



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:19 PM UTC

PDB ID : 3GG8 / pdb_00003gg8
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 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

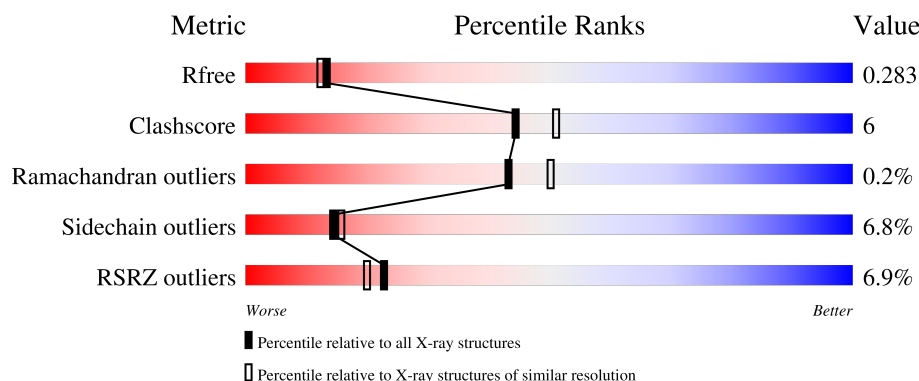
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (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 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	511	4% 78% 14% 6%
1	B	511	11% 73% 15% 9%
1	C	511	4% 80% 14% .
1	D	511	7% 80% 13% 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	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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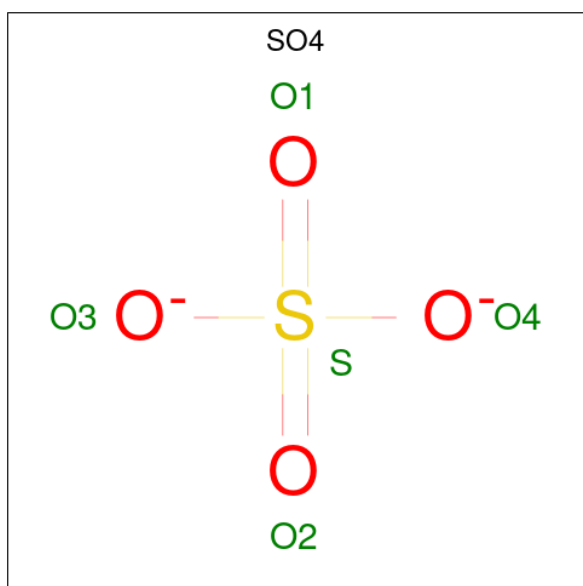
Chain	Residue	Modelled	Actual	Comment	Reference
B	24	HIS	-	expression tag	UNP Q969A2
B	25	HIS	-	expression tag	UNP Q969A2
B	26	HIS	-	expression tag	UNP Q969A2
B	27	HIS	-	expression tag	UNP Q969A2
B	28	SER	-	expression tag	UNP Q969A2
B	29	SER	-	expression tag	UNP Q969A2
B	30	GLY	-	expression tag	UNP Q969A2
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 (CCD ID: 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 (CCD ID: GOL) (formula: C₃H₈O₃).



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

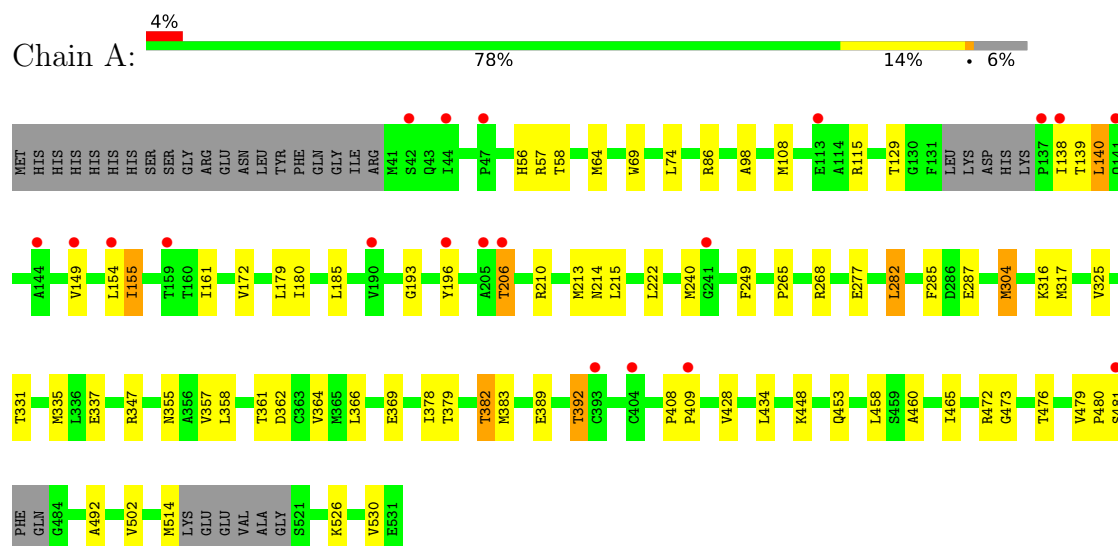
- Molecule 4 is water.

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		

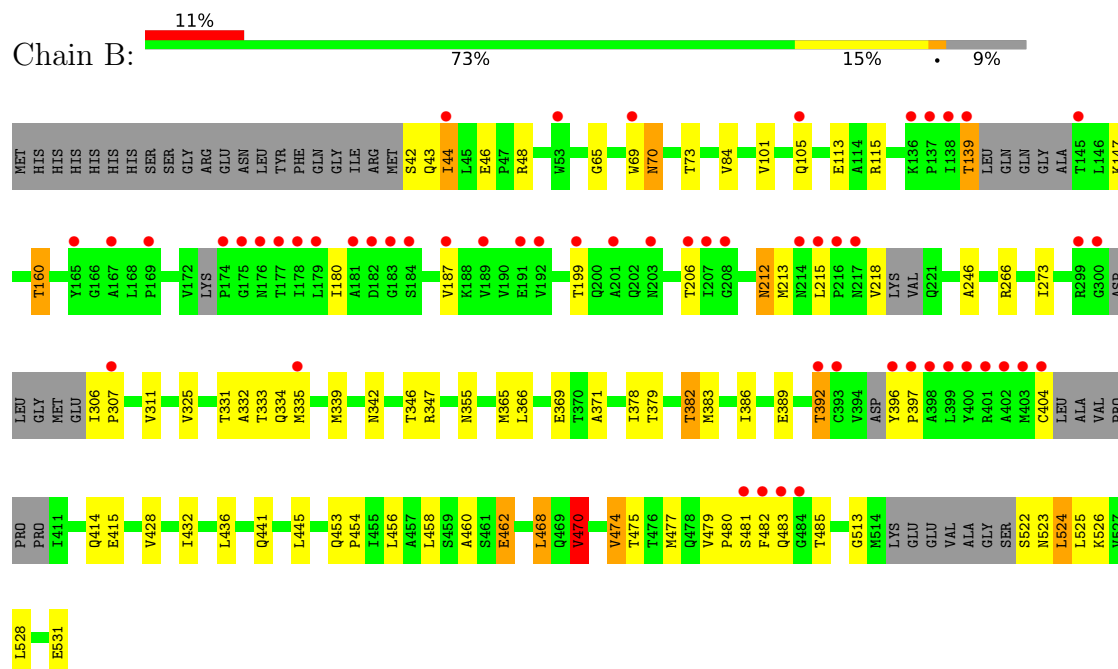
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

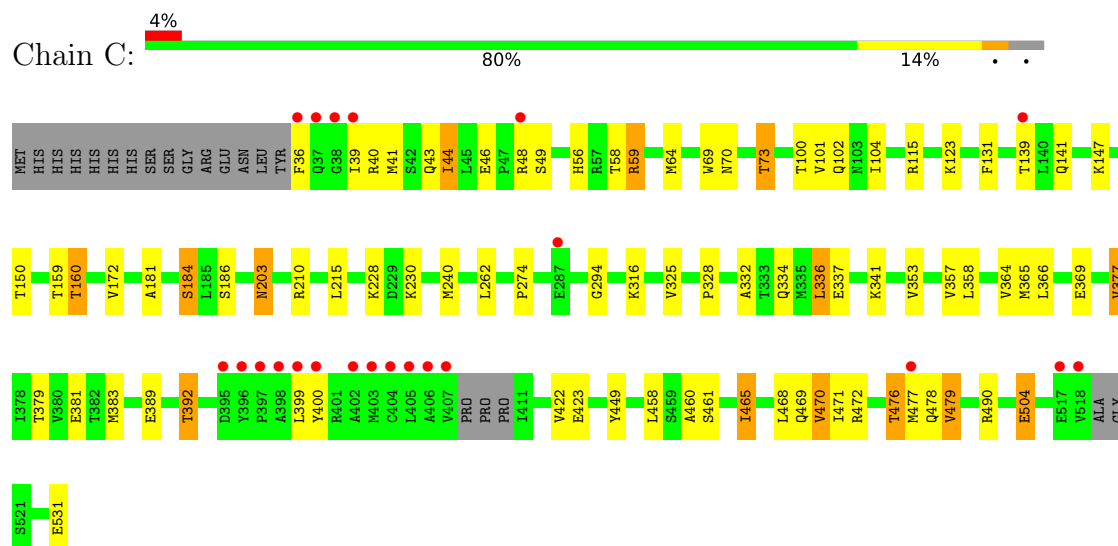
• Molecule 1: Pyruvate kinase



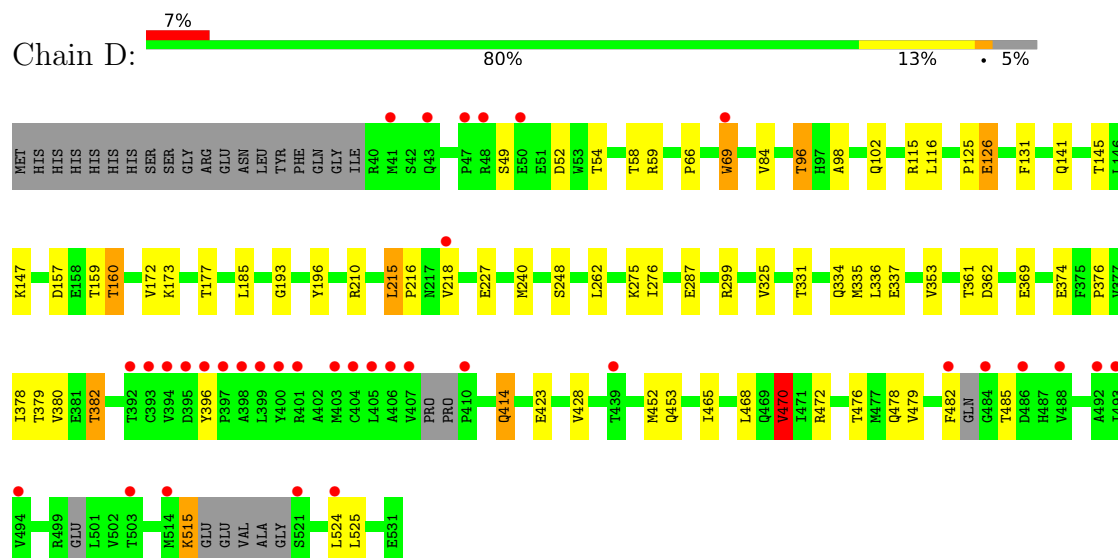
• Molecule 1: Pyruvate kinase



- 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 42.45 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.6 (42.45-2.21) 97.9 (42.45-2.21)	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 (4.86%)	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)	0.31 , 21.7	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	0.93	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: 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	0.66	0/3635	0.93	3/4937 (0.1%)
1	B	0.79	5/3458 (0.1%)	0.93	4/4697 (0.1%)
1	C	0.67	0/3794	0.91	0/5146
1	D	0.67	0/3630	0.92	1/4929 (0.0%)
All	All	0.70	5/14517 (0.0%)	0.92	8/19709 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	VAL	C-O	17.24	1.58	1.23
1	B	531	GLU	CD-OE1	10.06	1.44	1.25
1	B	139	THR	C-O	9.27	1.42	1.23
1	B	404	CYS	C-O	6.61	1.36	1.23
1	B	474	VAL	CA-CB	6.03	1.61	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	VAL	CA-C-O	-6.36	109.99	120.80
1	A	285	PHE	N-CA-C	5.88	118.17	111.11
1	B	470	VAL	CB-CA-C	5.72	118.30	111.20
1	D	470	VAL	CB-CA-C	5.29	117.76	111.20
1	B	306	ILE	CA-C-N	5.20	125.73	120.38
1	B	306	ILE	C-N-CA	5.20	125.73	120.38
1	A	222	LEU	CA-C-N	-5.01	114.59	119.76
1	A	222	LEU	C-N-CA	-5.01	114.59	119.76

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	45	0
1	B	3409	0	3347	45	0
1	C	3730	0	3785	53	0
1	D	3582	0	3584	37	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	6	0
All	All	14796	0	14329	172	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 6.

All (172) 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:HD3	1:D:515:LYS:H	1.49	0.77
1:D:414:GLN:H	1:D:414:GLN:HE21	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:H	1:A:155:ILE:HD13	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:H	1:B:212[A]:ASN:HD22	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:D:240:MET:HE1	4:D:577:HOH:O	1.98	0.62
1:C:101:VAL:HG11	1:C:240:MET:HE3	1.80	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:A:335:MET:HE3	1:A:364:VAL:HB	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:C:240:MET:HE1	4:C:614:HOH:O	2.07	0.55
1:D:414:GLN:H	1:D:414:GLN:NE2	2.03	0.54
1:B:366:LEU:HD21	1:B:383:MET:HE2	1.89	0.54
1:A:331:THR:O	1:A:335:MET:HE2	2.08	0.54
1:C:364:VAL:HG23	1:C:383:MET:HE3	1.89	0.53
1:A:369:GLU:HB3	1:A:379:THR:HG21	1.89	0.53
1:B:366:LEU:CD2	1:B:383:MET:HE2	2.38	0.53
1:A:98:ALA:HA	1:A:240:MET:HE2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LYS:HE2	1:C:358:LEU:HD13	1.91	0.52
1:D:396:TYR:HD2	1:D:452:MET:HE3	1.75	0.52
1:B:42:SER:C	1:B:44:ILE:H	2.17	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:B:332:ALA:HB1	1:B:365:MET:HE2	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
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:D:125:PRO:C	1:D:126:GLU:HG2	2.35	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:A:108:MET:HE3	1:A:115:ARG:HA	1.95	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:D:335:MET:HE3	1:D:353:VAL:HG22	1.95	0.48
1:C:64:MET:HA	1:C:64:MET:HE2	1.96	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: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:B:333:THR:C	1:B:334:GLN:HG2	2.40	0.47
1:A:57:ARG:HE	1:A:473:GLY:HA2	1.80	0.47
1:A:304:MET:HA	1:A:304:MET:HE2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:282:LEU:HD22	1:C:41:MET:HE2	2.00	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:A:366:LEU:HD21	1:A:383:MET:HE2	1.98	0.44
1:B:462:GLU:CD	1:B:462:GLU:H	2.26	0.44
1:C:460:ALA:HA	1:C:479:VAL:O	2.18	0.43
1:A:282:LEU:HD23	1:A:282:LEU:HA	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:B:331:THR:O	1:B:335:MET:HE2	2.18	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:B:524:LEU:C	1:B:524:LEU:HD23	2.44	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:D:215:LEU:HB3	1:D:218:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:LEU:HG	1:C:383:MET:HE1	2.01	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:A:317:MET:SD	1:C:44:ILE:CG2	3.09	0.41
1:B:65:GLY:HA3	1:B:371:ALA:HA	2.02	0.41
1:A:526:LYS:HG3	1:D:524:LEU:HG	2.01	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: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:58:THR:HA	1:A:472:ARG:HG3	2.02	0.41
1:A:389:GLU:O	1:A:392:THR:HB	2.21	0.41
1:B:468:LEU:C	1:B:470:VAL:H	2.29	0.41
1:C:332:ALA:HB1	1:C:365:MET:HE2	2.03	0.41
1:B:70:ASN:ND2	1:B:73:THR:OG1	2.53	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: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:B:456:LEU:HD21	1:B:477:MET:HE2	2.03	0.40
1:D:227:GLU:OE1	1:D:227:GLU:HA	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%)	18	18
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%)	43	50

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%)	361 (94%)	21 (6%)	19	23
1	B	352/428 (82%)	330 (94%)	22 (6%)	16	18
1	C	404/428 (94%)	376 (93%)	28 (7%)	14	15
1	D	379/428 (89%)	347 (92%)	32 (8%)	10	10
All	All	1517/1712 (89%)	1414 (93%)	103 (7%)	14	16

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	TRP
1	A	138	ILE
1	A	140	LEU

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Mol	Chain	Res	Type
1	A	155	ILE
1	A	161	ILE
1	A	172	VAL
1	A	206	THR
1	A	215	LEU
1	A	282	LEU
1	A	287	GLU
1	A	304	MET
1	A	325	VAL
1	A	337	GLU
1	A	361	THR
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	A	514	MET
1	B	44	ILE
1	B	69	TRP
1	B	70	ASN
1	B	113	GLU
1	B	160	THR
1	B	212[A]	ASN
1	B	212[B]	ASN
1	B	215	LEU
1	B	266	ARG
1	B	325	VAL
1	B	382	THR
1	B	392	THR
1	B	428	VAL
1	B	453	GLN
1	B	462	GLU
1	B	468	LEU
1	B	470	VAL
1	B	474	VAL
1	B	475	THR
1	B	485	THR
1	B	524	LEU
1	B	525	LEU
1	C	39	ILE
1	C	40	ARG

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Mol	Chain	Res	Type
1	C	44	ILE
1	C	46	GLU
1	C	49	SER
1	C	59	ARG
1	C	73	THR
1	C	139	THR
1	C	141	GLN
1	C	150	THR
1	C	160	THR
1	C	172	VAL
1	C	184	SER
1	C	203	ASN
1	C	215	LEU
1	C	325	VAL
1	C	336	LEU
1	C	341	LYS
1	C	377	VAL
1	C	392	THR
1	C	399	LEU
1	C	465	ILE
1	C	468	LEU
1	C	470	VAL
1	C	476	THR
1	C	479	VAL
1	C	490	ARG
1	C	504	GLU
1	D	54	THR
1	D	69	TRP
1	D	96	THR
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	276	ILE
1	D	287	GLU
1	D	325	VAL

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Mol	Chain	Res	Type
1	D	336	LEU
1	D	361	THR
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
1	D	525	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	176	ASN
1	A	235	ASN
1	A	512	HIS
1	B	70	ASN
1	B	105	GLN
1	B	176	ASN
1	B	251	GLN
1	B	334	GLN
1	B	342	ASN
1	B	355	ASN
1	B	429	ASN
1	B	469	GLN
1	B	523	ASN
1	C	43	GLN
1	C	91	HIS
1	C	141	GLN
1	C	203	ASN
1	C	441	GLN
1	C	483	GLN
1	D	200	GLN
1	D	235	ASN

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Mol	Chain	Res	Type
1	D	414	GLN
1	D	441	GLN
1	D	453	GLN

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 oligosaccharides 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	B	532	-	4,4,4	0.28	0	6,6,6	0.24	0
2	SO4	A	1	-	4,4,4	0.22	0	6,6,6	0.29	0
3	GOL	A	532	-	5,5,5	0.39	0	5,5,5	0.44	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%)	0.56	20 (4%) 40 37	20, 35, 41, 44	10 (2%)
1	B	463/511 (90%)	0.78	55 (11%) 9 7	20, 35, 42, 47	11 (2%)
1	C	491/511 (96%)	0.46	22 (4%) 38 35	19, 35, 40, 45	11 (2%)
1	D	483/511 (94%)	0.49	35 (7%) 21 19	24, 35, 41, 46	7 (1%)
All	All	1915/2044 (93%)	0.57	132 (6%) 23 20	19, 35, 41, 47	39 (2%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	38	GLY	5.7
1	B	400	TYR	4.7
1	B	397	PRO	4.7
1	B	216	PRO	4.7
1	B	167	ALA	4.6
1	B	396	TYR	4.6
1	B	404	CYS	4.5
1	D	393	CYS	4.4
1	B	399	LEU	4.2
1	D	484	GLY	4.2
1	D	439	THR	4.2
1	C	518	VAL	3.8
1	B	482	PHE	3.8
1	C	400	TYR	3.8
1	C	404	CYS	3.7
1	C	36	PHE	3.7
1	D	395	ASP	3.6
1	C	397	PRO	3.6
1	C	403	MET	3.5
1	A	47	PRO	3.5
1	B	402	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	406	ALA	3.4
1	B	191	GLU	3.4
1	B	165	TYR	3.3
1	D	399	LEU	3.3
1	D	405	LEU	3.3
1	B	136	LYS	3.2
1	B	53	TRP	3.2
1	B	393	CYS	3.2
1	C	396	TYR	3.2
1	D	47	PRO	3.2
1	A	190	VAL	3.1
1	A	154	LEU	3.1
1	C	37	GLN	3.1
1	B	401	ARG	3.1
1	A	42	SER	3.1
1	B	217	ASN	3.1
1	B	398	ALA	3.1
1	D	398	ALA	3.1
1	B	403	MET	3.1
1	D	400	TYR	3.0
1	C	407	VAL	3.0
1	B	182	ASP	3.0
1	B	299	ARG	2.9
1	D	486	ASP	2.9
1	C	405	LEU	2.9
1	D	407	VAL	2.9
1	A	149	VAL	2.9
1	D	394	VAL	2.9
1	B	138	ILE	2.9
1	C	399	LEU	2.8
1	B	208	GLY	2.8
1	B	481	SER	2.8
1	D	48	ARG	2.8
1	C	517	GLU	2.8
1	D	69	TRP	2.8
1	B	175	GLY	2.8
1	B	300	GLY	2.8
1	B	484	GLY	2.7
1	B	137	PRO	2.7
1	A	113	GLU	2.7
1	A	44	ILE	2.7
1	B	44	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	410	PRO	2.7
1	D	397	PRO	2.7
1	D	41	MET	2.7
1	B	183	GLY	2.7
1	A	404	CYS	2.7
1	A	481	SER	2.6
1	D	494	VAL	2.6
1	D	503	THR	2.6
1	C	477	MET	2.6
1	D	43	GLN	2.6
1	B	69	TRP	2.6
1	C	398	ALA	2.6
1	D	392	THR	2.6
1	B	181	ALA	2.5
1	C	395	ASP	2.5
1	A	409	PRO	2.5
1	B	483	GLN	2.5
1	B	189	VAL	2.5
1	D	50	GLU	2.5
1	D	482	PHE	2.5
1	A	393	CYS	2.4
1	B	206	THR	2.4
1	D	403	MET	2.4
1	B	176	ASN	2.4
1	B	203	ASN	2.4
1	B	184	SER	2.4
1	B	192	VAL	2.4
1	C	39	ILE	2.4
1	D	488	VAL	2.4
1	B	215	LEU	2.4
1	C	287	GLU	2.4
1	B	169	PRO	2.4
1	B	174	PRO	2.4
1	C	402	ALA	2.3
1	B	145	THR	2.3
1	D	396	TYR	2.3
1	D	521	SER	2.3
1	B	179	LEU	2.3
1	B	307	PRO	2.3
1	A	141	GLN	2.3
1	B	214	ASN	2.3
1	B	105	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	137	PRO	2.2
1	C	48	ARG	2.2
1	A	144	ALA	2.2
1	D	514	MET	2.2
1	B	177	THR	2.2
1	B	392	THR	2.2
1	A	196	TYR	2.2
1	D	404	CYS	2.2
1	D	406	ALA	2.1
1	D	401	ARG	2.1
1	B	207	ILE	2.1
1	D	524	LEU	2.1
1	B	187	VAL	2.1
1	B	199	THR	2.1
1	D	492	ALA	2.1
1	B	178	ILE	2.1
1	A	241	GLY	2.1
1	A	159	THR	2.1
1	A	205	ALA	2.1
1	A	138	ILE	2.1
1	A	206	THR	2.0
1	B	139	THR	2.0
1	C	139	THR	2.0
1	B	335	MET	2.0
1	D	493	ILE	2.0
1	D	218	VAL	2.0
1	B	201	ALA	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(Å ²)	Q<0.9
2	SO4	B	532	5/5	0.73	0.13	83,83,83,84	0
3	GOL	A	532	6/6	0.75	0.19	63,63,63,63	0
2	SO4	A	1	5/5	0.85	0.19	57,58,60,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.