



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:07 PM UTC

PDB ID : 5J0A / pdb_00005j0a
Title : Crystal structure of PDZ-binding kinase
Authors : Zou, Q.W.; Zhou, H.; Yang, X.
Deposited on : 2016-03-28
Resolution : 2.74 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

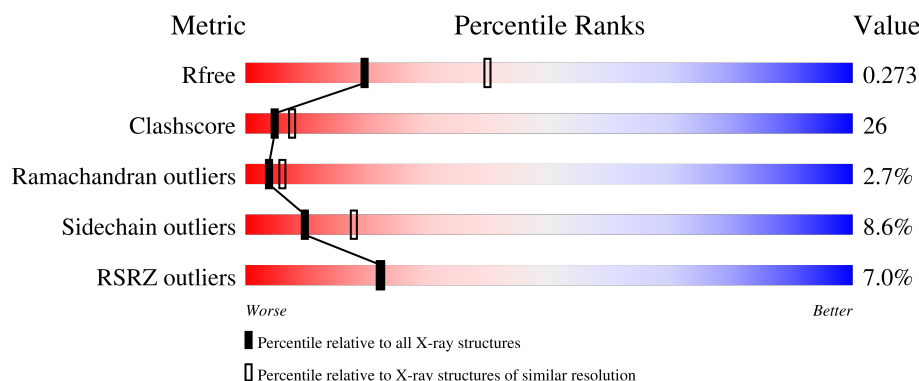
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	300	7% 53% 39% 7%
2	B	304	7% 50% 43% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	401	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4975 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 Lymphokine-activated killer T-cell-originated protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2355	1490	387	464	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q96KB5
A	198	GLU	THR	engineered mutation	UNP Q96KB5
A	321	ALA	-	expression tag	UNP Q96KB5

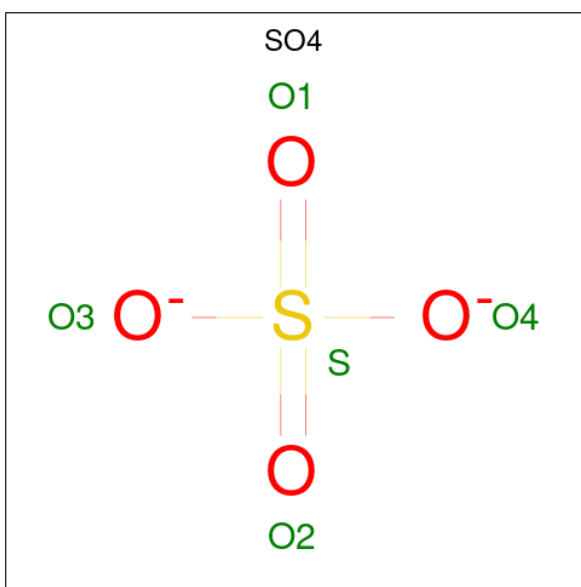
- Molecule 2 is a protein called Lymphokine-activated killer T-cell-originated protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2380	1506	391	468	15			

There are 4 discrepancies between the modelled and reference sequences:

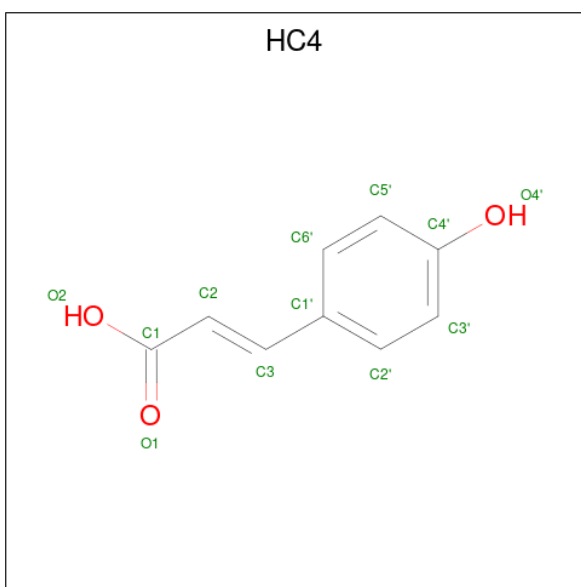
Chain	Residue	Modelled	Actual	Comment	Reference
B	18	GLY	-	expression tag	UNP Q96KB5
B	198	GLU	THR	engineered mutation	UNP Q96KB5
B	320	ALA	-	expression tag	UNP Q96KB5
B	321	ALA	-	expression tag	UNP Q96KB5

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 4'-HYDROXYCINNAMIC ACID (CCD ID: HC4) (formula: C₉H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	9	3		
4	A	1	Total	C	O	0	0
			12	9	3		
4	A	1	Total	C	O	0	0
			12	9	3		
4	B	1	Total	C	O	0	0
			12	9	3		

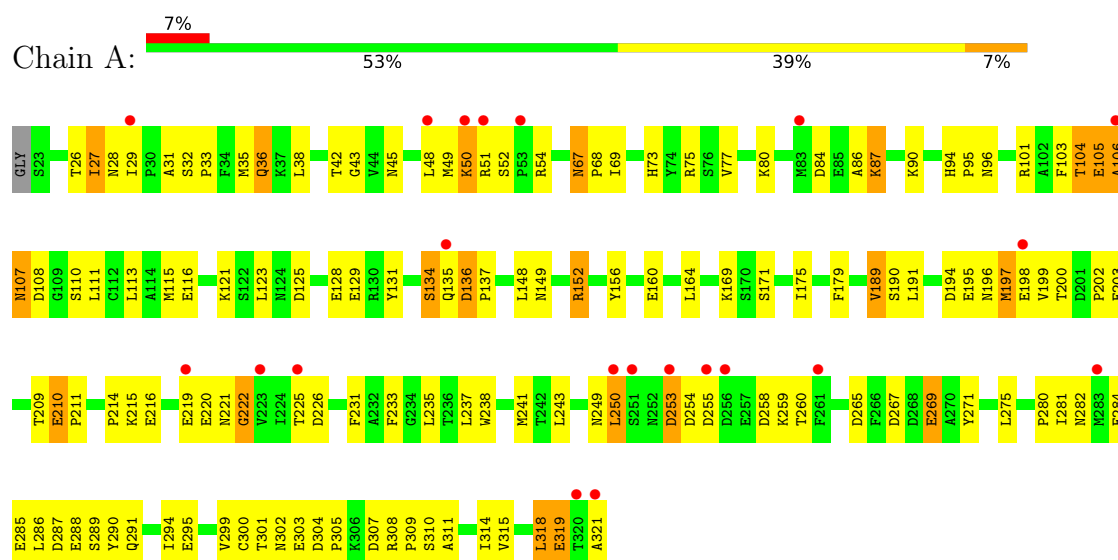
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	B	81	Total	O	0	0
			81	81		

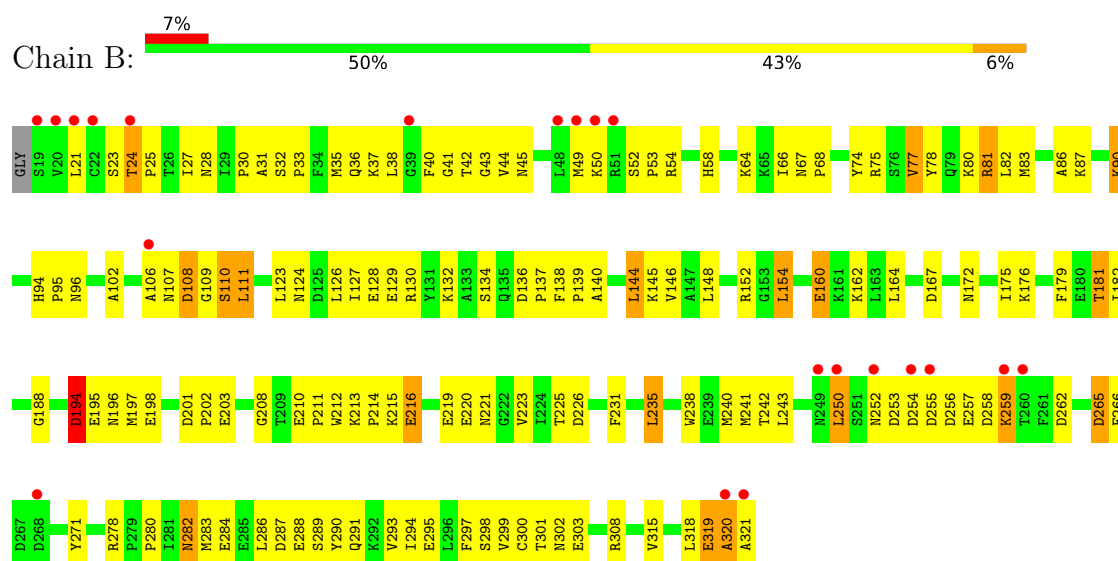
3 Residue-property plots [i](#)

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: Lymphokine-activated killer T-cell-originated protein kinase



- Molecule 2: Lymphokine-activated killer T-cell-originated protein kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.56Å 97.91Å 162.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.76 – 2.74 32.76 – 2.74	Depositor EDS
% Data completeness (in resolution range)	95.6 (32.76-2.74) 95.7 (32.76-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.96 (at 2.72Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.222 , 0.271 0.226 , 0.273	Depositor DCC
R_{free} test set	1580 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4975	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, HC4

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	0.41	0/2407	0.90	5/3262 (0.2%)
2	B	0.47	0/2432	0.99	7/3296 (0.2%)
All	All	0.44	0/4839	0.95	12/6558 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	195	GLU	N-CA-C	-10.93	99.96	113.18
2	B	129	GLU	N-CA-C	-9.43	101.08	111.36
1	A	135	GLN	N-CA-C	-9.03	102.21	113.23
1	A	107	ASN	N-CA-C	-8.77	99.02	110.33
2	B	319	GLU	N-CA-C	-8.57	103.33	112.93
2	B	253	ASP	N-CA-C	-7.51	103.11	111.82
2	B	160	GLU	N-CA-C	6.54	118.41	111.28
2	B	21	LEU	CB-CA-C	-6.10	108.53	115.79
1	A	67	ASN	CA-C-N	5.98	126.00	119.90
1	A	67	ASN	C-N-CA	5.98	126.00	119.90
2	B	289	SER	N-CA-C	-5.52	106.54	113.28
1	A	73	HIS	N-CA-C	5.48	116.94	110.97

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	2355	0	2303	118	0
2	B	2380	0	2331	144	0
3	A	25	0	0	2	0
3	B	25	0	0	3	0
4	A	36	0	18	3	0
4	B	12	0	6	0	0
5	A	61	0	0	2	0
5	B	81	0	0	4	0
All	All	4975	0	4658	242	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 26.

All (242) 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)
2:B:42:THR:HG22	2:B:43:GLY:H	1.21	1.02
1:A:105:GLU:CD	1:A:105:GLU:H	1.78	0.92
2:B:198:GLU:HG2	2:B:225:THR:HG22	1.51	0.90
1:A:94:HIS:HD2	1:A:96:ASN:H	1.19	0.87
2:B:167:ASP:HB3	2:B:208:GLY:HA2	1.59	0.84
2:B:167:ASP:CB	2:B:208:GLY:HA2	2.09	0.83
1:A:210:GLU:HB3	1:A:211:PRO:HD3	1.60	0.82
1:A:94:HIS:CD2	1:A:96:ASN:H	1.96	0.82
2:B:123:LEU:HD11	2:B:240:MET:HE3	1.61	0.81
1:A:69:ILE:HD11	1:A:75:ARG:HG3	1.64	0.79
2:B:94:HIS:HD2	2:B:96:ASN:H	1.31	0.78
2:B:176:LYS:HB3	2:B:181:THR:HB	1.65	0.78
2:B:194:ASP:HB3	2:B:196:ASN:H	1.49	0.78
2:B:220:GLU:CD	2:B:220:GLU:H	1.91	0.77
2:B:31:ALA:HA	2:B:42:THR:O	1.85	0.76
1:A:42:THR:HG22	1:A:43:GLY:O	1.85	0.76
1:A:250:LEU:H	1:A:250:LEU:HD12	1.50	0.76
2:B:194:ASP:HB2	2:B:198:GLU:H	1.50	0.76
2:B:94:HIS:CD2	2:B:96:ASN:H	2.04	0.76
1:A:267:ASP:OD1	1:A:269:GLU:HB2	1.85	0.75
1:A:50:LYS:H	1:A:50:LYS:HZ2	1.33	0.73
1:A:52:SER:HB2	1:A:54:ARG:NH1	2.04	0.72
1:A:321:ALA:HB1	2:B:37:LYS:NZ	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLU:HG3	2:B:50:LYS:HA	1.75	0.69
2:B:181:THR:HG22	5:B:507:HOH:O	1.92	0.69
2:B:42:THR:HG22	2:B:43:GLY:N	2.01	0.68
2:B:286:LEU:HD22	2:B:290:TYR:CD2	2.29	0.68
2:B:75:ARG:HD2	3:B:403:SO4:O2	1.94	0.67
2:B:36:GLN:HA	2:B:41:GLY:N	2.08	0.67
2:B:215:LYS:NZ	2:B:303:GLU:HB3	2.09	0.67
1:A:87:LYS:HE3	1:A:87:LYS:HA	1.77	0.66
2:B:23:SER:O	2:B:24:THR:HG23	1.96	0.66
2:B:130:ARG:NH2	2:B:139:PRO:HD3	2.11	0.66
1:A:219:GLU:HB2	1:A:222:GLY:H	1.61	0.65
1:A:156:TYR:O	1:A:160:GLU:HB2	1.97	0.65
2:B:210:GLU:HA	2:B:213:LYS:HG3	1.78	0.65
1:A:280:PRO:HG2	2:B:49:MET:HE3	1.79	0.65
1:A:32:SER:HB2	1:A:33:PRO:HD2	1.79	0.64
2:B:241:MET:HE1	2:B:294:ILE:HG12	1.78	0.64
2:B:77:VAL:HG22	2:B:78:TYR:CD2	2.33	0.63
1:A:94:HIS:HD2	1:A:96:ASN:N	1.95	0.62
2:B:67:ASN:N	2:B:68:PRO:HD3	2.14	0.62
2:B:282:ASN:HD22	2:B:282:ASN:N	1.97	0.62
1:A:238:TRP:HA	1:A:241:MET:HE3	1.81	0.62
2:B:250:LEU:HD12	2:B:250:LEU:H	1.65	0.62
1:A:131:TYR:CE2	2:B:54:ARG:HB3	2.35	0.61
2:B:188:GLY:HA3	3:B:401:SO4:O4	2.00	0.61
2:B:176:LYS:CB	2:B:181:THR:HB	2.31	0.61
1:A:105:GLU:CD	1:A:105:GLU:N	2.54	0.61
1:A:281:ILE:HD11	1:A:286:LEU:HD11	1.82	0.61
1:A:131:TYR:CD2	2:B:54:ARG:HB3	2.36	0.60
1:A:314:ILE:O	1:A:318:LEU:HB2	2.01	0.60
1:A:27:ILE:HG21	1:A:48:LEU:HD21	1.83	0.60
2:B:81:ARG:NH2	3:B:401:SO4:O1	2.33	0.60
1:A:290:TYR:O	1:A:294:ILE:HG13	2.02	0.60
1:A:197:MET:HG3	1:A:226:ASP:HB3	1.84	0.59
2:B:250:LEU:HA	2:B:265:ASP:O	2.02	0.59
1:A:38:LEU:HD13	2:B:299:VAL:HG21	1.85	0.59
1:A:214:PRO:HA	1:A:231:PHE:CD2	2.38	0.59
1:A:86:ALA:O	1:A:90:LYS:HG3	2.02	0.59
2:B:290:TYR:O	2:B:294:ILE:HG13	2.03	0.58
2:B:167:ASP:HB2	2:B:208:GLY:HA2	1.82	0.58
2:B:256:ASP:O	2:B:257:GLU:HB3	2.02	0.58
2:B:36:GLN:HA	2:B:41:GLY:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:PRO:HG2	2:B:50:LYS:NZ	2.18	0.58
2:B:215:LYS:HZ2	2:B:303:GLU:HB3	1.66	0.57
2:B:278:ARG:NH1	2:B:298:SER:O	2.37	0.57
2:B:201:ASP:OD1	2:B:202:PRO:HD2	2.03	0.57
1:A:194:ASP:CG	1:A:195:GLU:N	2.62	0.57
1:A:50:LYS:HZ2	1:A:50:LYS:N	2.03	0.56
1:A:299:VAL:HG21	2:B:38:LEU:HD13	1.88	0.56
2:B:127:ILE:C	2:B:127:ILE:HD12	2.30	0.56
2:B:300:CYS:O	2:B:308:ARG:HD3	2.06	0.56
2:B:278:ARG:HD3	2:B:301:THR:OG1	2.05	0.56
1:A:219:GLU:C	1:A:221:ASN:H	2.13	0.55
1:A:214:PRO:HA	1:A:231:PHE:CE2	2.42	0.55
2:B:106:ALA:HB2	2:B:111:LEU:HG	1.89	0.55
1:A:194:ASP:HB3	1:A:198:GLU:O	2.07	0.54
2:B:124:ASN:O	2:B:127:ILE:HG13	2.08	0.54
1:A:28:ASN:HA	1:A:45:ASN:HD22	1.72	0.54
1:A:169:LYS:HE3	1:A:171:SER:HB2	1.91	0.53
2:B:318:LEU:C	2:B:320:ALA:H	2.15	0.53
1:A:50:LYS:H	1:A:50:LYS:CD	2.21	0.52
1:A:67:ASN:N	1:A:68:PRO:HD3	2.24	0.52
2:B:145:LYS:HE2	2:B:179:PHE:O	2.09	0.52
1:A:196:ASN:O	1:A:198:GLU:HG3	2.09	0.52
1:A:203:GLU:OE2	1:A:203:GLU:HA	2.09	0.52
2:B:86:ALA:O	2:B:90:LYS:HB2	2.10	0.52
2:B:215:LYS:O	2:B:219:GLU:HG3	2.09	0.52
1:A:243:LEU:O	2:B:58:HIS:HE1	1.92	0.51
2:B:146:VAL:HA	2:B:182:ILE:HD13	1.92	0.51
1:A:164:LEU:HD13	1:A:226:ASP:HA	1.93	0.51
2:B:130:ARG:HH22	2:B:139:PRO:HD3	1.73	0.51
1:A:321:ALA:HB1	2:B:37:LYS:CE	2.41	0.51
2:B:259:LYS:HB2	5:B:542:HOH:O	2.11	0.51
2:B:35:MET:HE1	2:B:44:VAL:HG22	1.93	0.51
2:B:137:PRO:O	2:B:138:PHE:C	2.52	0.51
1:A:94:HIS:HD1	1:A:156:TYR:HB2	1.76	0.50
1:A:198:GLU:O	1:A:200:THR:HG23	2.10	0.50
1:A:107:ASN:OD1	1:A:108:ASP:N	2.45	0.50
1:A:131:TYR:CD1	1:A:131:TYR:C	2.90	0.50
1:A:194:ASP:CG	1:A:195:GLU:H	2.19	0.50
2:B:256:ASP:O	2:B:257:GLU:CB	2.60	0.49
1:A:282:ASN:HD22	1:A:285:GLU:HB2	1.78	0.49
2:B:291:GLN:O	2:B:295:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:ASP:O	2:B:259:LYS:C	2.55	0.49
1:A:189:VAL:N	3:A:402:SO4:O3	2.44	0.49
2:B:167:ASP:HB2	5:B:537:HOH:O	2.13	0.49
1:A:50:LYS:HG2	1:A:51:ARG:H	1.76	0.49
1:A:300:CYS:O	1:A:308:ARG:HD2	2.12	0.49
2:B:80:LYS:HE3	2:B:110:SER:OG	2.13	0.49
2:B:83:MET:HE3	2:B:83:MET:O	2.13	0.48
2:B:278:ARG:HH12	2:B:302:ASN:ND2	2.11	0.48
1:A:101:ARG:HB3	1:A:116:GLU:OE1	2.13	0.48
2:B:75:ARG:HA	2:B:75:ARG:HD3	1.62	0.48
2:B:259:LYS:NZ	2:B:259:LYS:HB3	2.28	0.48
2:B:108:ASP:CG	2:B:109:GLY:H	2.22	0.48
2:B:140:ALA:HB2	2:B:290:TYR:CD1	2.48	0.48
2:B:214:PRO:HB2	2:B:216:GLU:OE2	2.13	0.48
1:A:27:ILE:HG22	1:A:48:LEU:HG	1.96	0.47
1:A:50:LYS:H	1:A:50:LYS:HD3	1.79	0.47
2:B:28:ASN:O	2:B:30:PRO:HD3	2.14	0.47
2:B:42:THR:CG2	2:B:43:GLY:H	2.04	0.47
1:A:115:MET:CE	2:B:74:TYR:HA	2.45	0.47
2:B:126:LEU:C	2:B:128:GLU:H	2.23	0.47
2:B:194:ASP:HB3	2:B:196:ASN:N	2.25	0.47
1:A:103:PHE:O	1:A:104:THR:HG23	2.14	0.47
2:B:94:HIS:CD2	2:B:95:PRO:HD2	2.50	0.47
2:B:146:VAL:HG21	2:B:240:MET:HE1	1.96	0.47
1:A:225:THR:OG1	1:A:226:ASP:N	2.47	0.46
1:A:210:GLU:HB3	1:A:211:PRO:CD	2.39	0.46
1:A:258:ASP:OD2	1:A:260:THR:HB	2.15	0.46
2:B:148:LEU:HD21	2:B:152:ARG:NH2	2.31	0.46
1:A:215:LYS:O	1:A:219:GLU:HG2	2.16	0.46
2:B:32:SER:OG	2:B:33:PRO:HD2	2.16	0.46
2:B:287:ASP:OD1	2:B:288:GLU:N	2.49	0.46
1:A:104:THR:O	1:A:111:LEU:HD11	2.15	0.46
2:B:194:ASP:HB2	2:B:198:GLU:O	2.16	0.46
1:A:28:ASN:HB2	1:A:45:ASN:ND2	2.31	0.45
1:A:315:VAL:O	1:A:319:GLU:N	2.45	0.45
2:B:123:LEU:O	2:B:127:ILE:HG23	2.16	0.45
1:A:94:HIS:CD2	1:A:94:HIS:C	2.94	0.45
1:A:49:MET:HE3	2:B:280:PRO:HG2	1.98	0.45
1:A:307:ASP:OD1	2:B:40:PHE:HE1	1.99	0.45
2:B:134:SER:C	2:B:136:ASP:H	2.25	0.45
1:A:80:LYS:HE2	1:A:110:SER:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:PHE:HZ	2:B:271:TYR:CG	2.34	0.45
1:A:152:ARG:HG3	3:A:405:SO4:S	2.57	0.45
2:B:241:MET:HE2	2:B:286:LEU:HD13	1.98	0.45
2:B:315:VAL:O	2:B:319:GLU:HG3	2.16	0.45
1:A:94:HIS:CD2	1:A:95:PRO:N	2.85	0.45
2:B:162:LYS:NZ	2:B:197:MET:HE3	2.31	0.45
2:B:262:ASP:N	2:B:265:ASP:OD2	2.40	0.45
1:A:231:PHE:CD1	1:A:301:THR:HA	2.52	0.45
1:A:281:ILE:HD12	1:A:282:ASN:H	1.82	0.45
1:A:35:MET:HB2	2:B:295:GLU:OE1	2.16	0.45
4:A:408:HC4:H3'	5:A:505:HOH:O	2.16	0.44
2:B:52:SER:C	2:B:54:ARG:H	2.24	0.44
1:A:284:GLU:CD	2:B:50:LYS:HG3	2.42	0.44
2:B:126:LEU:C	2:B:128:GLU:N	2.73	0.44
2:B:137:PRO:HG3	2:B:241:MET:O	2.17	0.44
2:B:128:GLU:O	2:B:132:LYS:HG2	2.16	0.44
1:A:87:LYS:NZ	1:A:90:LYS:HE2	2.32	0.44
2:B:252:ASN:HB3	2:B:255:ASP:CG	2.43	0.44
2:B:28:ASN:ND2	2:B:45:ASN:OD1	2.51	0.44
1:A:304:ASP:HA	1:A:305:PRO:HD3	1.86	0.44
2:B:221:ASN:O	2:B:221:ASN:OD1	2.36	0.44
1:A:219:GLU:C	1:A:221:ASN:N	2.74	0.43
2:B:164:LEU:HD13	2:B:226:ASP:HA	2.00	0.43
2:B:175:ILE:HD12	2:B:182:ILE:HG12	2.00	0.43
1:A:321:ALA:HB1	2:B:37:LYS:HZ2	1.83	0.43
2:B:90:LYS:HD2	2:B:102:ALA:HB2	2.00	0.43
2:B:241:MET:HE2	2:B:286:LEU:CD1	2.48	0.43
1:A:235:LEU:O	1:A:238:TRP:HB3	2.18	0.43
2:B:108:ASP:CG	2:B:109:GLY:N	2.76	0.43
2:B:278:ARG:HH12	2:B:302:ASN:HD22	1.66	0.43
1:A:190:SER:O	1:A:191:LEU:HD23	2.18	0.43
2:B:212:TRP:HA	2:B:235:LEU:HD23	2.01	0.43
2:B:238:TRP:HB2	2:B:297:PHE:CE1	2.54	0.43
1:A:49:MET:HB2	2:B:280:PRO:HB2	2.01	0.43
2:B:52:SER:HA	2:B:53:PRO:HD3	1.87	0.43
2:B:282:ASN:N	2:B:282:ASN:ND2	2.64	0.43
1:A:54:ARG:HG3	1:A:54:ARG:HH11	1.84	0.43
1:A:125:ASP:O	1:A:129:GLU:HB2	2.18	0.43
1:A:216:GLU:HA	1:A:219:GLU:CG	2.49	0.43
1:A:289:SER:C	1:A:291:GLN:H	2.27	0.43
1:A:38:LEU:CD1	2:B:299:VAL:HG21	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:HD3	1:A:303:GLU:OE1	2.18	0.43
4:A:408:HC4:H2	2:B:66:ILE:HA	2.01	0.43
2:B:127:ILE:HG22	2:B:138:PHE:HE2	1.84	0.43
1:A:36:GLN:HG3	5:A:527:HOH:O	2.18	0.43
2:B:282:ASN:HD22	2:B:282:ASN:H	1.62	0.43
1:A:308:ARG:HA	1:A:309:PRO:HD3	1.94	0.42
1:A:94:HIS:ND1	1:A:156:TYR:HB2	2.34	0.42
2:B:64:LYS:HE3	2:B:64:LYS:HB2	1.87	0.42
1:A:216:GLU:OE1	1:A:308:ARG:NH2	2.52	0.42
2:B:198:GLU:CG	2:B:225:THR:HG22	2.37	0.42
1:A:121:LYS:NZ	1:A:129:GLU:OE2	2.53	0.42
1:A:175:ILE:HG12	1:A:179:PHE:CE1	2.54	0.42
2:B:201:ASP:OD1	2:B:202:PRO:CD	2.66	0.42
1:A:209:THR:HG22	1:A:211:PRO:HD2	2.02	0.42
1:A:216:GLU:HA	1:A:219:GLU:HG2	2.02	0.42
2:B:27:ILE:HG12	2:B:28:ASN:N	2.35	0.42
2:B:36:GLN:OE1	2:B:41:GLY:HA3	2.19	0.42
2:B:77:VAL:HG22	2:B:78:TYR:CE2	2.54	0.42
1:A:94:HIS:HD1	1:A:156:TYR:CB	2.32	0.42
2:B:238:TRP:CE2	2:B:242:THR:HG21	2.55	0.42
1:A:282:ASN:ND2	1:A:285:GLU:OE1	2.50	0.41
2:B:181:THR:CG2	5:B:507:HOH:O	2.60	0.41
1:A:219:GLU:O	1:A:220:GLU:HB3	2.20	0.41
1:A:80:LYS:HE2	1:A:110:SER:CB	2.51	0.41
1:A:96:ASN:OD1	1:A:149:ASN:HB3	2.21	0.41
1:A:282:ASN:ND2	1:A:285:GLU:HB2	2.34	0.41
2:B:320:ALA:O	2:B:321:ALA:HB3	2.20	0.41
2:B:215:LYS:HZ1	2:B:303:GLU:HB3	1.83	0.41
1:A:295:GLU:OE1	2:B:35:MET:HG3	2.21	0.41
1:A:48:LEU:CD2	2:B:283:MET:HB2	2.50	0.41
1:A:233:PHE:CE1	1:A:237:LEU:HD11	2.55	0.41
2:B:144:LEU:HD22	2:B:293:VAL:HG23	2.02	0.41
2:B:154:LEU:HD12	2:B:154:LEU:HA	1.92	0.41
2:B:242:THR:O	2:B:243:LEU:HB2	2.21	0.41
2:B:250:LEU:HD12	2:B:250:LEU:N	2.33	0.41
1:A:77:VAL:HG22	2:B:77:VAL:HB	2.02	0.41
1:A:284:GLU:H	1:A:284:GLU:HG2	1.66	0.41
4:A:408:HC4:H2	4:A:408:HC4:H6'	1.81	0.41
1:A:36:GLN:HA	1:A:36:GLN:HE21	1.84	0.41
1:A:94:HIS:CD2	1:A:95:PRO:HD2	2.56	0.41
1:A:106:ALA:C	1:A:107:ASN:O	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASP:OD1	1:A:288:GLU:N	2.54	0.41
1:A:310:SER:O	1:A:311:ALA:C	2.63	0.41
2:B:94:HIS:CG	2:B:95:PRO:HD2	2.56	0.41
1:A:29:ILE:O	1:A:43:GLY:HA2	2.21	0.40
1:A:134:SER:HB2	1:A:136:ASP:H	1.86	0.40
1:A:137:PRO:HD3	2:B:54:ARG:HH22	1.86	0.40
1:A:253:ASP:O	1:A:254:ASP:CB	2.69	0.40
2:B:83:MET:O	2:B:87:LYS:HG3	2.21	0.40
2:B:210:GLU:CB	2:B:211:PRO:HD3	2.52	0.40
2:B:221:ASN:O	2:B:221:ASN:CG	2.62	0.40
2:B:282:ASN:ND2	2:B:282:ASN:H	2.18	0.40
1:A:131:TYR:HE2	2:B:54:ARG:HB3	1.85	0.40
2:B:231:PHE:CD1	2:B:301:THR:HA	2.57	0.40
2:B:203:GLU:HA	2:B:203:GLU:OE2	2.22	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	297/300 (99%)	254 (86%)	32 (11%)	11 (4%)		
2	B	301/304 (99%)	265 (88%)	31 (10%)	5 (2%)		
All	All	598/604 (99%)	519 (87%)	63 (10%)	16 (3%)		

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
2	B	107	ASN
1	A	269	GLU
1	A	275	LEU

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Mol	Chain	Res	Type
2	B	259	LYS
1	A	31	ALA
2	B	108	ASP
2	B	320	ALA
1	A	210	GLU
1	A	253	ASP
1	A	271	TYR
1	A	106	ALA
2	B	194	ASP
1	A	199	VAL
1	A	202	PRO
1	A	222	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/261 (100%)	237 (91%)	24 (9%)	8	16
2	B	264/264 (100%)	243 (92%)	21 (8%)	11	20
All	All	525/525 (100%)	480 (91%)	45 (9%)	10	18

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	27	ILE
1	A	36	GLN
1	A	50	LYS
1	A	84	ASP
1	A	87	LYS
1	A	104	THR
1	A	105	GLU
1	A	113	LEU
1	A	123	LEU
1	A	128	GLU

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Mol	Chain	Res	Type
1	A	134	SER
1	A	136	ASP
1	A	148	LEU
1	A	152	ARG
1	A	189	VAL
1	A	197	MET
1	A	249	ASN
1	A	250	LEU
1	A	255	ASP
1	A	259	LYS
1	A	265	ASP
1	A	302	ASN
1	A	318	LEU
2	B	24	THR
2	B	77	VAL
2	B	81	ARG
2	B	82	LEU
2	B	90	LYS
2	B	110	SER
2	B	111	LEU
2	B	144	LEU
2	B	154	LEU
2	B	160	GLU
2	B	172	ASN
2	B	181	THR
2	B	194	ASP
2	B	216	GLU
2	B	223	VAL
2	B	235	LEU
2	B	250	LEU
2	B	254	ASP
2	B	265	ASP
2	B	282	ASN
2	B	284	GLU

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

Mol	Chain	Res	Type
1	A	36	GLN
1	A	45	ASN
1	A	67	ASN
1	A	79	GLN

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Mol	Chain	Res	Type
1	A	124	ASN
1	A	291	GLN
1	A	302	ASN
2	B	58	HIS
2	B	79	GLN
2	B	94	HIS
2	B	107	ASN
2	B	172	ASN
2	B	282	ASN
2	B	302	ASN

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 ⓘ

14 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	$\# Z > 2$
3	SO4	A	405	-	4,4,4	0.70	0	6,6,6	0.07	0
3	SO4	B	402	-	4,4,4	0.69	0	6,6,6	0.08	0
3	SO4	A	401	-	4,4,4	0.70	0	6,6,6	0.07	0
4	HC4	A	407	-	12,12,12	1.64	3 (25%)	15,15,15	0.92	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	403	-	4,4,4	0.70	0	6,6,6	0.07	0
4	HC4	A	406	-	12,12,12	1.67	4 (33%)	15,15,15	1.02	1 (6%)
4	HC4	B	406	-	12,12,12	1.64	3 (25%)	15,15,15	0.90	1 (6%)
3	SO4	B	404	-	4,4,4	0.70	0	6,6,6	0.06	0
3	SO4	A	403	-	4,4,4	0.69	0	6,6,6	0.05	0
3	SO4	B	401	-	4,4,4	0.69	0	6,6,6	0.09	0
3	SO4	B	405	-	4,4,4	0.70	0	6,6,6	0.07	0
3	SO4	A	402	-	4,4,4	0.70	0	6,6,6	1.66	0
3	SO4	A	404	-	4,4,4	0.69	0	6,6,6	0.08	0
4	HC4	A	408	-	12,12,12	1.70	3 (25%)	15,15,15	0.98	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HC4	A	406	-	-	0/5/5/5	0/1/1/1
4	HC4	A	408	-	-	0/5/5/5	0/1/1/1
4	HC4	A	407	-	-	0/5/5/5	0/1/1/1
4	HC4	B	406	-	-	0/5/5/5	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	406	HC4	C2-C1	-3.68	1.39	1.48
4	A	408	HC4	C2-C1	-3.67	1.39	1.48
4	A	407	HC4	C2-C1	-3.57	1.39	1.48
4	B	406	HC4	C2-C1	-3.55	1.39	1.48
4	A	408	HC4	C1'-C3	-2.95	1.39	1.47
4	A	407	HC4	C1'-C3	-2.82	1.39	1.47
4	B	406	HC4	C1'-C3	-2.82	1.39	1.47
4	A	406	HC4	C1'-C3	-2.79	1.39	1.47
4	A	408	HC4	C2-C3	2.64	1.39	1.33
4	A	406	HC4	C2-C3	2.54	1.39	1.33
4	B	406	HC4	C2-C3	2.53	1.39	1.33
4	A	407	HC4	C2-C3	2.51	1.39	1.33
4	A	406	HC4	O2-C1	-2.02	1.25	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	406	HC4	C1'-C3-C2	-3.30	119.71	126.92
4	A	408	HC4	C1'-C3-C2	-3.14	120.06	126.92
4	B	406	HC4	C1'-C3-C2	-2.71	121.00	126.92
4	A	407	HC4	C1'-C3-C2	-2.51	121.44	126.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	SO4	1	0
3	B	403	SO4	1	0
3	B	401	SO4	2	0
3	A	402	SO4	1	0
4	A	408	HC4	3	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	299/300 (99%)	0.52	21 (7%)	22 22	38, 74, 107, 132	0
2	B	303/304 (99%)	0.28	21 (6%)	23 22	36, 60, 107, 129	0
All	All	602/604 (99%)	0.40	42 (6%)	22 22	36, 67, 107, 132	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	20	VAL	6.2
1	A	135	GLN	5.3
1	A	198	GLU	5.2
2	B	21	LEU	4.6
2	B	321	ALA	3.7
1	A	320	THR	3.7
2	B	259	LYS	3.7
2	B	320	ALA	3.6
2	B	22	CYS	3.5
1	A	250	LEU	3.3
1	A	50	LYS	3.2
2	B	50	LYS	3.2
1	A	51	ARG	3.1
1	A	29	ILE	3.0
2	B	19	SER	2.9
1	A	256	ASP	2.9
1	A	321	ALA	2.9
2	B	250	LEU	2.8
1	A	106	ALA	2.8
2	B	51	ARG	2.7
2	B	24	THR	2.7
2	B	106	ALA	2.6
1	A	223	VAL	2.6
2	B	254	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	48	LEU	2.4
1	A	283	MET	2.4
2	B	255	ASP	2.4
2	B	48	LEU	2.3
2	B	260	THR	2.3
1	A	219	GLU	2.2
1	A	253	ASP	2.2
1	A	261	PHE	2.2
2	B	49	MET	2.2
1	A	225	THR	2.1
2	B	39	GLY	2.1
1	A	251	SER	2.1
2	B	249	ASN	2.1
1	A	255	ASP	2.1
1	A	83	MET	2.1
2	B	252	ASN	2.0
2	B	268	ASP	2.0
1	A	53	PRO	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
3	SO4	B	405	5/5	0.66	0.14	129,129,129,130	0
3	SO4	A	403	5/5	0.74	0.19	134,135,135,136	0
3	SO4	B	404	5/5	0.75	0.18	138,139,139,140	0
3	SO4	A	405	5/5	0.77	0.16	148,148,149,149	0
4	HC4	A	408	12/12	0.79	0.28	60,82,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	404	5/5	0.80	0.10	138,138,139,139	0
4	HC4	A	406	12/12	0.86	0.20	40,59,62,62	0
3	SO4	B	402	5/5	0.86	0.15	140,141,141,141	0
3	SO4	A	401	5/5	0.87	0.15	133,133,134,134	0
4	HC4	B	406	12/12	0.87	0.21	87,91,96,97	0
3	SO4	B	403	5/5	0.90	0.23	112,112,113,113	0
3	SO4	A	402	5/5	0.94	0.10	80,80,81,82	0
3	SO4	B	401	5/5	0.95	0.12	71,72,73,75	0
4	HC4	A	407	12/12	0.97	0.07	36,39,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.