



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:48 AM GMT

PDB ID : 3G2G
Title : S437Y Mutant of human muscle pyruvate kinase, isoform M2
Authors : Hong, B.; Dimov, S.; Allali-Hassani, A.; Tempel, W.; MacKenzie, F.; Arrow-smith, C.H.; Edwards, A.M.; Bountra, c.; Weigelt, J.; Bochkarev, A.; Vedadi, M.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2009-01-31
Resolution : 2.00 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

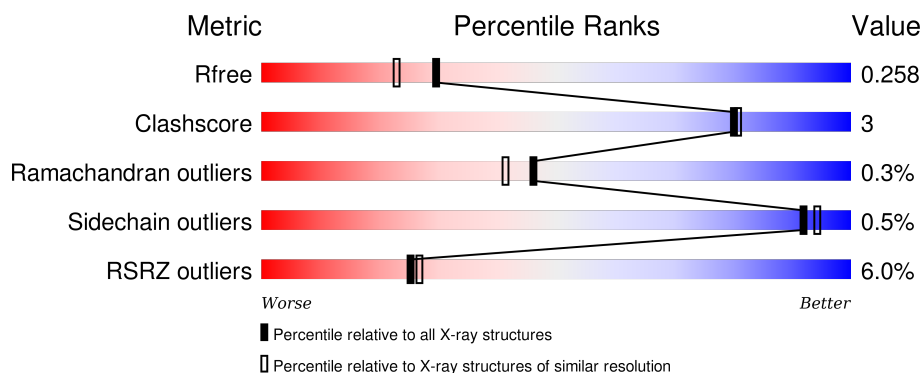
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	533	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>8%</div> <div>15%</div> </div> </div>
1	B	533	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>5%</div> </div> </div>
1	C	533	<div> <div>6%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>•</div> </div> </div>
1	D	533	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	534	-	-	-	X
3	UNX	A	534	-	-	-	X
3	UNX	A	535	-	-	-	X
3	UNX	A	536	-	-	-	X
3	UNX	A	537	-	-	-	X
3	UNX	B	535	-	-	-	X
3	UNX	B	539	-	-	-	X
3	UNX	B	540	-	-	-	X
3	UNX	B	541	-	-	-	X
3	UNX	B	542	-	-	-	X
3	UNX	B	543	-	-	-	X
3	UNX	B	544	-	-	-	X
3	UNX	C	537	-	-	-	X
3	UNX	C	538	-	-	-	X
3	UNX	C	539	-	-	-	X
3	UNX	C	540	-	-	-	X
3	UNX	C	541	-	-	-	X
3	UNX	C	542	-	-	-	X
3	UNX	D	538	-	-	-	X
3	UNX	D	541	-	-	-	X
3	UNX	D	542	-	-	-	X
3	UNX	D	543	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15165 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 isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3365	2120	589	634	22			
1	B	504	Total	C	N	O	S	0	1	0
			3759	2371	661	703	24			
1	C	510	Total	C	N	O	S	0	1	0
			3760	2377	651	707	25			
1	D	507	Total	C	N	O	S	0	0	0
			3720	2349	650	698	23			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P14618
A	0	SER	-	EXPRESSION TAG	UNP P14618
A	437	TYR	SER	ENGINEERED	UNP P14618
B	-1	GLY	-	EXPRESSION TAG	UNP P14618
B	0	SER	-	EXPRESSION TAG	UNP P14618
B	437	TYR	SER	ENGINEERED	UNP P14618
C	-1	GLY	-	EXPRESSION TAG	UNP P14618
C	0	SER	-	EXPRESSION TAG	UNP P14618
C	437	TYR	SER	ENGINEERED	UNP P14618
D	-1	GLY	-	EXPRESSION TAG	UNP P14618
D	0	SER	-	EXPRESSION TAG	UNP P14618
D	437	TYR	SER	ENGINEERED	UNP P14618

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	12	Total 12	X 12	0	0
3	A	4	Total 4	X 4	0	0
3	D	8	Total 8	X 8	0	0
3	C	7	Total 7	X 7	0	0

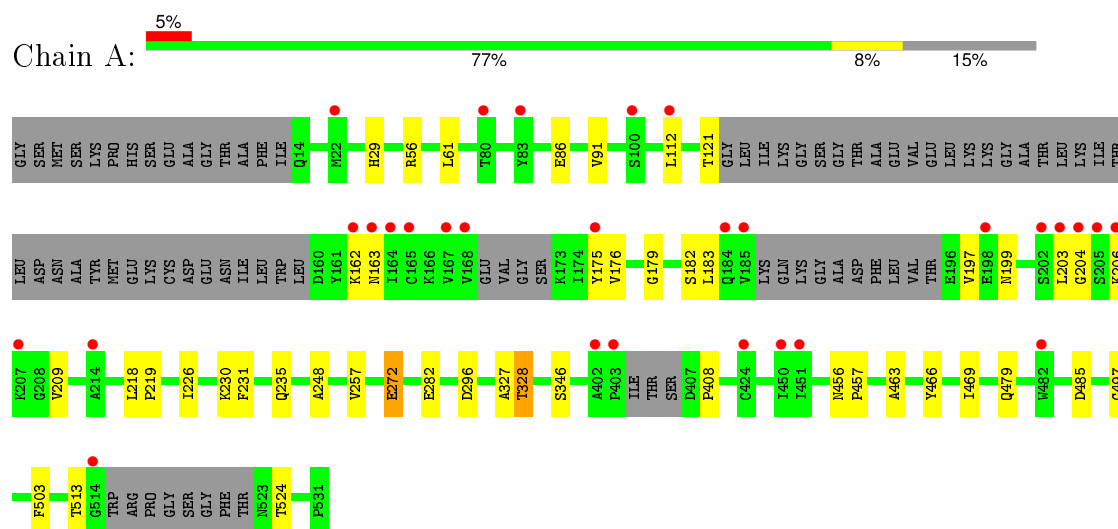
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total 92	O 92	0	0
4	B	151	Total 151	O 151	0	0
4	C	120	Total 120	O 120	0	0
4	D	102	Total 102	O 102	0	0

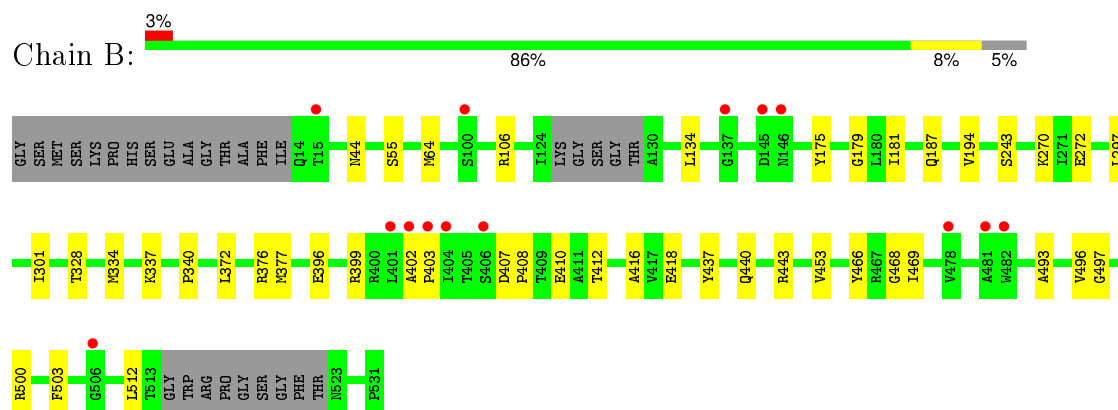
3 Residue-property plots [i](#)

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.

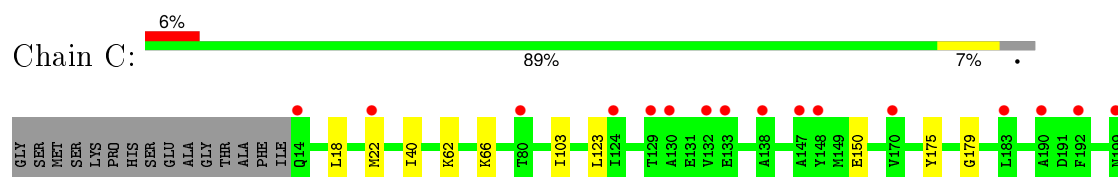
• Molecule 1: Pyruvate kinase isozymes M1/M2

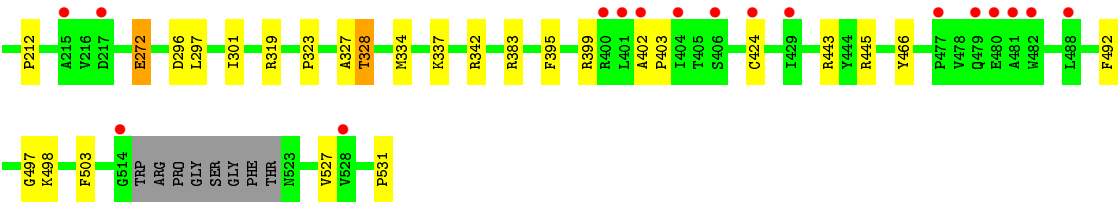


• Molecule 1: Pyruvate kinase isozymes M1/M2

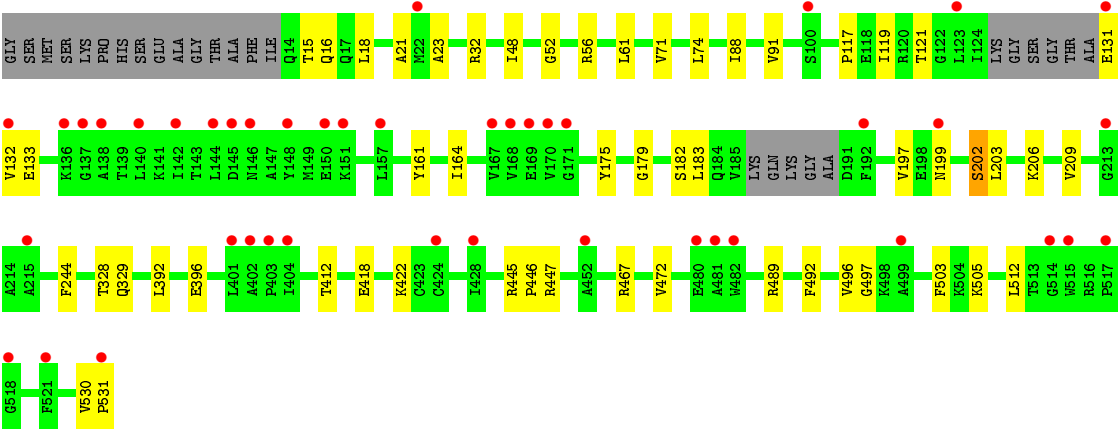
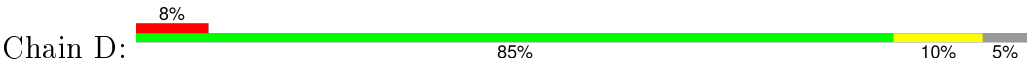


• Molecule 1: Pyruvate kinase isozymes M1/M2





● Molecule 1: Pyruvate kinase isozymes M1/M2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.55Å 137.88Å 155.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.96 – 2.00 21.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (21.96-2.00) 99.6 (21.96-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine), coot, molprobity	Depositor
R, R_{free}	0.227 , 0.260 0.224 , 0.258	Depositor DCC
R_{free} test set	2097 reflections (1.39%)	DCC
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 152544 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15165	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: UNX, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/3417	0.49	0/4632
1	B	0.36	0/3820	0.51	0/5178
1	C	0.34	0/3823	0.51	0/5186
1	D	0.34	0/3782	0.50	0/5135
All	All	0.34	0/14842	0.50	0/20131

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 [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	3365	0	3284	25	0
1	B	3759	0	3722	25	0
1	C	3760	0	3682	20	0
1	D	3720	0	3597	34	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	0	0
3	A	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	0	0	0
3	C	7	0	0	0	0
3	D	8	0	0	0	0
4	A	92	0	0	1	0
4	B	151	0	0	0	0
4	C	120	0	0	0	0
4	D	102	0	0	1	0
All	All	15165	0	14285	98	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 (98) 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:D:175:TYR:HB3	1:D:179:GLY:HA2	1.74	0.70
1:B:410:GLU:CG	1:D:422:LYS:HE2	2.31	0.61
1:B:340:PRO:HG3	1:B:377:MET:HG2	1.84	0.59
1:B:410:GLU:HG3	1:D:422:LYS:HE2	1.83	0.59
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.84	0.59
1:A:203:LEU:HD12	1:A:204:GLY:H	1.69	0.58
1:D:182:SER:OG	1:D:199:ASN:HB3	2.03	0.57
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.87	0.57
1:C:395:PHE:CZ	1:C:399:ARG:HD2	2.40	0.56
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.87	0.56
1:D:446:PRO:HD2	4:D:564:HOH:O	2.06	0.54
1:A:272:GLU:HB3	1:A:296:ASP:HB2	1.89	0.54
1:C:175:TYR:HB3	1:C:179:GLY:HA2	1.90	0.53
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.43	0.53
1:D:119:ILE:HG23	1:D:161:TYR:HB2	1.92	0.52
1:B:418:GLU:OE2	1:D:418:GLU:OE2	2.28	0.52
1:D:445:ARG:NH2	1:D:467:ARG:HB3	2.25	0.51
1:C:319:ARG:O	1:C:443:ARG:NH2	2.43	0.51
1:A:183:LEU:HD23	1:A:197:VAL:HA	1.92	0.51
1:A:61:LEU:HD13	1:A:91:VAL:HA	1.93	0.51
1:A:226:ILE:O	1:A:230:LYS:HG2	2.10	0.51
1:B:496:VAL:O	1:B:500:ARG:HG2	2.11	0.51
1:C:18:LEU:O	1:C:22:MET:HG3	2.12	0.50
1:C:123:LEU:HB2	1:C:150:GLU:HA	1.92	0.50
1:A:176:VAL:HG22	1:A:209:VAL:HG22	1.93	0.49
1:D:52:GLY:O	1:D:56:ARG:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:GLU:HA	1:D:203:LEU:O	2.13	0.49
1:D:392:LEU:O	1:D:396:GLU:HG3	2.13	0.49
1:A:121:THR:O	1:A:206:LYS:HA	2.14	0.48
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.96	0.48
1:A:182:SER:HB3	1:A:199:ASN:HB2	1.94	0.48
1:B:44:ASN:HB3	1:B:468:GLY:HA2	1.96	0.48
1:C:297:LEU:O	1:C:301:ILE:HG12	2.14	0.47
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.96	0.47
1:C:40:ILE:O	1:C:383:ARG:HD2	2.15	0.47
1:C:103:ILE:HD13	1:C:492:PHE:CE1	2.50	0.47
1:D:74:LEU:N	1:D:74:LEU:HD23	2.30	0.47
1:D:164:ILE:O	1:D:164:ILE:HG12	2.15	0.47
1:B:55:SER:HB2	1:B:64:MET:SD	2.55	0.46
1:C:272:GLU:HB3	1:C:296:ASP:HB2	1.97	0.46
1:B:410:GLU:HG2	1:D:422:LYS:HE2	1.97	0.46
1:B:243:SER:HA	1:B:270:LYS:HD3	1.98	0.46
1:C:327:ALA:O	1:C:328:THR:HB	2.16	0.46
1:C:175:TYR:CE1	1:C:212:PRO:HG3	2.51	0.46
1:D:489:ARG:O	1:D:492:PHE:HB3	2.16	0.46
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.51	0.45
1:D:412:THR:HG22	1:D:512:LEU:HD22	1.98	0.45
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.52	0.45
1:A:248:ALA:HB2	1:A:282:GLU:HG3	1.99	0.45
1:D:132:VAL:HG23	1:D:132:VAL:O	2.18	0.45
1:D:16:GLN:HB2	1:D:447:ARG:NH1	2.32	0.44
1:A:163:ASN:OD1	1:A:163:ASN:C	2.55	0.44
1:B:440:GLN:O	1:B:443:ARG:HG2	2.18	0.44
1:B:396:GLU:O	1:B:399:ARG:HB2	2.18	0.44
1:A:218:LEU:HB3	1:A:219:PRO:HD2	2.00	0.43
1:B:466:TYR:HB2	1:B:469:ILE:HD12	2.00	0.43
1:B:402:ALA:HA	1:B:403:PRO:HD3	1.91	0.43
1:A:230:LYS:HE2	1:A:257:VAL:HG13	1.99	0.43
1:D:74:LEU:HD11	1:D:88:ILE:HG13	2.01	0.43
1:D:183:LEU:HD23	1:D:197:VAL:HA	2.00	0.43
1:C:498:LYS:NZ	1:C:531:PRO:O	2.43	0.43
1:A:327:ALA:O	1:A:328:THR:HB	2.19	0.42
1:D:505:LYS:HA	1:D:530:VAL:HG12	1.99	0.42
1:B:372:LEU:O	1:B:376:ARG:HG3	2.18	0.42
1:B:187:GLN:HB2	1:B:194:VAL:HB	2.01	0.42
1:A:408:PRO:HB3	1:C:527:VAL:CG1	2.49	0.42
1:C:445[B]:ARG:HA	1:C:445[B]:ARG:HD3	1.81	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:LEU:O	1:B:301:ILE:HG12	2.20	0.42
1:B:134:LEU:HD12	1:B:181:ILE:HD13	2.00	0.42
1:D:121:THR:O	1:D:206:LYS:HA	2.20	0.42
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.55	0.42
1:A:479:GLN:HB2	1:A:485:ASP:HB2	2.02	0.42
1:C:334:MET:HA	1:C:337:LYS:O	2.20	0.41
1:B:407:ASP:HA	1:B:408:PRO:HD3	1.73	0.41
1:C:342:ARG:HG2	1:D:329:GLN:OE1	2.20	0.41
1:A:56:ARG:HH22	1:A:86:GLU:HB3	1.85	0.41
1:D:61:LEU:HD13	1:D:91:VAL:HA	2.01	0.41
1:B:334:MET:HA	1:B:337:LYS:O	2.21	0.41
1:B:106:ARG:NH2	1:B:500:ARG:HH22	2.18	0.41
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.51	0.41
1:A:231:PHE:CE2	1:A:235:GLN:HG3	2.56	0.41
1:A:456:ASN:HA	1:A:457:PRO:HD3	1.95	0.41
1:B:416:ALA:HB2	1:B:512:LEU:HD21	2.03	0.41
1:A:112:LEU:HD23	1:A:112:LEU:C	2.41	0.41
1:D:175:TYR:O	1:D:209:VAL:HA	2.21	0.41
1:D:530:VAL:HA	1:D:531:PRO:HD3	1.90	0.41
1:B:412:THR:HG22	1:B:512:LEU:HD22	2.02	0.41
1:A:29:HIS:HE1	4:A:606:HOH:O	2.04	0.41
1:C:323:PRO:HG3	1:C:466:TYR:CE1	2.56	0.41
1:C:62:LYS:O	1:C:66:LYS:HG3	2.20	0.40
1:A:513:THR:OG1	1:A:524:THR:HB	2.20	0.40
1:D:48:ILE:HG12	1:D:71:VAL:HB	2.02	0.40
1:D:23:ALA:HB2	1:D:32:ARG:HD2	2.04	0.40
1:D:117:PRO:HD2	1:D:244:PHE:HB2	2.03	0.40
1:D:15:THR:C	1:D:16:GLN:HG2	2.42	0.40
1:D:18:LEU:O	1:D:21:ALA:HB3	2.21	0.40
1:D:133:GLU:HA	1:D:202:SER:HA	2.04	0.40
1:C:402:ALA:HA	1:C:403:PRO:HD3	1.94	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	443/533 (83%)	432 (98%)	9 (2%)	2 (0%)	34	26
1	B	499/533 (94%)	490 (98%)	8 (2%)	1 (0%)	52	48
1	C	507/533 (95%)	491 (97%)	15 (3%)	1 (0%)	52	48
1	D	501/533 (94%)	482 (96%)	18 (4%)	1 (0%)	52	48
All	All	1950/2132 (92%)	1895 (97%)	50 (3%)	5 (0%)	46	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	LYS
1	A	328	THR
1	C	328	THR
1	D	328	THR
1	B	328	THR

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	338/437 (77%)	336 (99%)	2 (1%)	90	93
1	B	381/437 (87%)	379 (100%)	2 (0%)	92	94
1	C	373/437 (85%)	371 (100%)	2 (0%)	92	94
1	D	365/437 (84%)	364 (100%)	1 (0%)	94	96
All	All	1457/1748 (83%)	1450 (100%)	7 (0%)	92	94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	GLU
1	A	346	SER
1	B	272	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	437	TYR
1	C	272	GLU
1	C	424	CYS
1	D	202	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 44 ligands modelled in this entry, 31 are unknown - 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	$\# Z > 2$
2	SO4	A	532	-	4,4,4	0.32	0	6,6,6	0.30	0
2	SO4	A	533	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	B	532	-	4,4,4	0.38	0	6,6,6	0.20	0
2	SO4	B	533	-	4,4,4	0.19	0	6,6,6	0.13	0
2	SO4	B	534	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	C	532	-	4,4,4	0.21	0	6,6,6	0.22	0
2	SO4	C	533	-	4,4,4	0.17	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	534	-	4,4,4	0.17	0	6,6,6	0.10	0
2	SO4	C	535	-	4,4,4	0.15	0	6,6,6	0.41	0
2	SO4	D	532	-	4,4,4	0.23	0	6,6,6	0.20	0
2	SO4	D	533	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	D	534	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	D	535	-	4,4,4	0.16	0	6,6,6	0.25	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	532	-	-	0/0/0/0	0/0/0/0
2	SO4	A	533	-	-	0/0/0/0	0/0/0/0
2	SO4	B	532	-	-	0/0/0/0	0/0/0/0
2	SO4	B	533	-	-	0/0/0/0	0/0/0/0
2	SO4	B	534	-	-	0/0/0/0	0/0/0/0
2	SO4	C	532	-	-	0/0/0/0	0/0/0/0
2	SO4	C	533	-	-	0/0/0/0	0/0/0/0
2	SO4	C	534	-	-	0/0/0/0	0/0/0/0
2	SO4	C	535	-	-	0/0/0/0	0/0/0/0
2	SO4	D	532	-	-	0/0/0/0	0/0/0/0
2	SO4	D	533	-	-	0/0/0/0	0/0/0/0
2	SO4	D	534	-	-	0/0/0/0	0/0/0/0
2	SO4	D	535	-	-	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.

No monomer is involved in short contacts.

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	455/533 (85%)	0.28	29 (6%) 23 24	19, 33, 64, 75	0
1	B	504/533 (94%)	0.00	14 (2%) 56 57	17, 28, 44, 67	0
1	C	510/533 (95%)	0.20	33 (6%) 22 23	19, 30, 54, 68	0
1	D	507/533 (95%)	0.40	43 (8%) 13 14	20, 32, 67, 77	0
All	All	1976/2132 (92%)	0.22	119 (6%) 25 27	17, 31, 59, 77	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	404	ILE	7.9
1	D	192	PHE	7.7
1	D	404	ILE	6.7
1	C	404	ILE	6.2
1	C	190	ALA	5.0
1	D	215	ALA	4.7
1	D	481	ALA	4.6
1	A	203	LEU	4.6
1	D	521	PHE	4.6
1	D	403	PRO	4.4
1	D	167	VAL	4.3
1	D	517	PRO	4.3
1	D	482	TRP	4.3
1	D	138	ALA	4.2
1	C	215	ALA	4.2
1	D	402	ALA	4.2
1	C	148	TYR	4.1
1	D	424	CYS	4.0
1	A	204	GLY	4.0
1	A	112	LEU	3.8
1	D	171	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	401	LEU	3.7
1	C	170	VAL	3.7
1	D	518	GLY	3.5
1	A	185	VAL	3.5
1	A	165	CYS	3.5
1	A	424	CYS	3.5
1	A	198	GLU	3.5
1	A	202	SER	3.5
1	D	137	GLY	3.4
1	C	424	CYS	3.3
1	A	402	ALA	3.3
1	A	207	LYS	3.2
1	A	403	PRO	3.2
1	C	401	LEU	3.2
1	A	214	ALA	3.2
1	A	514	GLY	3.2
1	D	142	ILE	3.1
1	A	168	VAL	3.0
1	C	482	TRP	3.0
1	C	402	ALA	3.0
1	A	163	ASN	3.0
1	B	146	ASN	3.0
1	D	150	GLU	2.9
1	B	403	PRO	2.9
1	D	22	MET	2.9
1	A	205	SER	2.9
1	B	482	TRP	2.9
1	D	146	ASN	2.9
1	A	162	LYS	2.9
1	D	499	ALA	2.9
1	D	148	TYR	2.9
1	C	132	VAL	2.8
1	A	206	LYS	2.8
1	B	401	LEU	2.8
1	D	123	LEU	2.8
1	D	151	LYS	2.7
1	B	406	SER	2.7
1	C	192	PHE	2.7
1	A	164	ILE	2.7
1	C	124	ILE	2.6
1	D	100	SER	2.6
1	B	481	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	132	VAL	2.6
1	D	168	VAL	2.6
1	C	217	ASP	2.5
1	C	514	GLY	2.5
1	C	528	VAL	2.5
1	D	515	TRP	2.5
1	A	22	MET	2.5
1	C	199	ASN	2.4
1	C	406	SER	2.4
1	C	400	ARG	2.4
1	D	140	LEU	2.4
1	D	145	ASP	2.4
1	C	130	ALA	2.4
1	C	479	GLN	2.4
1	B	145	ASP	2.4
1	C	147	ALA	2.4
1	B	478	VAL	2.4
1	A	184	GLN	2.4
1	C	129	THR	2.4
1	C	481	ALA	2.3
1	D	213	GLY	2.3
1	C	488	LEU	2.3
1	D	157	LEU	2.3
1	A	83	TYR	2.3
1	C	133	GLU	2.3
1	C	429	ILE	2.3
1	B	506	GLY	2.3
1	D	199	ASN	2.3
1	A	451	ILE	2.3
1	A	100	SER	2.3
1	B	137	GLY	2.3
1	D	144	LEU	2.3
1	D	514	GLY	2.3
1	C	22	MET	2.3
1	A	450	ILE	2.3
1	B	402	ALA	2.3
1	D	131	GLU	2.2
1	D	480	GLU	2.2
1	A	482	TRP	2.2
1	C	14	GLN	2.2
1	D	170	VAL	2.1
1	A	80	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	183	LEU	2.1
1	C	138	ALA	2.1
1	D	452	ALA	2.1
1	D	136	LYS	2.1
1	C	477	PRO	2.1
1	D	531	PRO	2.1
1	C	480	GLU	2.1
1	A	175	TYR	2.1
1	B	100	SER	2.1
1	B	15	THR	2.0
1	C	80	THR	2.0
1	D	169	GLU	2.0
1	D	428	ILE	2.0
1	A	167	VAL	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(\AA^2)	Q<0.9
3	UNX	D	542	1/1	-0.30	4.07	197.77	28,28,28,28	1
3	UNX	A	536	1/1	0.34	3.21	196.38	20,20,20,20	1
3	UNX	D	543	1/1	0.37	2.68	179.45	33,33,33,33	1
3	UNX	C	537	1/1	0.28	2.84	178.06	28,28,28,28	1
3	UNX	B	539	1/1	0.42	2.02	168.02	19,19,19,19	1
3	UNX	C	540	1/1	0.39	3.31	166.12	24,24,24,24	1
3	UNX	A	537	1/1	0.00	3.10	135.88	38,38,38,38	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	UNX	B	535	1/1	-0.00	2.29	134.94	21,21,21,21	1
3	UNX	B	541	1/1	0.19	2.82	134.01	21,21,21,21	1
3	UNX	C	539	1/1	-0.19	2.90	132.68	27,27,27,27	1
3	UNX	C	542	1/1	0.63	2.61	125.32	21,21,21,21	1
3	UNX	C	538	1/1	0.50	2.29	110.77	25,25,25,25	1
3	UNX	B	540	1/1	0.02	2.66	109.69	22,22,22,22	1
3	UNX	B	543	1/1	0.05	2.81	106.68	19,19,19,19	1
3	UNX	A	535	1/1	-0.17	2.00	95.85	28,28,28,28	1
3	UNX	A	534	1/1	0.24	2.38	95.53	37,37,37,37	1
3	UNX	C	541	1/1	0.17	3.13	92.94	29,29,29,29	1
3	UNX	B	542	1/1	0.60	2.98	92.56	23,23,23,23	1
3	UNX	D	541	1/1	0.27	3.37	85.67	25,25,25,25	1
3	UNX	D	538	1/1	-0.16	2.09	81.35	25,25,25,25	1
3	UNX	B	544	1/1	0.47	2.16	68.03	29,29,29,29	1
2	SO4	C	534	5/5	0.96	0.20	2.86	49,50,56,59	0
2	SO4	A	532	5/5	0.98	0.10	-0.06	29,30,34,34	0
2	SO4	D	532	5/5	0.99	0.07	-1.26	33,33,37,38	0
2	SO4	C	532	5/5	0.98	0.07	-1.70	24,27,31,34	0
2	SO4	B	532	5/5	0.99	0.09	-1.72	29,29,32,32	0
3	UNX	C	536	1/1	0.35	1.85	-	29,29,29,29	1
3	UNX	B	537	1/1	0.11	1.37	-	30,30,30,30	1
2	SO4	B	534	5/5	0.97	0.07	-	27,28,32,32	0
3	UNX	D	540	1/1	-0.24	4.34	-	29,29,29,29	1
3	UNX	B	546	1/1	0.45	2.41	-	22,22,22,22	1
3	UNX	D	537	1/1	0.45	1.65	-	26,26,26,26	1
2	SO4	A	533	5/5	0.93	0.28	-	49,50,60,62	0
3	UNX	B	538	1/1	-0.07	1.35	-	32,32,32,32	1
2	SO4	D	534	5/5	0.92	0.27	-	52,60,64,72	0
2	SO4	D	533	5/5	0.96	0.28	-	46,48,56,61	0
3	UNX	B	536	1/1	0.32	1.76	-	22,22,22,22	1
3	UNX	B	545	1/1	-0.09	3.35	-	25,25,25,25	1
2	SO4	C	535	5/5	0.94	0.25	-	38,43,50,58	0
3	UNX	D	539	1/1	-0.27	1.74	-	36,36,36,36	1
2	SO4	C	533	5/5	0.96	0.17	-	46,50,51,57	0
2	SO4	D	535	5/5	0.94	0.16	-	45,45,48,49	0
2	SO4	B	533	5/5	0.96	0.21	-	49,50,59,60	0
3	UNX	D	536	1/1	0.16	1.98	-	26,26,26,26	1

6.5 Other polymers ⓘ

There are no such residues in this entry.