
1	D	159	LEU	2.7
1	B	166	LYS	2.7
1	A	130	ALA	2.7
1	D	158	TRP	2.7
1	C	203	LEU	2.7
1	B	163	ASN	2.7
1	D	183	LEU	2.7
1	C	144	LEU	2.7
1	C	206	LYS	2.7
1	A	126	GLY	2.7
1	D	126	GLY	2.7
1	A	151	LYS	2.6
1	D	150	GLU	2.6
1	B	147	ALA	2.6
1	B	188	LYS	2.6
1	B	143	THR	2.6
1	C	161	TYR	2.6
1	D	125	LYS	2.6
1	D	146	ASN	2.5
1	C	133	GLU	2.5
1	B	207	LYS	2.5
1	C	151	LYS	2.5
1	D	141	LYS	2.5
1	B	400	ARG	2.5
1	B	169	GLU	2.5
1	D	121	THR	2.5
1	C	196	GLU	2.5
1	B	203	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	217	ASP	2.5
1	C	188	LYS	2.5
1	C	326	CYS	2.4
1	B	41	THR	2.4
1	A	124	ILE	2.4
1	C	218	LEU	2.4
1	C	146	ASN	2.4
1	B	162	LYS	2.4
1	B	145	ASP	2.4
1	C	406	SER	2.4
1	D	480	GLU	2.4
1	C	200	GLY	2.4
1	C	132	VAL	2.4
1	D	516	ARG	2.3
1	C	175	TYR	2.3
1	C	160	ASP	2.3
1	B	187	GLN	2.3
1	C	198	GLU	2.3
1	D	131	GLU	2.3
1	A	402	ALA	2.3
1	D	204	GLY	2.2
1	D	195	THR	2.2
1	B	208	GLY	2.2
1	B	401	LEU	2.2
1	A	24	ASP	2.2
1	A	156	ILE	2.1
1	D	185	VAL	2.1
1	B	149	MET	2.1
1	C	150	GLU	2.1
1	D	145	ASP	2.1
1	B	40	ILE	2.1
1	B	159	LEU	2.1
1	C	182	SER	2.1
1	C	325	ILE	2.1
1	D	193	LEU	2.1
1	D	165	CYS	2.1
1	A	521	PHE	2.1
1	D	174	ILE	2.1
1	C	405	THR	2.1
1	D	138	ALA	2.1
1	D	170	VAL	2.1
1	C	181	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	119	ILE	2.0
1	A	129	THR	2.0
1	D	173	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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	C	1004	6/6	0.77	0.30	6.63	41,44,61,63	0
4	GOL	D	1004	6/6	0.87	0.25	3.76	38,41,49,50	0
4	GOL	B	1004	6/6	0.66	0.26	3.62	38,41,42,44	0
4	GOL	A	1005	6/6	0.87	0.17	0.77	38,41,43,44	0
2	K	A	1001	1/1	0.98	0.13	-0.06	33,33,33,33	0
3	SO4	A	1003	5/5	0.98	0.13	-0.46	27,38,49,65	0
3	SO4	D	1002	5/5	0.97	0.09	-1.13	46,51,63,70	0
3	SO4	C	1003	5/5	0.97	0.11	-1.16	43,52,55,67	0
2	K	B	1001	1/1	0.97	0.11	-1.27	37,37,37,37	0
3	SO4	A	1004	5/5	0.94	0.10	-1.34	54,56,60,64	0
3	SO4	B	1003	5/5	0.97	0.09	-1.40	37,45,57,60	0
2	K	C	1001	1/1	0.99	0.11	-1.43	27,27,27,27	0
3	SO4	B	1002	5/5	0.99	0.11	-1.61	22,26,31,35	0
3	SO4	D	1003	5/5	0.99	0.09	-1.88	35,36,39,46	0
3	SO4	A	1002	5/5	0.98	0.07	-2.12	37,45,56,57	0
3	SO4	C	1002	5/5	0.98	0.09	-3.45	25,31,45,45	0
2	K	D	1001	1/1	0.96	0.07	-4.35	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.