



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:11 PM UTC

PDB ID : 4QGC / pdb_00004qgc
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

<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

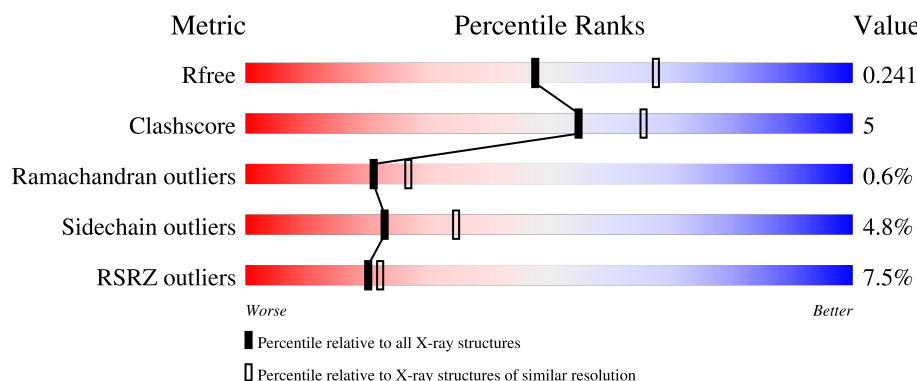
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	535	2% 81% 12% • 6%
1	B	535	10% 79% 13% • 7%
1	C	535	8% 79% 13% • 7%
1	D	535	7% 78% 14% • 7%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	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			

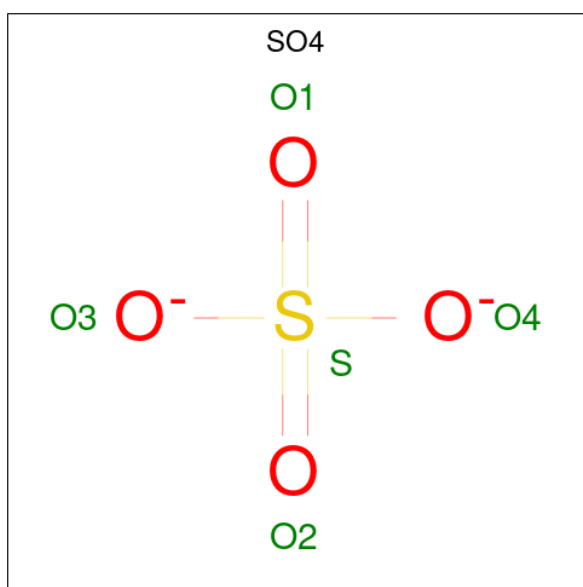
There are 20 discrepancies between the modelled and reference sequences:

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 (CCD ID: K) (formula: K).

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

- Molecule 3 is SULFATE ION (CCD ID: 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 (CCD ID: 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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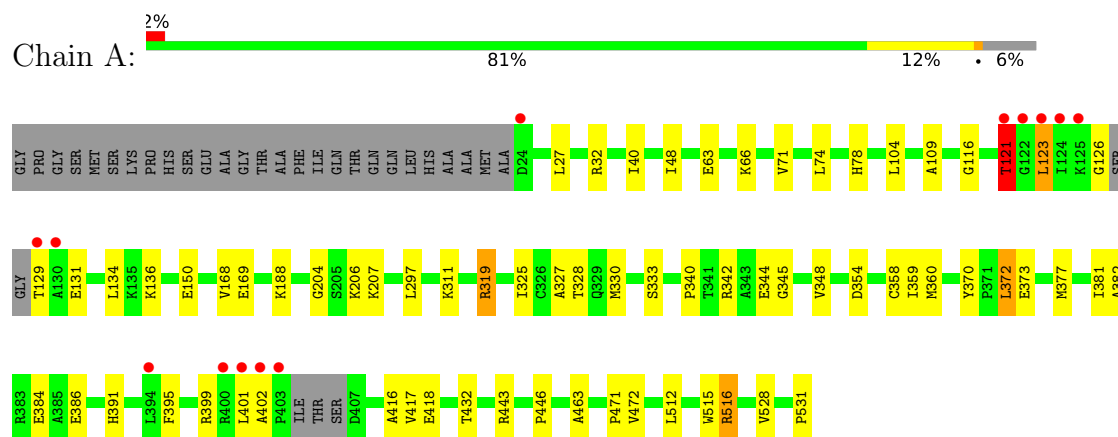
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	136	Total 136	O 136	0	0

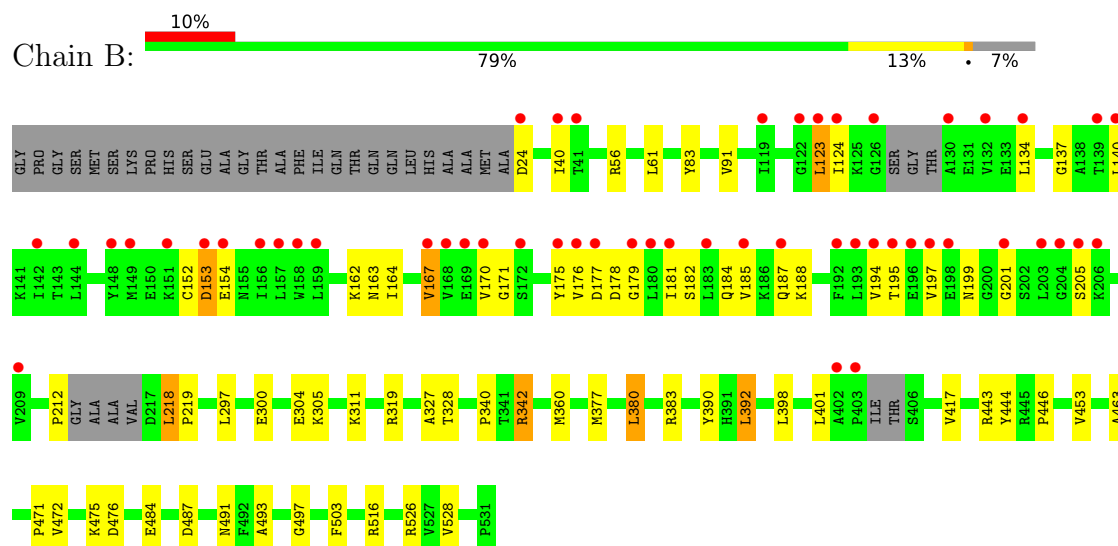
3 Residue-property plots

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.

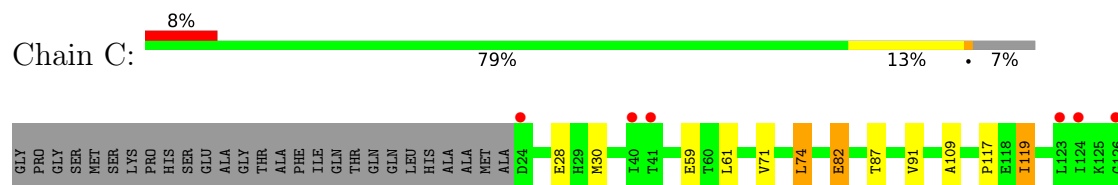
• Molecule 1: Pyruvate kinase PKM

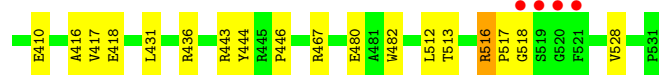
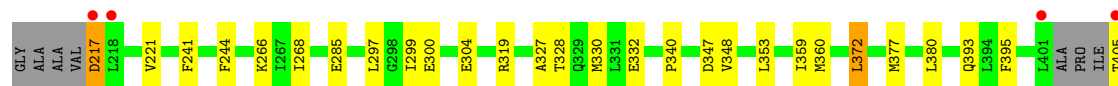


• Molecule 1: Pyruvate kinase PKM

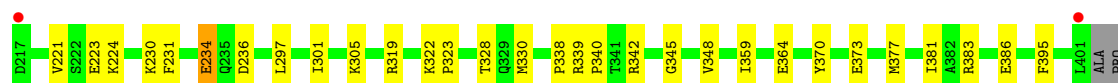
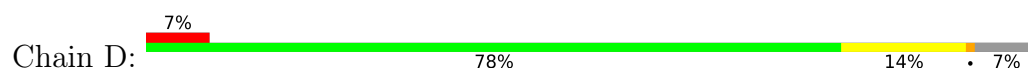


• Molecule 1: Pyruvate kinase PKM





- 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 0.199 , 0.241	Depositor DCC
R_{free} test set	4930 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.4	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: K, SO4, GOL

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	0.27	0/3922	0.73	2/5293 (0.0%)
1	B	0.27	0/3899	0.72	0/5259
1	C	0.27	0/3893	0.74	0/5250
1	D	0.28	0/3900	0.73	0/5261
All	All	0.27	0/15614	0.73	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	A	121	THR	N-CA-C	-5.48	103.67	110.41
1	A	391	HIS	N-CA-C	5.12	116.86	111.28

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	40	0
1	B	3839	0	3917	43	0
1	C	3834	0	3912	37	0
1	D	3840	0	3924	41	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	3	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	150	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 5.

All (150) 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:D:330:MET:HE3	1:D:348:VAL:HG22	1.74	0.69
1:C:330:MET:HE3	1:C:348:VAL:HG22	1.75	0.68
1:A:330:MET:HE3	1:A:348:VAL:HG22	1.78	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:330:MET:HE2	1:C:359:ILE:HG23	1.86	0.57
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:330:MET:HE2	1:D:359:ILE:HG23	1.91	0.53
1:D:145:ASP:HB3	1:D:148:TYR:HB2	1.90	0.53
1:A:330:MET:HE2	1:A:359:ILE:HG23	1.92	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:384:GLU:OE1	1:D:305:LYS:NZ	2.43	0.47
1:A:416:ALA:HB2	1:A:512:LEU:HD21	1.97	0.47
1:B:154:GLU:N	1:B:154:GLU:OE2	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:327:ALA:HB1	1:C:360:MET:HE2	1.97	0.45
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:C:82:GLU:CD	1:C:82:GLU:H	2.25	0.44
1:A:121:THR:HG22	1:A:207:LYS:N	2.22	0.44
1:B:311:LYS:HE3	1:C:30:MET:HE1	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE2	1:B:188:LYS:HB3	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
1:C:416:ALA:HB2	1:C:512:LEU:HD21	2.01	0.42
1:C:417:VAL:HG13	1:C:446:PRO:HB3	2.00	0.42
1:C:131:GLU:HG2	1:C:204:GLY:HA2	2.00	0.42
1:B:327:ALA:HB1	1:B:360:MET:HE2	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:432:THR:OG1	3:A:1003:SO4:O4	2.33	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:A:311:LYS:HD3	1:D:30:MET:HE1	2.01	0.41
1:A:333:SER:OG	1:A:344:GLU:OE1	2.34	0.41
1:D:132:VAL:HB	1:D:154:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:A:372:LEU:HA	1.91	0.40
1:A:327:ALA:HB1	1:A:360:MET:HE2	2.03	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:HE2	1:D:166:LYS:HB3	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

5.3.1 Protein backbone

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%)	43	55
1	B	491/535 (92%)	466 (95%)	20 (4%)	5 (1%)	12	15
1	C	490/535 (92%)	476 (97%)	11 (2%)	3 (1%)	21	27
1	D	494/535 (92%)	470 (95%)	21 (4%)	3 (1%)	21	27
All	All	1972/2140 (92%)	1897 (96%)	63 (3%)	12 (1%)	21	27

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	399 (96%)	16 (4%)	28	43
1	B	414/438 (94%)	396 (96%)	18 (4%)	26	39
1	C	414/438 (94%)	391 (94%)	23 (6%)	19	28
1	D	413/438 (94%)	390 (94%)	23 (6%)	19	28
All	All	1656/1752 (94%)	1576 (95%)	80 (5%)	23	35

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	40	ILE
1	A	74	LEU
1	A	104	LEU
1	A	121	THR
1	A	123	LEU
1	A	134	LEU
1	A	168	VAL
1	A	297	LEU
1	A	319	ARG
1	A	342	ARG
1	A	372	LEU
1	A	401	LEU
1	A	472	VAL
1	A	516	ARG

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Mol	Chain	Res	Type
1	A	528	VAL
1	B	40	ILE
1	B	123	LEU
1	B	153	ASP
1	B	167	VAL
1	B	170	VAL
1	B	177	ASP
1	B	178	ASP
1	B	184	GLN
1	B	218	LEU
1	B	297	LEU
1	B	342	ARG
1	B	380	LEU
1	B	392	LEU
1	B	472	VAL
1	B	476	ASP
1	B	491	ASN
1	B	516	ARG
1	B	528	VAL
1	C	59	GLU
1	C	74	LEU
1	C	82	GLU
1	C	119	ILE
1	C	151	LYS
1	C	164	ILE
1	C	168	VAL
1	C	173	LYS
1	C	180	LEU
1	C	187	GLN
1	C	217	ASP
1	C	221	VAL
1	C	266	LYS
1	C	297	LEU
1	C	299	ILE
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

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Mol	Chain	Res	Type
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	168	VAL
1	D	182	SER
1	D	195	THR
1	D	209	VAL
1	D	221	VAL
1	D	223	GLU
1	D	234	GLU
1	D	297	LEU
1	D	301	ILE
1	D	339	ARG
1	D	342	ARG
1	D	443	ARG
1	D	472	VAL
1	D	521	PHE
1	D	528	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	HIS
1	A	393	GLN
1	B	163	ASN
1	B	210	ASN
1	B	318	ASN
1	B	440	GLN
1	B	479	GLN
1	C	29	HIS
1	C	391	HIS
1	C	458	GLN
1	C	479	GLN
1	D	318	ASN
1	D	393	GLN
1	D	479	GLN

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 ⓘ

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	D	1002	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	C	1002	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	C	1003	-	4,4,4	0.23	0	6,6,6	0.08	0
4	GOL	A	1005	-	5,5,5	0.37	0	5,5,5	0.38	0
3	SO4	A	1004	-	4,4,4	0.22	0	6,6,6	0.16	0
3	SO4	B	1002	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	D	1003	-	4,4,4	0.24	0	6,6,6	0.10	0
4	GOL	C	1004	-	5,5,5	0.38	0	5,5,5	0.34	0
4	GOL	D	1004	-	5,5,5	0.37	0	5,5,5	0.38	0
4	GOL	B	1004	-	5,5,5	0.36	0	5,5,5	0.36	0
3	SO4	A	1003	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	A	1002	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	1003	-	4,4,4	0.24	0	6,6,6	0.08	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
4	GOL	D	1004	-	-	3/4/4/4	-
4	GOL	B	1004	-	-	4/4/4/4	-
4	GOL	C	1004	-	-	3/4/4/4	-
4	GOL	A	1005	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1004	GOL	O1-C1-C2-C3
4	B	1004	GOL	C1-C2-C3-O3
4	B	1004	GOL	O2-C2-C3-O3
4	C	1004	GOL	O1-C1-C2-O2
4	C	1004	GOL	O1-C1-C2-C3
4	D	1004	GOL	O1-C1-C2-O2
4	A	1005	GOL	O1-C1-C2-C3
4	D	1004	GOL	O1-C1-C2-C3
4	B	1004	GOL	O1-C1-C2-O2
4	A	1005	GOL	O1-C1-C2-O2
4	C	1004	GOL	O2-C2-C3-O3
4	D	1004	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1004	SO4	2	0
3	A	1003	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	503/535 (94%)	0.03	13 (2%) 57 59	14, 27, 58, 82	0
1	B	499/535 (93%)	0.33	53 (10%) 11 12	12, 27, 100, 111	0
1	C	498/535 (93%)	0.35	44 (8%) 15 17	12, 30, 89, 106	0
1	D	500/535 (93%)	0.36	40 (8%) 18 20	14, 31, 91, 114	0
All	All	2000/2140 (93%)	0.27	150 (7%) 20 22	12, 29, 91, 114	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	152	CYS	7.1
1	C	165	CYS	5.0
1	C	123	LEU	5.0
1	D	147	ALA	5.0
1	B	170	VAL	4.8
1	C	144	LEU	4.7
1	D	203	LEU	4.6
1	D	123	LEU	4.4
1	B	130	ALA	4.2
1	C	168	VAL	4.1
1	B	201	GLY	4.0
1	C	192	PHE	4.0
1	B	134	LEU	4.0
1	B	167	VAL	3.9
1	B	185	VAL	3.9
1	C	521	PHE	3.9
1	B	181	ILE	3.9
1	D	130	ALA	3.9
1	B	180	LEU	3.8
1	C	136	LYS	3.8
1	D	153	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	164	ILE	3.7
1	C	24	ASP	3.6
1	B	402	ALA	3.6
1	D	197	VAL	3.6
1	C	167	VAL	3.6
1	A	122	GLY	3.6
1	B	177	ASP	3.6
1	C	170	VAL	3.5
1	D	202	SER	3.5
1	B	142	ILE	3.5
1	D	140	LEU	3.5
1	B	204	GLY	3.5
1	B	195	THR	3.4
1	D	190	ALA	3.4
1	D	138	ALA	3.4
1	B	140	LEU	3.4
1	D	157	LEU	3.3
1	C	148	TYR	3.3
1	B	176	VAL	3.3
1	B	197	VAL	3.3
1	D	139	THR	3.2
1	B	126	GLY	3.2
1	C	405	THR	3.2
1	A	130	ALA	3.2
1	C	134	LEU	3.2
1	B	194	VAL	3.1
1	D	180	LEU	3.1
1	B	124	ILE	3.1
1	B	403	PRO	3.1
1	B	193	LEU	3.1
1	A	401	LEU	3.0
1	D	148	TYR	3.0
1	A	129	THR	3.0
1	C	172	SER	3.0
1	B	192	PHE	3.0
1	C	143	THR	2.9
1	D	195	THR	2.9
1	A	400	ARG	2.9
1	C	203	LEU	2.9
1	D	124	ILE	2.9
1	C	157	LEU	2.9
1	D	401	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	132	VAL	2.9
1	C	210	ASN	2.8
1	C	130	ALA	2.8
1	C	188	LYS	2.8
1	B	198	GLU	2.8
1	A	121	THR	2.7
1	C	401	LEU	2.7
1	C	190	ALA	2.7
1	D	122	GLY	2.7
1	B	205	SER	2.7
1	B	123	LEU	2.7
1	B	157	LEU	2.7
1	B	168	VAL	2.7
1	C	189	GLY	2.7
1	C	187	GLN	2.6
1	B	24	ASP	2.6
1	D	132	VAL	2.6
1	B	179	GLY	2.6
1	A	403	PRO	2.6
1	B	144	LEU	2.6
1	C	520	GLY	2.6
1	A	402	ALA	2.6
1	C	147	ALA	2.5
1	B	40	ILE	2.5
1	B	119	ILE	2.5
1	A	123	LEU	2.5
1	C	206	LYS	2.5
1	D	156	ILE	2.5
1	B	183	LEU	2.5
1	D	191	ASP	2.5
1	B	158	TRP	2.5
1	C	124	ILE	2.5
1	C	138	ALA	2.5
1	B	172	SER	2.4
1	D	135	LYS	2.4
1	B	153	ASP	2.4
1	D	155	ASN	2.4
1	D	126	GLY	2.4
1	D	144	LEU	2.4
1	B	139	THR	2.4
1	B	149	MET	2.4
1	B	175	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	191	ASP	2.4
1	B	41	THR	2.3
1	A	394	LEU	2.3
1	D	136	LYS	2.3
1	D	158	TRP	2.3
1	D	189	GLY	2.3
1	D	100	SER	2.3
1	B	209	VAL	2.3
1	C	197	VAL	2.3
1	D	217	ASP	2.3
1	B	203	LEU	2.3
1	D	207	LYS	2.3
1	C	145	ASP	2.3
1	B	206	LYS	2.3
1	D	188	LYS	2.3
1	D	134	LEU	2.2
1	C	212	PRO	2.2
1	B	122	GLY	2.2
1	B	169	GLU	2.2
1	B	196	GLU	2.2
1	A	124	ILE	2.2
1	B	159	LEU	2.2
1	C	126	GLY	2.2
1	C	518	GLY	2.2
1	C	41	THR	2.2
1	D	142	ILE	2.2
1	B	148	TYR	2.1
1	B	132	VAL	2.1
1	C	217	ASP	2.1
1	B	154	GLU	2.1
1	A	125	LYS	2.1
1	D	204	GLY	2.1
1	D	520	GLY	2.1
1	B	151	LYS	2.1
1	B	187	GLN	2.1
1	C	156	ILE	2.1
1	C	161	TYR	2.1
1	D	175	TYR	2.1
1	C	519	SER	2.0
1	A	24	ASP	2.0
1	C	218	LEU	2.0
1	B	156	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	41	THR	2.0
1	D	146	ASN	2.0
1	C	40	ILE	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
4	GOL	C	1004	6/6	0.67	0.22	41,44,61,63	0
4	GOL	B	1004	6/6	0.76	0.18	38,41,42,44	0
4	GOL	D	1004	6/6	0.76	0.19	38,41,49,50	0
4	GOL	A	1005	6/6	0.81	0.13	38,41,43,44	0
3	SO4	A	1004	5/5	0.90	0.12	54,56,60,64	0
3	SO4	D	1002	5/5	0.90	0.11	46,51,63,70	0
3	SO4	B	1003	5/5	0.91	0.10	37,45,57,60	0
3	SO4	C	1003	5/5	0.92	0.10	43,52,55,67	0
2	K	D	1001	1/1	0.94	0.10	39,39,39,39	0
3	SO4	A	1002	5/5	0.94	0.09	37,45,56,57	0
2	K	B	1001	1/1	0.95	0.06	37,37,37,37	0
3	SO4	A	1003	5/5	0.95	0.10	27,38,49,65	0
3	SO4	C	1002	5/5	0.97	0.09	25,31,45,45	0
3	SO4	D	1003	5/5	0.97	0.07	35,36,39,46	0
2	K	A	1001	1/1	0.97	0.05	33,33,33,33	0
2	K	C	1001	1/1	0.98	0.03	27,27,27,27	0
3	SO4	B	1002	5/5	0.99	0.04	22,26,31,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.