



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:21 AM UTC

PDB ID : 3G2G / pdb_00003g2g
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

<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

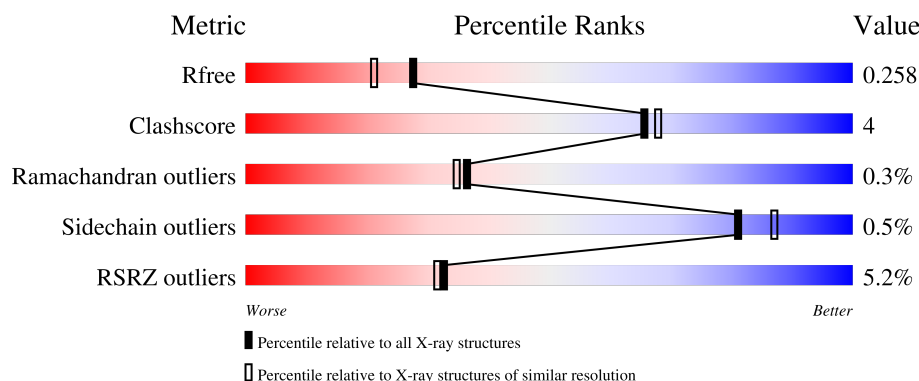
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	533	5% 76% 9% 15%
1	B	533	% 85% 9% 5%
1	C	533	4% 88% 7% .
1	D	533	10% 83% 11% 5%

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	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	536	-	-	-	X
3	UNX	B	537	-	-	-	X
3	UNX	B	538	-	-	-	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	B	545	-	-	-	X
3	UNX	B	546	-	-	-	X
3	UNX	C	536	-	-	-	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	536	-	-	-	X
3	UNX	D	537	-	-	-	X
3	UNX	D	538	-	-	-	X
3	UNX	D	539	-	-	-	X
3	UNX	D	540	-	-	-	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 mutation	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
B	437	TYR	SER	engineered mutation	UNP P14618
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
C	437	TYR	SER	engineered mutation	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618
D	437	TYR	SER	engineered mutation	UNP P14618

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	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 (CCD ID: UNX) (formula: X).

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

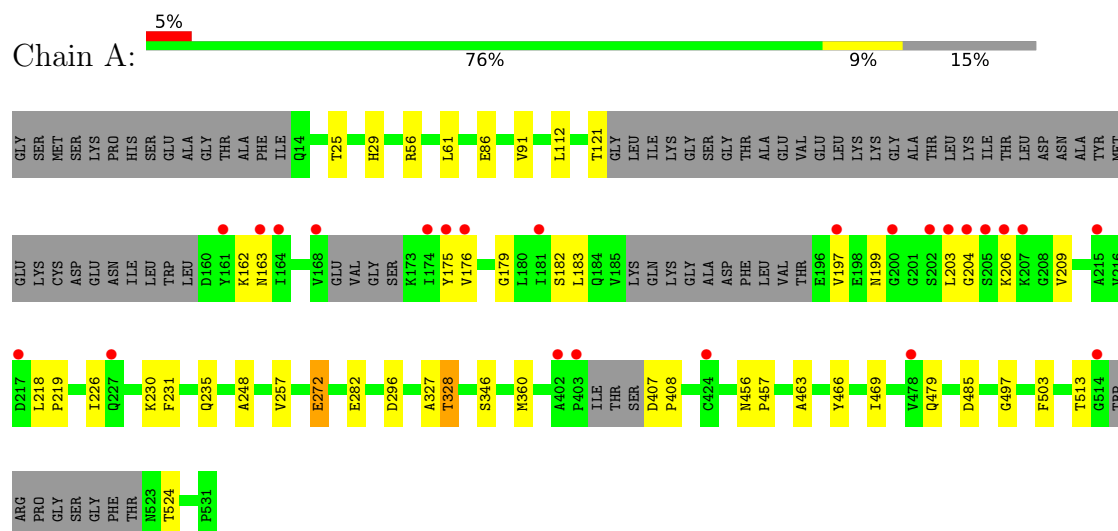
- Molecule 4 is water.

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

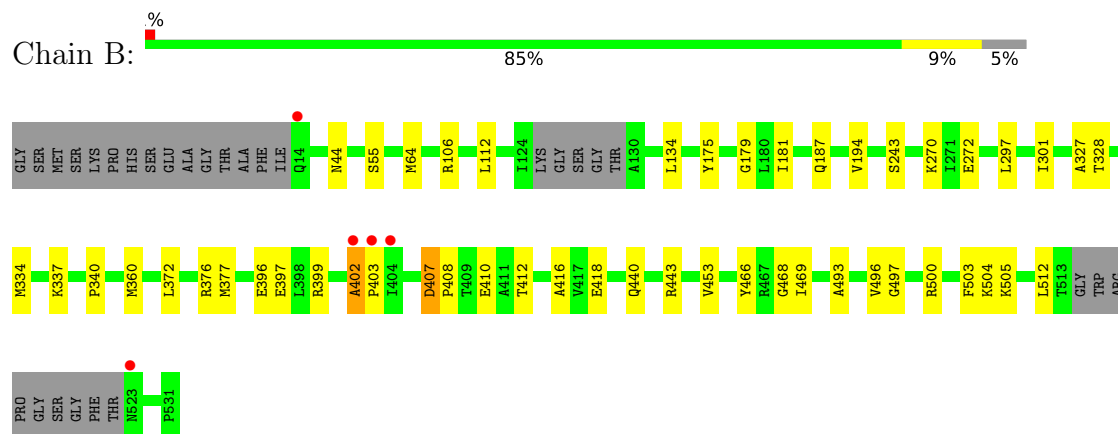
3 Residue-property plots

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.

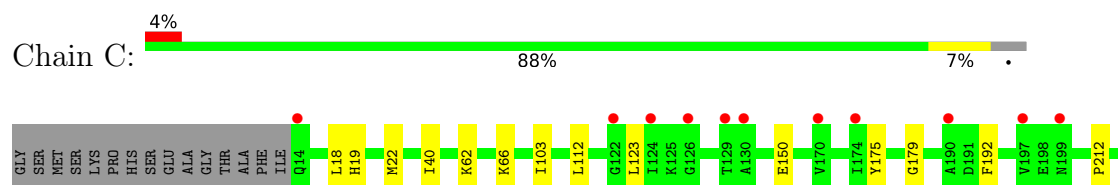
• Molecule 1: Pyruvate kinase isozymes M1/M2

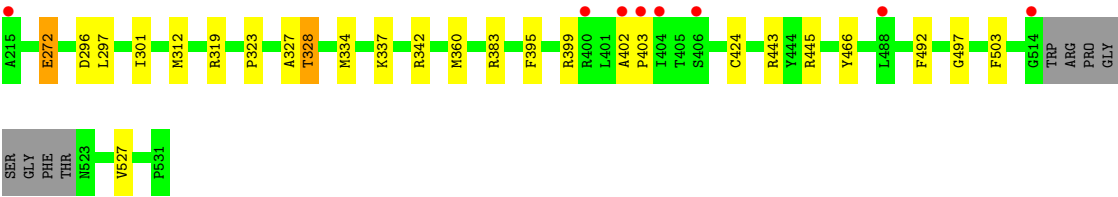


• Molecule 1: Pyruvate kinase isozymes M1/M2

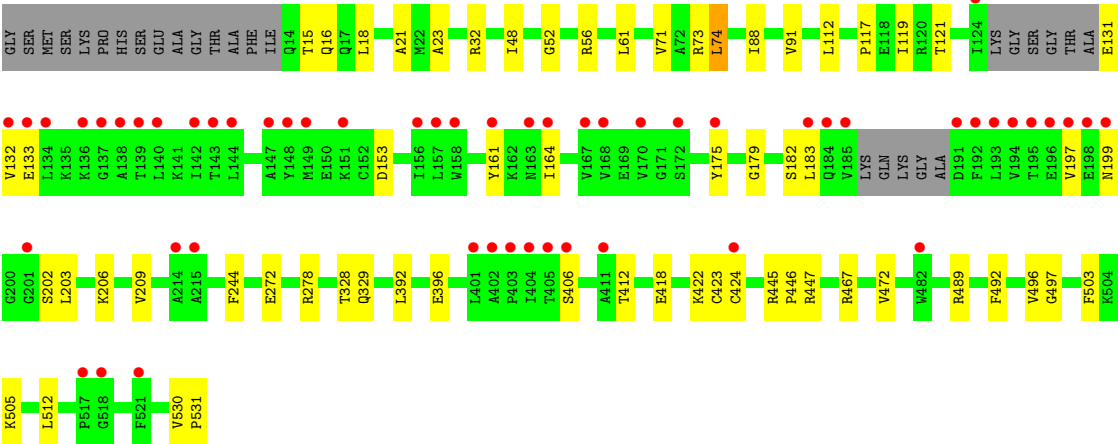
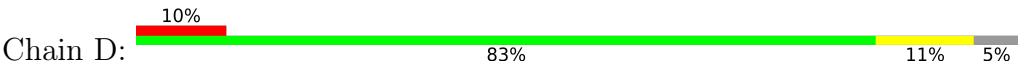


• Molecule 1: Pyruvate kinase isozymes M1/M2





● 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) 99.5 (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	Depositor
R, R_{free}	0.227 , 0.260 0.224 , 0.258	Depositor DCC
R_{free} test set	2097 reflections (1.37%)	wwPDB-VP
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 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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, UNX

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	0.42	0/3417	0.75	2/4632 (0.0%)
1	B	0.45	0/3820	0.76	4/5178 (0.1%)
1	C	0.44	0/3823	0.76	1/5186 (0.0%)
1	D	0.42	0/3782	0.76	1/5135 (0.0%)
All	All	0.43	0/14842	0.76	8/20131 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	407	ASP	CA-C-N	5.97	125.52	119.19
1	B	407	ASP	C-N-CA	5.97	125.52	119.19
1	D	406	SER	N-CA-C	-5.60	106.44	113.72
1	C	192	PHE	N-CA-C	5.42	116.51	108.60
1	A	407	ASP	CA-C-N	5.32	125.13	119.28
1	A	407	ASP	C-N-CA	5.32	125.13	119.28
1	B	402	ALA	CA-C-N	5.22	125.47	119.83
1	B	402	ALA	C-N-CA	5.22	125.47	119.83

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	3365	0	3284	27	0
1	B	3759	0	3722	29	0
1	C	3760	0	3682	23	0
1	D	3720	0	3597	39	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
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	111	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 (111) 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:C:19:HIS:HA	1:C:22:MET:HE2	1.74	0.70
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:A:272:GLU:HB3	1:A:296:ASP:HB2	1.89	0.54
1:D:446:PRO:HD2	4:D:564:HOH:O	2.06	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:C:319:ARG:O	1:C:443:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:ARG:NH2	1:D:467:ARG:HB3	2.25	0.51
1:A:61:LEU:HD13	1:A:91:VAL:HA	1.93	0.51
1:A:183:LEU:HD23	1:A:197:VAL:HA	1.92	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
1:D:131:GLU:HA	1:D:203:LEU:O	2.13	0.49
1:A:163:ASN:OD1	1:A:163:ASN:C	2.55	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:B:327:ALA:HB1	1:B:360:MET:HE2	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:HD23	1:D:74:LEU:N	2.30	0.47
1:D:164:ILE:HG12	1:D:164:ILE:O	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:A:327:ALA:HB1	1:A:360:MET:HE2	1.96	0.46
1:A:112:LEU:C	1:A:112:LEU:HD23	2.41	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:C:327:ALA:HB1	1:C:360:MET:HE2	1.98	0.45
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:A:248:ALA:HB2	1:A:282:GLU:HG3	1.99	0.45
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.52	0.45
1:D:132:VAL:O	1:D:132:VAL:HG23	2.18	0.45
1:D:15:THR:C	1:D:16:GLN:HG2	2.42	0.44
1:C:327:ALA:O	1:C:328:THR:HB	2.16	0.44
1:D:16:GLN:HB2	1:D:447:ARG:NH1	2.32	0.44
1:D:182:SER:HG	1:D:199:ASN:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:GLN:O	1:B:443:ARG:HG2	2.18	0.44
1:D:73:ARG:C	1:D:74:LEU:HD23	2.42	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:D:423:CYS:O	1:D:424:CYS:C	2.61	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:B:187:GLN:HB2	1:B:194:VAL:HB	2.01	0.42
1:B:372:LEU:O	1:B:376:ARG:HG3	2.18	0.42
1:D:505:LYS:HA	1:D:530:VAL:HG12	1.99	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
1:B:112:LEU:HD23	1:B:112:LEU:C	2.44	0.42
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:A:56:ARG:HH22	1:A:86:GLU:HB3	1.85	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:B:334:MET:HA	1:B:337:LYS:O	2.21	0.41
1:B:504:LYS:O	1:B:505:LYS:C	2.63	0.41
1:D:61:LEU:HD13	1:D:91:VAL:HA	2.01	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:A:25:THR:HB	1:B:397:GLU:CD	2.46	0.41
1:B:416:ALA:HB2	1:B:512:LEU:HD21	2.03	0.41
1:B:412:THR:HG22	1:B:512:LEU:HD22	2.02	0.41
1:D:153:ASP:OD2	1:D:153:ASP:C	2.64	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:A:29:HIS:HE1	4:A:606:HOH:O	2.04	0.41
1:A:327:ALA:O	1:A:328:THR:HB	2.19	0.41
1:C:312:MET:C	1:C:312:MET:SD	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:PRO:HG3	1:C:466:TYR:CE1	2.56	0.41
1:A:513:THR:OG1	1:A:524:THR:HB	2.20	0.40
1:C:62:LYS:O	1:C:66:LYS:HG3	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:112:LEU:HD23	1:D:112:LEU:C	2.47	0.40
1:D:117:PRO:HD2	1:D:244:PHE:HB2	2.03	0.40
1:C:112:LEU:C	1:C:112:LEU:HD23	2.46	0.40
1:C:402:ALA:HA	1:C:403:PRO:HD3	1.94	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

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	443/533 (83%)	432 (98%)	9 (2%)	2 (0%)	24	21
1	B	499/533 (94%)	490 (98%)	8 (2%)	1 (0%)	43	42
1	C	507/533 (95%)	491 (97%)	15 (3%)	1 (0%)	43	42
1	D	501/533 (94%)	482 (96%)	18 (4%)	1 (0%)	43	42
All	All	1950/2132 (92%)	1895 (97%)	50 (3%)	5 (0%)	36	35

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

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Mol	Chain	Res	Type
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%)	78	85
1	B	381/437 (87%)	380 (100%)	1 (0%)	86	91
1	C	373/437 (85%)	371 (100%)	2 (0%)	81	87
1	D	365/437 (84%)	362 (99%)	3 (1%)	73	80
All	All	1457/1748 (83%)	1449 (100%)	8 (0%)	81	87

All (8) 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
1	C	272	GLU
1	C	424	CYS
1	D	74	LEU
1	D	272	GLU
1	D	278	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	78	HIS
1	A	199	ASN
1	A	252	HIS
1	A	393	GLN
1	A	439	HIS
1	A	491	ASN

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Mol	Chain	Res	Type
1	B	44	ASN
1	B	393	GLN
1	B	458	GLN
1	C	44	ASN
1	C	458	GLN
1	D	16	GLN
1	D	210	ASN
1	D	235	GLN
1	D	252	HIS
1	D	458	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 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	B	532	-	4,4,4	0.27	0	6,6,6	0.27	0
2	SO4	A	532	-	4,4,4	0.19	0	6,6,6	0.21	0
2	SO4	C	532	-	4,4,4	0.22	0	6,6,6	0.27	0
2	SO4	D	532	-	4,4,4	0.26	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	533	-	4,4,4	0.28	0	6,6,6	0.14	0
2	SO4	B	534	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	A	533	-	4,4,4	0.27	0	6,6,6	0.18	0
2	SO4	D	533	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	B	533	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	D	534	-	4,4,4	0.25	0	6,6,6	0.14	0
2	SO4	C	534	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	D	535	-	4,4,4	0.24	0	6,6,6	0.31	0
2	SO4	C	535	-	4,4,4	0.22	0	6,6,6	0.32	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 [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	455/533 (85%)	0.26	24 (5%) 32 31	19, 33, 64, 75	0
1	B	504/533 (94%)	-0.12	5 (0%) 79 79	14, 28, 44, 67	1 (0%)
1	C	510/533 (95%)	0.09	19 (3%) 45 44	15, 30, 54, 68	1 (0%)
1	D	507/533 (95%)	0.33	54 (10%) 11 10	20, 32, 67, 77	0
All	All	1976/2132 (92%)	0.14	102 (5%) 33 31	14, 31, 59, 77	2 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	404	ILE	4.9
1	D	424	CYS	4.8
1	C	404	ILE	4.4
1	D	167	VAL	4.3
1	D	405	THR	4.2
1	B	404	ILE	4.1
1	D	192	PHE	4.1
1	C	190	ALA	4.0
1	A	164	ILE	4.0
1	A	403	PRO	3.9
1	A	424	CYS	3.9
1	D	403	PRO	3.8
1	D	139	THR	3.7
1	C	14	GLN	3.6
1	A	197	VAL	3.6
1	D	194	VAL	3.6
1	D	148	TYR	3.5
1	D	185	VAL	3.5
1	D	482	TRP	3.3
1	D	156	ILE	3.2
1	A	514	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	142	ILE	3.1
1	A	200	GLY	3.0
1	D	402	ALA	3.0
1	A	168	VAL	3.0
1	A	202	SER	3.0
1	C	402	ALA	3.0
1	D	140	LEU	3.0
1	D	172	SER	3.0
1	D	193	LEU	2.9
1	D	124	ILE	2.9
1	C	400	ARG	2.9
1	D	215	ALA	2.9
1	D	168	VAL	2.8
1	B	523	ASN	2.8
1	A	204	GLY	2.8
1	D	143	THR	2.8
1	B	403	PRO	2.8
1	D	163	ASN	2.7
1	A	206	LYS	2.7
1	B	402	ALA	2.7
1	D	198	GLU	2.7
1	B	14	GLN	2.7
1	D	517	PRO	2.7
1	A	402	ALA	2.6
1	D	151	LYS	2.6
1	C	215	ALA	2.6
1	C	403	PRO	2.6
1	D	521	PHE	2.5
1	C	514	GLY	2.5
1	A	203	LEU	2.5
1	C	199	ASN	2.5
1	D	144	LEU	2.5
1	D	199	ASN	2.5
1	D	149	MET	2.4
1	D	401	LEU	2.4
1	D	518	GLY	2.4
1	A	181	ILE	2.4
1	A	227	GLN	2.4
1	D	197	VAL	2.4
1	A	217	ASP	2.4
1	D	147	ALA	2.4
1	D	214	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	207	LYS	2.4
1	A	175	TYR	2.3
1	D	138	ALA	2.3
1	D	157	LEU	2.3
1	A	205	SER	2.3
1	A	163	ASN	2.3
1	C	129	THR	2.3
1	C	488	LEU	2.3
1	C	124	ILE	2.3
1	A	176	VAL	2.3
1	D	195	THR	2.3
1	C	130	ALA	2.3
1	D	411	ALA	2.3
1	D	183	LEU	2.3
1	A	161	TYR	2.3
1	D	184	GLN	2.2
1	A	174	ILE	2.2
1	D	170	VAL	2.2
1	D	164	ILE	2.2
1	C	122	GLY	2.2
1	D	134	LEU	2.2
1	D	161	TYR	2.2
1	D	136	LYS	2.2
1	D	196	GLU	2.1
1	C	406	SER	2.1
1	D	175	TYR	2.1
1	D	158	TRP	2.1
1	C	126	GLY	2.1
1	D	191	ASP	2.1
1	D	201	GLY	2.1
1	A	478	VAL	2.1
1	C	170	VAL	2.1
1	D	406	SER	2.1
1	D	133	GLU	2.1
1	C	197	VAL	2.1
1	D	132	VAL	2.1
1	D	137	GLY	2.0
1	C	174	ILE	2.0
1	A	215	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
3	UNX	B	537	1/1	-0.51	1.09	30,30,30,30	1
3	UNX	A	534	1/1	-0.48	1.01	37,37,37,37	1
3	UNX	D	537	1/1	-0.46	1.05	26,26,26,26	1
3	UNX	C	536	1/1	-0.43	1.09	29,29,29,29	1
3	UNX	C	541	1/1	-0.30	2.05	29,29,29,29	1
3	UNX	D	536	1/1	-0.22	1.23	26,26,26,26	1
3	UNX	D	542	1/1	-0.21	1.34	28,28,28,28	1
3	UNX	C	539	1/1	-0.19	1.65	27,27,27,27	1
3	UNX	B	536	1/1	-0.14	1.09	22,22,22,22	1
3	UNX	A	537	1/1	-0.12	1.40	38,38,38,38	1
3	UNX	D	538	1/1	-0.10	1.34	25,25,25,25	1
3	UNX	B	538	1/1	-0.08	1.05	32,32,32,32	1
3	UNX	D	543	1/1	-0.07	1.57	33,33,33,33	1
3	UNX	B	544	1/1	-0.02	1.98	29,29,29,29	1
3	UNX	B	545	1/1	-0.02	1.63	25,25,25,25	1
3	UNX	C	537	1/1	0.00	1.50	28,28,28,28	1
3	UNX	A	535	1/1	-0.00	1.35	28,28,28,28	1
3	UNX	B	535	1/1	0.01	1.37	21,21,21,21	1
3	UNX	D	540	1/1	0.02	1.48	29,29,29,29	1
3	UNX	B	546	1/1	0.06	1.53	22,22,22,22	1
3	UNX	B	543	1/1	0.09	1.85	19,19,19,19	1
3	UNX	D	541	1/1	0.10	1.51	25,25,25,25	1
3	UNX	B	541	1/1	0.18	1.70	21,21,21,21	1
3	UNX	B	540	1/1	0.19	1.78	22,22,22,22	1
3	UNX	C	540	1/1	0.21	1.53	24,24,24,24	1
3	UNX	D	539	1/1	0.34	1.17	36,36,36,36	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UNX	C	538	1/1	0.50	1.65	25,25,25,25	1
3	UNX	A	536	1/1	0.51	1.71	20,20,20,20	1
3	UNX	B	542	1/1	0.51	1.88	23,23,23,23	1
3	UNX	C	542	1/1	0.52	1.75	21,21,21,21	1
3	UNX	B	539	1/1	0.55	1.27	19,19,19,19	1
2	SO4	D	534	5/5	0.79	0.10	52,60,64,72	0
2	SO4	A	533	5/5	0.84	0.18	49,50,60,62	0
2	SO4	D	533	5/5	0.88	0.14	46,48,56,61	0
2	SO4	C	535	5/5	0.90	0.17	38,43,50,58	0
2	SO4	B	533	5/5	0.91	0.10	49,50,59,60	0
2	SO4	C	534	5/5	0.91	0.13	49,50,56,59	0
2	SO4	D	535	5/5	0.92	0.10	45,45,48,49	0
2	SO4	C	533	5/5	0.95	0.09	46,50,51,57	0
2	SO4	C	532	5/5	0.96	0.07	24,27,31,34	0
2	SO4	A	532	5/5	0.97	0.08	29,30,34,34	0
2	SO4	B	534	5/5	0.97	0.06	27,28,32,32	0
2	SO4	B	532	5/5	0.98	0.05	29,29,32,32	0
2	SO4	D	532	5/5	0.98	0.05	33,33,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.