



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:42 am BST

PDB ID : 3GG8
Title : Crystal structure of the Toxoplasma gondii Pyruvate Kinase N terminal truncated
Authors : Wernimont, A.K.; Lew, J.; Allali-Hassani, A.; Vedadi, M.; Bochkarev, A.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Hills, T.; Schapira, M.; Hui, R.; Pizarro, J.C.; Structural Genomics Consortium (SGC)
Deposited on : 2009-02-27
Resolution : 2.21 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

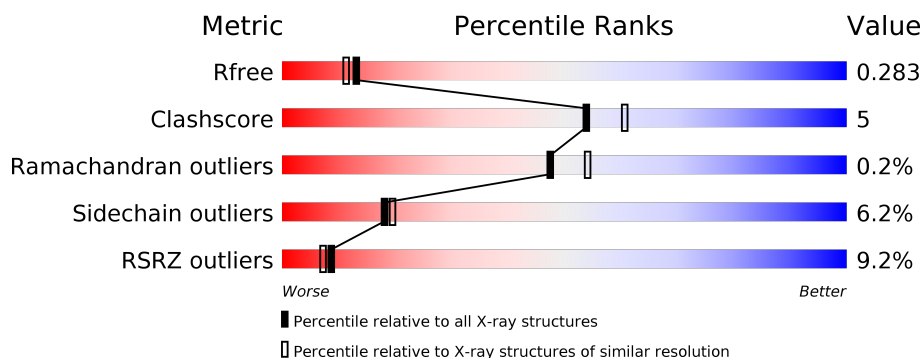
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 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	511	<div> <div>7%</div> <div>80% 13% • 6%</div> </div>
1	B	511	<div> <div>16%</div> <div>75% 14% • 9%</div> </div>
1	C	511	<div> <div>7%</div> <div>81% 13% • •</div> </div>
1	D	511	<div> <div>5%</div> <div>81% 11% • 5%</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	GOL	A	532	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14796 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	4	0
			3575	2240	627	678	30			
1	B	463	Total	C	N	O	S	0	2	0
			3409	2134	592	655	28			
1	C	491	Total	C	N	O	S	0	4	0
			3730	2339	652	709	30			
1	D	483	Total	C	N	O	S	0	0	0
			3582	2245	625	683	29			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	EXPRESSION TAG	UNP Q969A2
A	22	HIS	-	EXPRESSION TAG	UNP Q969A2
A	23	HIS	-	EXPRESSION TAG	UNP Q969A2
A	24	HIS	-	EXPRESSION TAG	UNP Q969A2
A	25	HIS	-	EXPRESSION TAG	UNP Q969A2
A	26	HIS	-	EXPRESSION TAG	UNP Q969A2
A	27	HIS	-	EXPRESSION TAG	UNP Q969A2
A	28	SER	-	EXPRESSION TAG	UNP Q969A2
A	29	SER	-	EXPRESSION TAG	UNP Q969A2
A	30	GLY	-	EXPRESSION TAG	UNP Q969A2
A	31	ARG	-	EXPRESSION TAG	UNP Q969A2
A	32	GLU	-	EXPRESSION TAG	UNP Q969A2
A	33	ASN	-	EXPRESSION TAG	UNP Q969A2
A	34	LEU	-	EXPRESSION TAG	UNP Q969A2
A	35	TYR	-	EXPRESSION TAG	UNP Q969A2
A	36	PHE	-	EXPRESSION TAG	UNP Q969A2
A	37	GLN	-	EXPRESSION TAG	UNP Q969A2
A	38	GLY	-	EXPRESSION TAG	UNP Q969A2
B	21	MET	-	EXPRESSION TAG	UNP Q969A2
B	22	HIS	-	EXPRESSION TAG	UNP Q969A2
B	23	HIS	-	EXPRESSION TAG	UNP Q969A2

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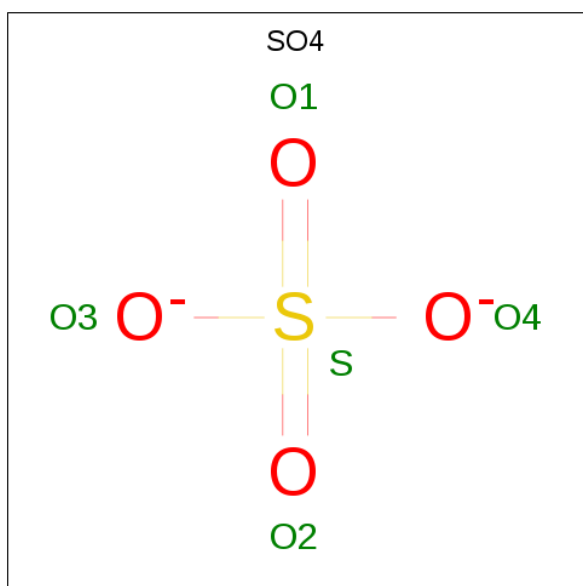
Chain	Residue	Modelled	Actual	Comment	Reference
B	24	HIS	-	EXPRESSION TAG	UNP Q969A2
B	25	HIS	-	EXPRESSION TAG	UNP Q969A2
B	26	HIS	-	EXPRESSION TAG	UNP Q969A2
B	27	HIS	-	EXPRESSION TAG	UNP Q969A2
B	28	SER	-	EXPRESSION TAG	UNP Q969A2
B	29	SER	-	EXPRESSION TAG	UNP Q969A2
B	30	GLY	-	EXPRESSION TAG	UNP Q969A2
B	31	ARG	-	EXPRESSION TAG	UNP Q969A2
B	32	GLU	-	EXPRESSION TAG	UNP Q969A2
B	33	ASN	-	EXPRESSION TAG	UNP Q969A2
B	34	LEU	-	EXPRESSION TAG	UNP Q969A2
B	35	TYR	-	EXPRESSION TAG	UNP Q969A2
B	36	PHE	-	EXPRESSION TAG	UNP Q969A2
B	37	GLN	-	EXPRESSION TAG	UNP Q969A2
B	38	GLY	-	EXPRESSION TAG	UNP Q969A2
C	21	MET	-	EXPRESSION TAG	UNP Q969A2
C	22	HIS	-	EXPRESSION TAG	UNP Q969A2
C	23	HIS	-	EXPRESSION TAG	UNP Q969A2
C	24	HIS	-	EXPRESSION TAG	UNP Q969A2
C	25	HIS	-	EXPRESSION TAG	UNP Q969A2
C	26	HIS	-	EXPRESSION TAG	UNP Q969A2
C	27	HIS	-	EXPRESSION TAG	UNP Q969A2
C	28	SER	-	EXPRESSION TAG	UNP Q969A2
C	29	SER	-	EXPRESSION TAG	UNP Q969A2
C	30	GLY	-	EXPRESSION TAG	UNP Q969A2
C	31	ARG	-	EXPRESSION TAG	UNP Q969A2
C	32	GLU	-	EXPRESSION TAG	UNP Q969A2
C	33	ASN	-	EXPRESSION TAG	UNP Q969A2
C	34	LEU	-	EXPRESSION TAG	UNP Q969A2
C	35	TYR	-	EXPRESSION TAG	UNP Q969A2
C	36	PHE	-	EXPRESSION TAG	UNP Q969A2
C	37	GLN	-	EXPRESSION TAG	UNP Q969A2
C	38	GLY	-	EXPRESSION TAG	UNP Q969A2
D	21	MET	-	EXPRESSION TAG	UNP Q969A2
D	22	HIS	-	EXPRESSION TAG	UNP Q969A2
D	23	HIS	-	EXPRESSION TAG	UNP Q969A2
D	24	HIS	-	EXPRESSION TAG	UNP Q969A2
D	25	HIS	-	EXPRESSION TAG	UNP Q969A2
D	26	HIS	-	EXPRESSION TAG	UNP Q969A2
D	27	HIS	-	EXPRESSION TAG	UNP Q969A2
D	28	SER	-	EXPRESSION TAG	UNP Q969A2
D	29	SER	-	EXPRESSION TAG	UNP Q969A2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	30	GLY	-	EXPRESSION TAG	UNP Q969A2
D	31	ARG	-	EXPRESSION TAG	UNP Q969A2
D	32	GLU	-	EXPRESSION TAG	UNP Q969A2
D	33	ASN	-	EXPRESSION TAG	UNP Q969A2
D	34	LEU	-	EXPRESSION TAG	UNP Q969A2
D	35	TYR	-	EXPRESSION TAG	UNP Q969A2
D	36	PHE	-	EXPRESSION TAG	UNP Q969A2
D	37	GLN	-	EXPRESSION TAG	UNP Q969A2
D	38	GLY	-	EXPRESSION TAG	UNP Q969A2

- 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	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

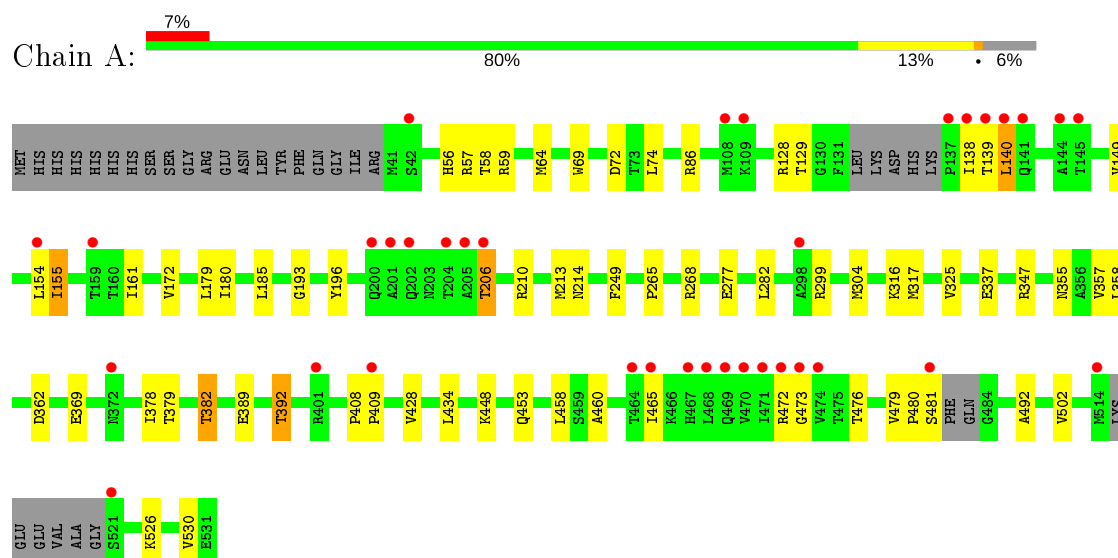
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total	O	0	0
			124	124		
4	B	73	Total	O	0	0
			73	73		
4	C	147	Total	O	0	0
			147	147		
4	D	140	Total	O	0	0
			140	140		

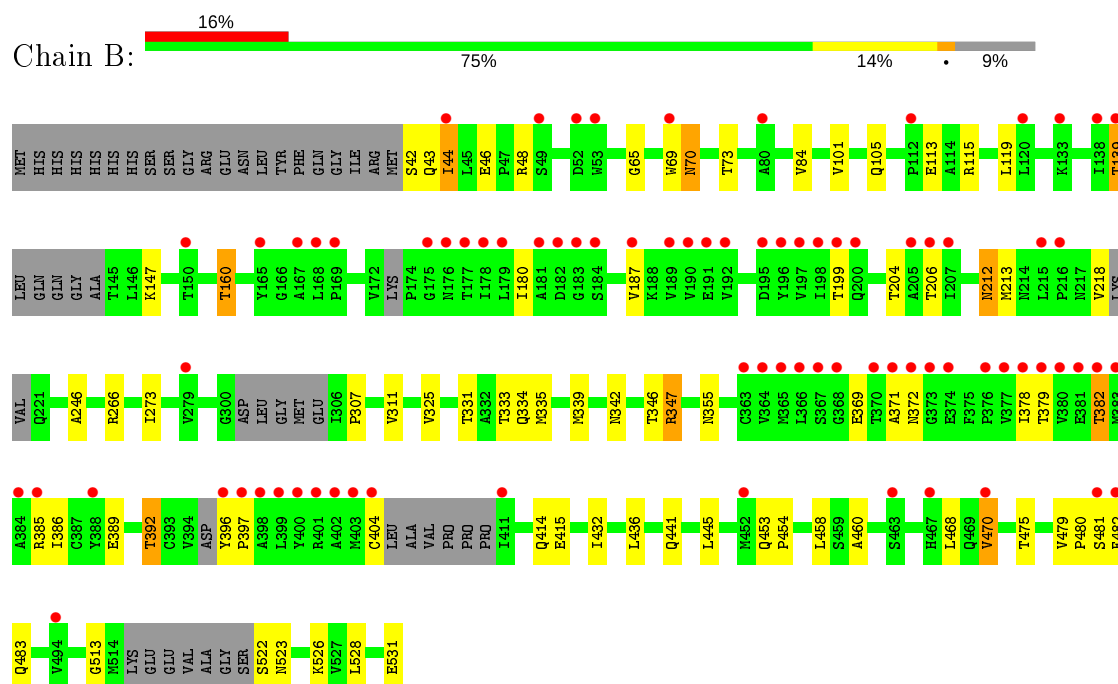
3 Residue-property plots [i](#)

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.

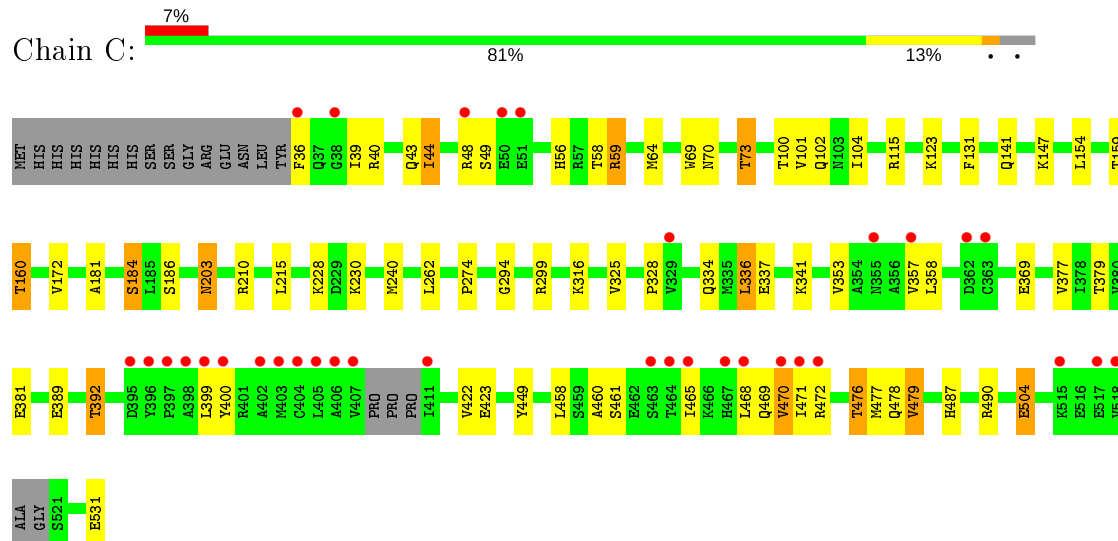
• Molecule 1: Pyruvate kinase



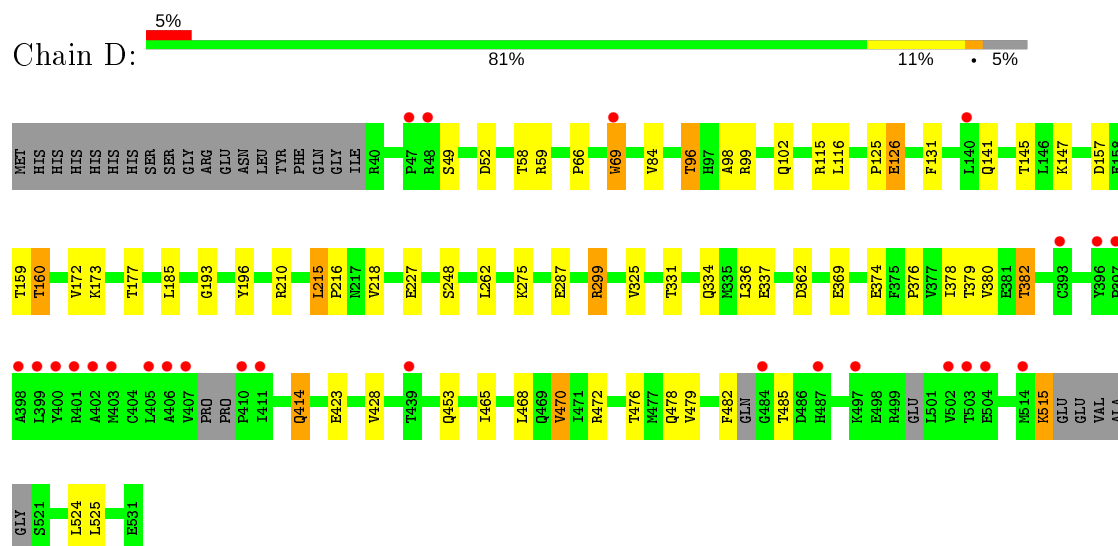
• Molecule 1: Pyruvate kinase



- Molecule 1: Pyruvate kinase



- Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.02Å 92.31Å 112.44Å 90.00° 105.57° 90.00°	Depositor
Resolution (Å)	42.45 – 2.21 42.46 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.6 (42.45-2.21) 97.6 (42.46-2.21)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.206 , 0.265 0.233 , 0.283	Depositor DCC
R_{free} test set	5263 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14796	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: GOL, 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	0.48	0/3635	0.63	0/4937
1	B	0.72	6/3458 (0.2%)	0.63	1/4697 (0.0%)
1	C	0.51	0/3794	0.63	1/5146 (0.0%)
1	D	0.49	0/3630	0.64	1/4929 (0.0%)
All	All	0.55	6/14517 (0.0%)	0.63	3/19709 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	VAL	C-O	18.25	1.58	1.23
1	B	531	GLU	CD-OE1	17.11	1.44	1.25
1	B	139	THR	C-O	9.86	1.42	1.23
1	B	531	GLU	CB-CG	8.01	1.67	1.52
1	B	404	CYS	C-O	7.07	1.36	1.23
1	B	531	GLU	CG-CD	6.82	1.62	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	525	LEU	CA-CB-CG	5.65	128.29	115.30
1	B	119	LEU	CA-CB-CG	5.61	128.20	115.30
1	C	154	LEU	CA-CB-CG	5.04	126.89	115.30

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	3575	0	3605	38	0
1	B	3409	0	3347	38	0
1	C	3730	0	3785	48	0
1	D	3582	0	3584	34	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	6	0	8	4	0
4	A	124	0	0	1	0
4	B	73	0	0	2	0
4	C	147	0	0	6	0
4	D	140	0	0	5	0
All	All	14796	0	14329	151	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 (151) 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:A:86:ARG:HH12	3:A:532:GOL:H11	1.24	1.00
1:B:415:GLU:HG3	1:B:445:LEU:HD12	1.46	0.98
1:D:378:ILE:O	1:D:382:THR:HG23	1.70	0.91
1:A:378:ILE:O	1:A:382:THR:HG23	1.82	0.80
1:B:378:ILE:O	1:B:382:THR:HG23	1.82	0.79
1:D:515:LYS:H	1:D:515:LYS:HD3	1.49	0.77
1:D:414:GLN:HE21	1:D:414:GLN:H	1.31	0.77
1:C:465:ILE:HG23	1:C:476:THR:HG21	1.71	0.73
1:D:126:GLU:OE1	4:D:816:HOH:O	2.08	0.71
1:A:86:ARG:HH22	3:A:532:GOL:H31	1.55	0.71
1:D:96:THR:CG2	4:D:623:HOH:O	2.40	0.70
1:A:502:VAL:HG21	1:A:530:VAL:HG21	1.73	0.69
1:A:155:ILE:HD13	1:A:155:ILE:H	1.58	0.69
1:C:389:GLU:O	1:C:392:THR:HB	1.94	0.68
1:A:458:LEU:HD21	1:A:492:ALA:HB2	1.75	0.67
1:B:212[A]:ASN:HD22	1:B:212[A]:ASN:H	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLU:HG3	1:B:445:LEU:CD1	2.25	0.66
1:D:96:THR:HG23	4:D:623:HOH:O	1.96	0.65
1:A:502:VAL:CG2	1:A:530:VAL:HG21	2.28	0.63
1:A:86:ARG:HH12	3:A:532:GOL:C1	2.06	0.62
1:C:240:MET:HE1	4:C:614:HOH:O	2.01	0.61
1:C:465:ILE:HG23	1:C:476:THR:CG2	2.30	0.60
1:C:69:TRP:CE3	1:C:70:ASN:HB3	2.35	0.60
1:A:149:VAL:HG21	1:A:154:LEU:HD12	1.84	0.60
1:A:265:PRO:HA	1:A:268:ARG:HG3	1.84	0.59
1:D:369:GLU:HB3	1:D:379:THR:HG21	1.84	0.59
1:C:186:SER:H	1:C:203:ASN:HD21	1.49	0.59
1:D:59:ARG:NH2	4:D:663:HOH:O	2.35	0.59
1:B:187:VAL:HB	1:B:199:THR:HB	1.84	0.58
1:A:480:PRO:O	1:A:481:SER:CB	2.52	0.57
1:D:465:ILE:HD13	1:D:478:GLN:HB2	1.86	0.57
1:B:389:GLU:O	1:B:392:THR:HB	2.04	0.57
1:B:347:ARG:HD2	1:D:299:ARG:HB3	1.86	0.57
1:D:248:SER:HA	1:D:275:LYS:HD3	1.86	0.57
1:C:131:PHE:CE1	1:C:210:ARG:HD2	2.40	0.57
1:C:70:ASN:OD1	1:C:73:THR:HG23	2.05	0.56
1:A:56:HIS:NE2	4:A:783:HOH:O	2.33	0.56
1:B:180:ILE:HG12	1:B:213:MET:HG2	1.87	0.55
1:A:193:GLY:HA3	1:A:196:TYR:CE2	2.40	0.55
1:D:157:ASP:HB3	1:D:159:THR:H	1.71	0.55
1:B:346:THR:HB	4:B:604:HOH:O	2.05	0.55
1:C:59:ARG:HG3	1:C:469:GLN:O	2.07	0.55
1:D:414:GLN:NE2	1:D:414:GLN:H	2.03	0.54
1:C:101:VAL:HG11	1:C:240:MET:HE3	1.88	0.54
1:A:369:GLU:HB3	1:A:379:THR:HG21	1.89	0.53
1:C:115:ARG:NH1	1:C:478:GLN:OE1	2.36	0.52
1:B:396:TYR:N	1:B:397:PRO:CD	2.72	0.52
1:B:436:LEU:HD12	1:B:458:LEU:HD12	1.90	0.52
1:C:43:GLN:NE2	4:C:714:HOH:O	2.43	0.52
1:B:355:ASN:ND2	4:B:649:HOH:O	2.43	0.52
1:A:316:LYS:HE2	1:C:358:LEU:HD13	1.91	0.52
1:A:362:ASP:HA	1:A:472:ARG:HB2	1.91	0.51
1:B:432:ILE:HG22	1:B:454:PRO:HB2	1.93	0.51
1:A:140:LEU:HD11	1:A:185:LEU:HD21	1.91	0.51
1:C:461:SER:O	1:C:465:ILE:HD12	2.11	0.51
1:B:382:THR:O	1:B:386:ILE:HG13	2.11	0.51
1:C:336:LEU:HD13	1:C:353:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:THR:HA	1:D:472:ARG:HG3	1.93	0.51
1:D:193:GLY:HA3	1:D:196:TYR:CE1	2.45	0.50
1:A:180:ILE:HG12	1:A:213:MET:HG2	1.94	0.50
1:C:181:ALA:HB3	1:C:184:SER:HB2	1.93	0.50
1:C:36:PHE:N	4:C:637:HOH:O	2.44	0.50
1:C:377:VAL:O	1:C:381:GLU:HG3	2.12	0.49
1:A:460:ALA:HA	1:A:479:VAL:O	2.12	0.49
1:C:369:GLU:HB3	1:C:379:THR:HG21	1.94	0.49
1:A:465:ILE:HD12	1:A:476:THR:HB	1.94	0.49
1:C:58:THR:HA	1:C:472:ARG:HG3	1.94	0.49
1:A:317:MET:SD	1:C:44:ILE:HG21	2.53	0.49
1:B:526:LYS:HE2	1:B:528:LEU:HD23	1.95	0.48
1:C:100:THR:O	1:C:104:ILE:HG12	2.13	0.48
1:C:69:TRP:CZ3	1:C:70:ASN:HB3	2.48	0.48
1:A:179:LEU:HB2	1:A:214:ASN:HB2	1.95	0.48
1:C:422:VAL:HG21	1:C:449:TYR:HB2	1.96	0.47
1:C:147:LYS:HB3	1:C:160:THR:HB	1.95	0.47
1:B:46:GLU:HB2	1:B:48:ARG:HH12	1.78	0.47
1:A:347:ARG:HH21	1:C:334:GLN:HB2	1.79	0.47
1:B:42:SER:C	1:B:44:ILE:H	2.17	0.47
1:B:480:PRO:O	1:B:482:PHE:N	2.43	0.47
1:C:230:LYS:HD2	1:C:262:LEU:HD11	1.96	0.47
1:D:334:GLN:HA	1:D:337:GLU:HG3	1.96	0.47
1:A:57:ARG:HE	1:A:473:GLY:HA2	1.80	0.47
1:A:129:THR:O	1:A:210:ARG:HA	2.15	0.46
1:C:504:GLU:HG2	1:C:531:GLU:O	2.16	0.46
1:C:48:ARG:HD2	1:C:389:GLU:OE2	2.16	0.46
1:D:362:ASP:HA	1:D:472:ARG:HB2	1.98	0.46
1:B:441:GLN:HG3	1:B:445:LEU:HD23	1.97	0.45
1:C:400:TYR:OH	1:C:423:GLU:HG3	2.16	0.45
1:B:460:ALA:HA	1:B:479:VAL:O	2.15	0.45
1:D:125:PRO:C	1:D:126:GLU:HG2	2.35	0.45
1:D:299:ARG:HD2	1:D:331:THR:HG23	1.97	0.45
1:C:101:VAL:HG11	1:C:240:MET:CE	2.46	0.45
1:C:334:GLN:HA	1:C:337:GLU:HG3	1.98	0.45
1:A:139:THR:HG23	1:A:206:THR:HG22	1.98	0.45
1:B:307:PRO:O	1:B:311:VAL:HG23	2.17	0.45
1:C:274:PRO:HD2	1:C:294:GLY:O	2.17	0.45
1:D:147:LYS:HB3	1:D:160:THR:HB	1.99	0.45
1:C:159:THR:OG1	1:C:160:THR:HG22	2.17	0.45
1:C:64:MET:SD	1:C:104:ILE:HD11	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:GLU:HB3	1:B:379:THR:HG21	1.99	0.44
1:C:59:ARG:CG	1:C:469:GLN:O	2.64	0.44
1:D:159:THR:OG1	1:D:160:THR:HG22	2.17	0.44
1:D:66:PRO:O	1:D:69:TRP:HB3	2.17	0.44
1:A:358:LEU:HD13	1:C:316:LYS:HE2	1.98	0.44
1:D:177:THR:O	1:D:216:PRO:HD2	2.16	0.44
1:C:357:VAL:O	1:C:472:ARG:NH2	2.40	0.44
1:B:414:GLN:HG2	1:B:523:ASN:HD21	1.83	0.44
1:C:460:ALA:HA	1:C:479:VAL:O	2.18	0.43
1:A:282:LEU:HA	1:A:282:LEU:HD23	1.82	0.43
1:C:102[A]:GLN:HG3	4:C:614:HOH:O	2.19	0.43
1:D:131:PHE:CZ	1:D:210:ARG:HD2	2.53	0.43
1:B:84:VAL:HG21	1:B:470:VAL:HG23	1.99	0.43
1:D:84:VAL:HG21	1:D:470:VAL:HG23	2.01	0.43
1:A:64:MET:SD	1:A:74:LEU:HD21	2.58	0.43
1:C:203:ASN:HD22	1:C:203:ASN:N	2.16	0.43
1:D:49:SER:O	1:D:52:ASP:HB2	2.19	0.43
1:A:249:PHE:N	1:A:277:GLU:OE1	2.50	0.42
1:B:522:SER:CB	4:C:721:HOH:O	2.68	0.42
1:C:123:LYS:HD2	1:C:228:LYS:HE2	2.01	0.42
1:B:115:ARG:HD3	1:B:115:ARG:HA	1.81	0.42
1:B:333:THR:C	1:B:334:GLN:HG2	2.40	0.42
1:D:215:LEU:HB3	1:D:218:VAL:HB	2.02	0.42
1:A:357:VAL:O	1:A:472:ARG:NH2	2.41	0.42
1:B:101:VAL:HG12	1:B:105:GLN:HE21	1.84	0.42
1:D:465:ILE:HD11	1:D:478:GLN:HA	2.01	0.42
1:B:246:ALA:HA	1:B:273:ILE:O	2.20	0.41
1:D:376:PRO:O	1:D:380:VAL:HG23	2.20	0.41
1:A:408:PRO:HA	1:A:409:PRO:HD3	1.97	0.41
1:B:513:GLY:HA2	1:B:523:ASN:ND2	2.35	0.41
1:C:336:LEU:O	1:C:369:GLU:HG2	2.20	0.41
1:C:328:PRO:CB	1:C:470:VAL:HG13	2.51	0.41
1:B:331:THR:O	1:B:335:MET:HE2	2.21	0.41
1:B:65:GLY:HA3	1:B:371:ALA:HA	2.02	0.41
1:A:317:MET:SD	1:C:44:ILE:CG2	3.09	0.41
1:B:333:THR:O	1:B:334:GLN:HG2	2.20	0.41
1:D:472:ARG:HD3	4:D:533:HOH:O	2.19	0.41
1:A:526:LYS:HG3	1:D:524:LEU:HG	2.01	0.41
1:C:458:LEU:HD23	1:C:477:MET:HB3	2.02	0.41
1:D:115:ARG:NH1	1:D:478:GLN:OE1	2.53	0.41
1:A:389:GLU:O	1:A:392:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HA	1:A:472:ARG:HG3	2.02	0.41
1:B:101:VAL:HG12	1:B:105:GLN:NE2	2.36	0.41
1:B:139:THR:HG22	1:B:206:THR:HB	2.02	0.41
1:B:70:ASN:ND2	1:B:73:THR:OG1	2.53	0.41
1:A:86:ARG:NH1	3:A:532:GOL:H11	2.09	0.40
1:D:98:ALA:O	1:D:102:GLN:HG3	2.21	0.40
1:C:56:HIS:HE1	4:C:586:HOH:O	2.05	0.40
1:B:339:MET:HA	1:B:342:ASN:O	2.21	0.40
1:D:227:GLU:HA	1:D:227:GLU:OE1	2.21	0.40
1:B:147:LYS:HB3	1:B:160:THR:HB	2.03	0.40
1:C:59:ARG:HD3	1:C:471:ILE:O	2.21	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	474/511 (93%)	459 (97%)	15 (3%)	0	100	100
1	B	449/511 (88%)	423 (94%)	23 (5%)	3 (1%)	22	21
1	C	489/511 (96%)	476 (97%)	13 (3%)	0	100	100
1	D	473/511 (93%)	456 (96%)	17 (4%)	0	100	100
All	All	1885/2044 (92%)	1814 (96%)	68 (4%)	3 (0%)	47	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	43	GLN
1	B	481	SER
1	B	483	GLN

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	382/428 (89%)	362 (95%)	20 (5%)	23	27
1	B	352/428 (82%)	333 (95%)	19 (5%)	22	25
1	C	404/428 (94%)	379 (94%)	25 (6%)	18	19
1	D	379/428 (89%)	349 (92%)	30 (8%)	12	11
All	All	1517/1712 (89%)	1423 (94%)	94 (6%)	18	19

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	69	TRP
1	A	72	ASP
1	A	128	ARG
1	A	138	ILE
1	A	140	LEU
1	A	155	ILE
1	A	161	ILE
1	A	172	VAL
1	A	206	THR
1	A	299	ARG
1	A	304	MET
1	A	325	VAL
1	A	337	GLU
1	A	382	THR
1	A	392	THR
1	A	428	VAL
1	A	434	LEU
1	A	448	LYS
1	A	453	GLN
1	B	44	ILE
1	B	69	TRP
1	B	70	ASN
1	B	113	GLU

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Mol	Chain	Res	Type
1	B	160	THR
1	B	204	THR
1	B	212[A]	ASN
1	B	212[B]	ASN
1	B	266	ARG
1	B	325	VAL
1	B	347	ARG
1	B	372	ASN
1	B	382	THR
1	B	385	ARG
1	B	392	THR
1	B	453	GLN
1	B	468	LEU
1	B	470	VAL
1	B	475	THR
1	C	39	ILE
1	C	40	ARG
1	C	44	ILE
1	C	49	SER
1	C	59	ARG
1	C	73	THR
1	C	141	GLN
1	C	160	THR
1	C	172	VAL
1	C	184	SER
1	C	203	ASN
1	C	215	LEU
1	C	299	ARG
1	C	325	VAL
1	C	336	LEU
1	C	341	LYS
1	C	392	THR
1	C	399	LEU
1	C	468	LEU
1	C	470	VAL
1	C	476	THR
1	C	479	VAL
1	C	487	HIS
1	C	490	ARG
1	C	504	GLU
1	D	69	TRP
1	D	96	THR

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Mol	Chain	Res	Type
1	D	99	ARG
1	D	116	LEU
1	D	126	GLU
1	D	141	GLN
1	D	145	THR
1	D	160	THR
1	D	172	VAL
1	D	173	LYS
1	D	185	LEU
1	D	215	LEU
1	D	262	LEU
1	D	287	GLU
1	D	299	ARG
1	D	325	VAL
1	D	336	LEU
1	D	374	GLU
1	D	382	THR
1	D	414	GLN
1	D	423	GLU
1	D	428	VAL
1	D	453	GLN
1	D	468	LEU
1	D	470	VAL
1	D	476	THR
1	D	479	VAL
1	D	482	PHE
1	D	485	THR
1	D	515	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	235	ASN
1	B	70	ASN
1	B	105	GLN
1	B	176	ASN
1	B	323	ASN
1	B	355	ASN
1	B	414	GLN
1	B	429	ASN
1	B	523	ASN

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Mol	Chain	Res	Type
1	C	43	GLN
1	C	203	ASN
1	C	235	ASN
1	C	523	ASN
1	D	200	GLN
1	D	235	ASN
1	D	414	GLN
1	D	453	GLN
1	D	491	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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1	-	4,4,4	0.15	0	6,6,6	0.31	0
2	SO4	B	532	-	4,4,4	0.19	0	6,6,6	0.22	0
3	GOL	A	532	-	5,5,5	0.38	0	5,5,5	0.42	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	GOL	A	532	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	532	GOL	O2-C2-C3-O3
3	A	532	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	532	GOL	4	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	478/511 (93%)	0.46	35 (7%) 15 13	29, 35, 41, 44	6 (1%)
1	B	463/511 (90%)	1.09	81 (17%) 1 1	29, 35, 42, 47	9 (1%)
1	C	491/511 (96%)	0.25	34 (6%) 16 15	26, 35, 40, 45	7 (1%)
1	D	483/511 (94%)	0.10	26 (5%) 25 24	30, 35, 41, 46	7 (1%)
All	All	1915/2044 (93%)	0.47	176 (9%) 9 7	26, 35, 41, 47	29 (1%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	378	ILE	19.3
1	B	379	THR	18.7
1	B	383	MET	17.3
1	B	376	PRO	16.5
1	B	380	VAL	16.2
1	B	377	VAL	15.8
1	B	384	ALA	15.3
1	B	382	THR	14.9
1	B	385	ARG	11.1
1	B	381	GLU	9.1
1	B	399	LEU	9.0
1	B	404	CYS	8.6
1	A	470	VAL	8.5
1	B	397	PRO	7.5
1	C	470	VAL	6.9
1	B	138	ILE	6.8
1	B	403	MET	6.6
1	B	400	TYR	6.0
1	B	365	MET	6.0
1	B	402	ALA	5.8
1	B	396	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	405	LEU	5.7
1	B	199	THR	5.5
1	B	192	VAL	5.5
1	B	363	CYS	5.4
1	B	216	PRO	5.4
1	B	53	TRP	5.2
1	D	410	PRO	5.1
1	B	371	ALA	5.1
1	D	484	GLY	5.0
1	B	167	ALA	5.0
1	A	140	LEU	5.0
1	A	471	ILE	4.9
1	D	399	LEU	4.9
1	C	397	PRO	4.8
1	B	398	ALA	4.7
1	B	401	ARG	4.6
1	C	399	LEU	4.6
1	B	215	LEU	4.3
1	D	47	PRO	4.3
1	B	178	ILE	4.2
1	B	177	THR	4.1
1	A	468	LEU	3.9
1	D	398	ALA	3.9
1	A	141	GLN	3.9
1	A	205	ALA	3.9
1	C	395	ASP	3.8
1	D	411	ILE	3.7
1	C	396	TYR	3.7
1	A	144	ALA	3.7
1	D	497	LYS	3.7
1	C	400	TYR	3.7
1	C	464	THR	3.6
1	B	367	SER	3.6
1	B	150	THR	3.6
1	B	187	VAL	3.5
1	B	191	GLU	3.5
1	A	139	THR	3.4
1	C	467	HIS	3.4
1	B	197	VAL	3.4
1	B	370	THR	3.4
1	C	403	MET	3.4
1	C	471	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	402	ALA	3.3
1	B	189	VAL	3.3
1	B	200	GLN	3.3
1	B	207	ILE	3.3
1	C	38	GLY	3.3
1	B	494	VAL	3.3
1	A	154	LEU	3.2
1	B	372	ASN	3.2
1	A	467	HIS	3.2
1	B	198	ILE	3.2
1	A	206	THR	3.2
1	B	183	GLY	3.2
1	B	179	LEU	3.1
1	B	190	VAL	3.1
1	C	468	LEU	3.1
1	B	165	TYR	3.1
1	C	406	ALA	3.0
1	C	363	CYS	3.0
1	B	366	LEU	3.0
1	B	373	GLY	3.0
1	C	518	VAL	3.0
1	B	206	THR	3.0
1	B	368	GLY	2.9
1	B	175	GLY	2.9
1	B	182	ASP	2.9
1	A	469	GLN	2.9
1	A	473	GLY	2.9
1	A	145	THR	2.9
1	C	36	PHE	2.9
1	C	398	ALA	2.8
1	B	196	TYR	2.8
1	C	407	VAL	2.8
1	D	400	TYR	2.8
1	D	406	ALA	2.7
1	B	482	PHE	2.7
1	D	439	THR	2.7
1	D	503	THR	2.7
1	A	138	ILE	2.7
1	A	200	GLN	2.7
1	B	139	THR	2.7
1	B	205	ALA	2.7
1	C	48	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	329	VAL	2.7
1	A	204	THR	2.7
1	B	169	PRO	2.7
1	C	515	LYS	2.6
1	D	397	PRO	2.6
1	B	52	ASP	2.6
1	A	474	VAL	2.6
1	A	159	THR	2.6
1	D	48	ARG	2.5
1	D	69	TRP	2.5
1	B	168	LEU	2.5
1	B	467	HIS	2.5
1	A	464	THR	2.5
1	B	112	PRO	2.5
1	A	409	PRO	2.5
1	A	372[A]	ASN	2.5
1	B	176	ASN	2.5
1	C	405	LEU	2.5
1	C	357	VAL	2.5
1	C	517	GLU	2.5
1	D	514	MET	2.5
1	B	481	SER	2.4
1	D	502	VAL	2.4
1	B	452	MET	2.4
1	B	411	ILE	2.4
1	A	521	SER	2.4
1	D	393	CYS	2.4
1	D	407	VAL	2.4
1	C	411	ILE	2.4
1	A	472	ARG	2.4
1	D	140	LEU	2.4
1	C	402	ALA	2.4
1	B	364	VAL	2.4
1	B	195	ASP	2.3
1	C	404	CYS	2.3
1	B	374	GLU	2.3
1	B	181	ALA	2.3
1	B	463	SER	2.3
1	A	42	SER	2.3
1	C	362	ASP	2.3
1	C	355[A]	ASN	2.3
1	C	465	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	133	LYS	2.2
1	B	279	VAL	2.2
1	C	472	ARG	2.2
1	D	401	ARG	2.2
1	A	201	ALA	2.2
1	B	44	ILE	2.2
1	A	465	ILE	2.2
1	B	388	TYR	2.2
1	C	50	GLU	2.2
1	A	108	MET	2.2
1	A	109	LYS	2.1
1	D	504	GLU	2.1
1	A	298	ALA	2.1
1	B	120	LEU	2.1
1	B	69	TRP	2.1
1	A	202	GLN	2.1
1	B	49	SER	2.1
1	D	487	HIS	2.1
1	A	401	ARG	2.1
1	D	396	TYR	2.1
1	A	137	PRO	2.1
1	A	481	SER	2.1
1	C	463	SER	2.1
1	C	51	GLU	2.1
1	B	80	ALA	2.1
1	B	470	VAL	2.1
1	A	514	MET	2.0
1	D	403	MET	2.0
1	B	184	SER	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 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. 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(\AA^2)	Q<0.9
3	GOL	A	532	6/6	0.69	0.30	63,63,63,63	0
2	SO4	B	532	5/5	0.86	0.15	83,83,83,84	0
2	SO4	A	1	5/5	0.91	0.23	57,58,60,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.