



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:29 am BST

PDB ID : 5YF9
Title : Crystal structure of CK2a2 form-2
Authors : Tsuyuguchi, M.; Kinoshita, T.
Deposited on : 2017-09-20
Resolution : 1.89 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

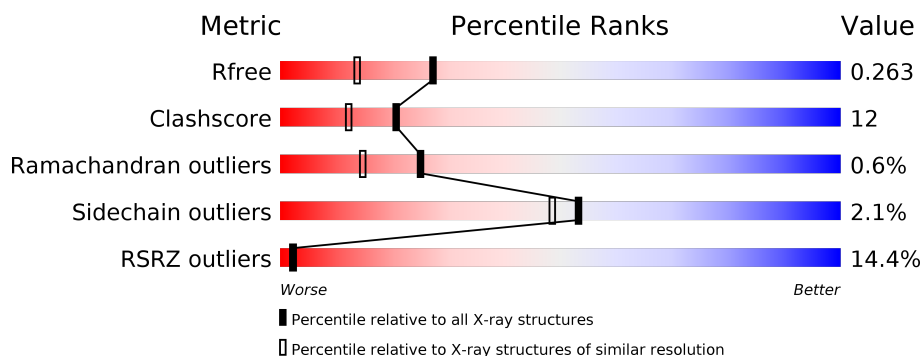
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	B	339	<div> <div>19%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>6%</div> </div> </div>
1	X	339	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>6%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	X	402	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6473 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.

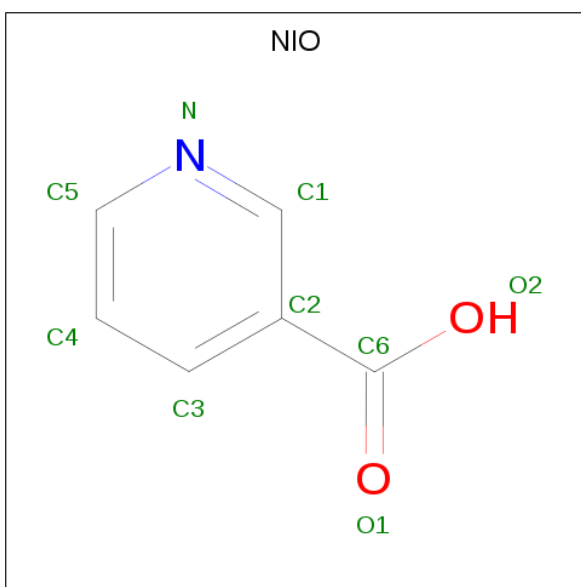
- Molecule 1 is a protein called Casein kinase II subunit alpha'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	319	Total	C	N	O	S	0	3	0
			2715	1749	474	481	11			
1	B	319	Total	C	N	O	S	0	2	0
			2708	1746	471	481	10			

There are 10 discrepancies between the modelled and reference sequences:

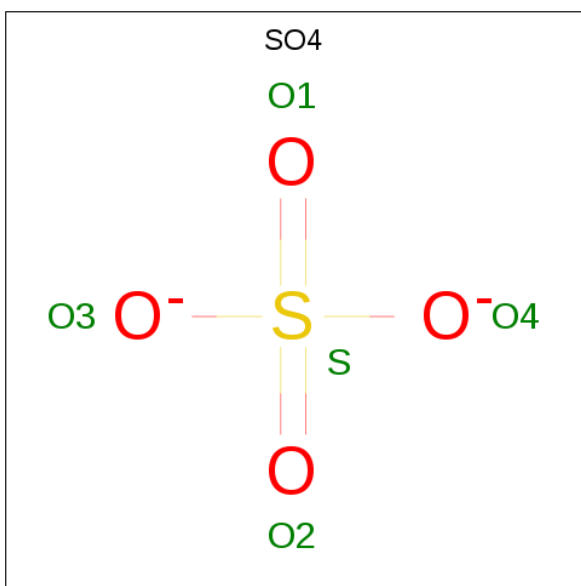
Chain	Residue	Modelled	Actual	Comment	Reference
X	-4	GLY	-	expression tag	UNP P19784
X	-3	PRO	-	expression tag	UNP P19784
X	-2	LEU	-	expression tag	UNP P19784
X	-1	GLY	-	expression tag	UNP P19784
X	0	SER	-	expression tag	UNP P19784
B	-4	GLY	-	expression tag	UNP P19784
B	-3	PRO	-	expression tag	UNP P19784
B	-2	LEU	-	expression tag	UNP P19784
B	-1	GLY	-	expression tag	UNP P19784
B	0	SER	-	expression tag	UNP P19784

- Molecule 2 is NICOTINIC ACID (three-letter code: NIO) (formula: C₆H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	X	1	Total	C	N	O	0	0
			9	6	1	2		
2	B	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

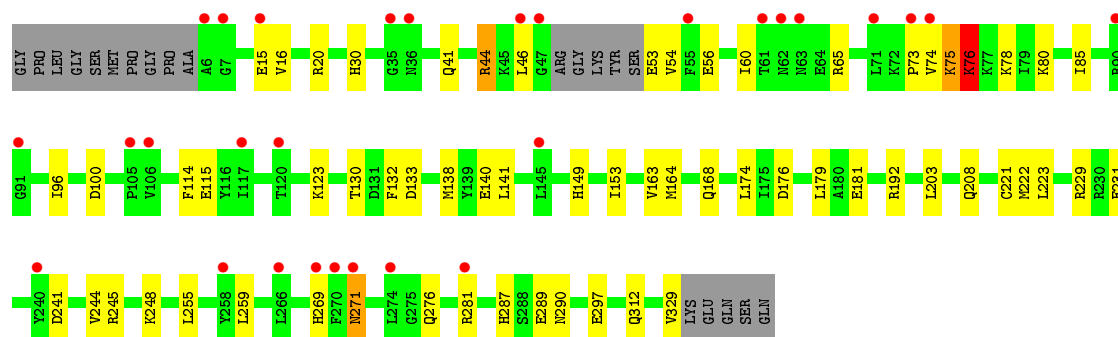
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	517	Total	O	0	0
			517	517		
4	B	475	Total	O	0	0
			475	475		

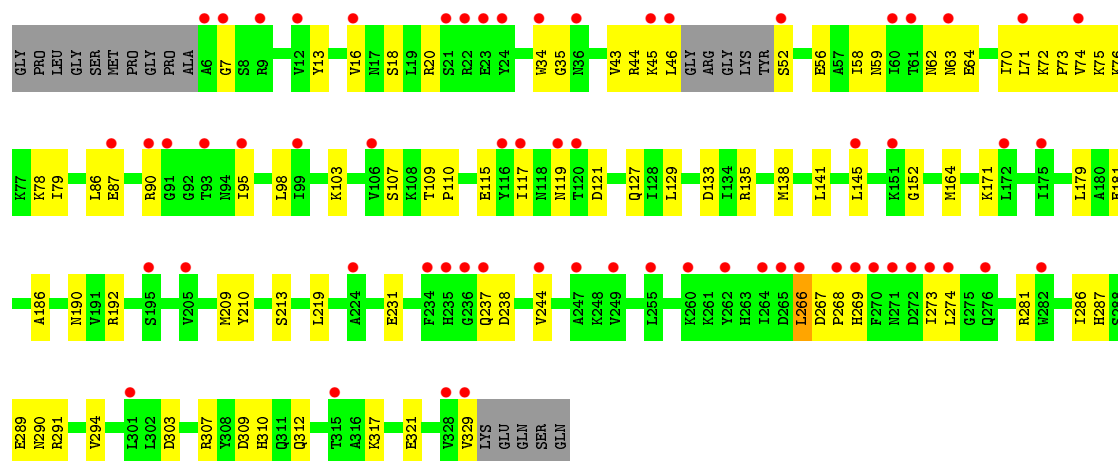
3 Residue-property plots [i](#)

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: Casein kinase II subunit alpha'



• Molecule 1: Casein kinase II subunit alpha'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.47Å 102.42Å 72.23Å 90.00° 95.02° 90.00°	Depositor
Resolution (Å)	46.29 – 1.89 46.29 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.29-1.89) 99.9 (46.29-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.211 , 0.263 0.212 , 0.263	Depositor DCC
R_{free} test set	2736 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.1	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	0.92	EDS
Total number of atoms	6473	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.16% 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, NIO

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	B	0.39	0/2777	0.54	0/3750
1	X	0.43	0/2784	0.55	0/3759
All	All	0.41	0/5561	0.54	0/7509

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	B	2708	0	2686	74	0
1	X	2715	0	2690	57	0
2	B	9	0	4	0	0
2	X	9	0	4	0	0
3	B	15	0	0	1	0
3	X	25	0	0	3	0
4	B	475	0	0	44	7
4	X	517	0	0	41	7
All	All	6473	0	5384	134	10

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 12.

All (134) 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:X:168:GLN:O	4:X:501:HOH:O	1.85	0.92
1:X:65:ARG:NH2	4:X:502:HOH:O	1.98	0.87
1:X:65:ARG:NH1	4:X:506:HOH:O	2.08	0.86
1:B:90:ARG:NH2	4:B:506:HOH:O	2.10	0.84
1:X:85:ILE:HG23	1:X:153:ILE:HD13	1.58	0.82
1:X:192:ARG:NE	4:X:507:HOH:O	2.11	0.82
1:X:15:GLU:OE1	4:X:503:HOH:O	1.98	0.81
1:B:281:ARG:NH1	4:B:510:HOH:O	2.14	0.80
1:X:290:ASN:HB3	4:X:629:HOH:O	1.82	0.80
1:X:100:ASP:OD2	4:X:504:HOH:O	2.00	0.79
1:X:269:HIS:O	4:X:505:HOH:O	2.01	0.78
1:B:52:SER:OG	1:B:72:LYS:NZ	2.15	0.78
1:B:13:TYR:HB3	4:B:533:HOH:O	1.85	0.76
1:B:231:GLU:OE2	4:B:503:HOH:O	2.03	0.76
3:X:402:SO4:S	4:X:508:HOH:O	2.42	0.76
1:X:96:ILE:HG13	4:X:600:HOH:O	1.84	0.75
1:X:179:LEU:HB3	4:X:515:HOH:O	1.84	0.74
1:B:63:ASN:ND2	4:B:509:HOH:O	2.12	0.73
1:X:168:GLN:HG2	4:X:631:HOH:O	1.87	0.73
1:B:90:ARG:NH2	4:B:505:HOH:O	2.09	0.72
1:X:149:HIS:ND1	4:X:514:HOH:O	2.21	0.71
1:X:174:LEU:HB2	4:X:645:HOH:O	1.90	0.70
1:X:114:PHE:HB3	4:X:600:HOH:O	1.91	0.70
1:B:190:ASN:ND2	4:B:521:HOH:O	2.24	0.69
1:X:221:CYS:SG	4:X:939:HOH:O	2.38	0.69
1:B:7:GLY:N	4:B:525:HOH:O	2.25	0.68
1:B:181:GLU:OE1	4:B:508:HOH:O	2.11	0.68
1:X:312:GLN:HA	4:X:552:HOH:O	1.94	0.68
1:B:317:LYS:NZ	4:B:526:HOH:O	2.26	0.68
1:B:59:ASN:ND2	4:B:528:HOH:O	2.27	0.67
1:B:62:ASN:ND2	4:B:520:HOH:O	2.23	0.67
1:B:109:THR:HG21	4:B:809:HOH:O	1.94	0.66
3:X:402:SO4:O3	4:X:508:HOH:O	2.13	0.65
1:B:127:GLN:NE2	4:B:530:HOH:O	2.28	0.65
1:B:303:ASP:OD2	4:B:511:HOH:O	2.15	0.65
1:B:119:ASN:HB2	1:B:164:MET:HE2	1.79	0.65
1:B:317:LYS:NZ	4:B:532:HOH:O	2.29	0.64
1:X:78:LYS:NZ	4:X:524:HOH:O	2.31	0.64
1:X:141:LEU:HB2	4:X:922:HOH:O	1.99	0.63
1:B:73:PRO:O	4:B:512:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LYS:O	1:B:46:LEU:HB2	2.00	0.61
1:X:287:HIS:CE1	1:X:289:GLU:HB2	2.36	0.61
1:X:297:GLU:HA	4:X:815:HOH:O	2.00	0.61
1:B:63:ASN:CG	4:B:534:HOH:O	2.40	0.61
1:B:58:ILE:HD11	4:B:861:HOH:O	2.01	0.60
1:B:76:LYS:HD3	4:B:512:HOH:O	2.02	0.59
1:B:307:ARG:NH1	4:B:531:HOH:O	2.36	0.58
1:X:231:GLU:OE1	4:X:510:HOH:O	2.17	0.58
1:X:192:ARG:CZ	4:X:507:HOH:O	2.49	0.58
1:X:65:ARG:HD2	4:X:502:HOH:O	2.02	0.58
1:B:70:ILE:HG21	4:B:958:HOH:O	2.03	0.58
1:X:130:THR:HG21	4:X:917:HOH:O	2.03	0.58
1:X:53:GLU:OE1	4:X:512:HOH:O	2.17	0.57
3:X:406:SO4:O4	4:X:511:HOH:O	2.17	0.57
4:X:507:HOH:O	1:B:192:ARG:NH1	2.37	0.57
1:X:229:ARG:HB2	4:X:629:HOH:O	2.04	0.57
1:X:130:THR:HG23	1:X:133:ASP:H	1.70	0.56
1:X:41:GLN:HB2	1:X:60:ILE:HD11	1.88	0.56
1:B:287:HIS:CE1	1:B:289:GLU:HB2	2.41	0.56
1:B:87:GLU:HG2	1:B:90:ARG:HH11	1.70	0.55
1:B:115:GLU:OE1	4:B:514:HOH:O	2.18	0.55
1:X:123:LYS:HA	4:X:638:HOH:O	2.07	0.55
1:X:164[B]:MET:SD	4:X:714:HOH:O	2.58	0.55
1:X:30:HIS:O	1:X:80:LYS:NZ	2.37	0.54
1:B:127:GLN:N	4:B:523:HOH:O	2.34	0.54
1:B:287:HIS:HE1	1:B:289:GLU:HB2	1.74	0.53
1:B:238:ASP:HB2	4:B:709:HOH:O	2.09	0.53
1:X:281[B]:ARG:HG3	4:X:798:HOH:O	2.07	0.53
1:B:107:SER:O	4:B:515:HOH:O	2.19	0.53
1:X:75:LYS:O	1:X:76:LYS:HB2	2.08	0.52
1:X:16[B]:VAL:O	1:X:20:ARG:HG3	2.10	0.52
3:B:402:SO4:O1	4:B:516:HOH:O	2.19	0.52
1:B:35:GLY:HA3	4:B:658:HOH:O	2.10	0.52
1:X:141:LEU:HD22	4:X:922:HOH:O	2.09	0.51
1:B:86:LEU:HD22	4:B:529:HOH:O	2.11	0.51
1:X:115:GLU:HG2	4:X:600:HOH:O	2.11	0.51
1:X:56:GLU:OE1	1:X:65:ARG:NH1	2.37	0.50
1:B:312:GLN:OE1	4:B:517:HOH:O	2.19	0.50
1:X:130:THR:CG2	1:X:133:ASP:H	2.24	0.49
1:B:62:ASN:CG	1:B:64:GLU:HG3	2.33	0.49
1:X:46:LEU:HB3	1:X:54:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ILE:HD13	1:B:110:PRO:HG2	1.95	0.49
1:X:74:VAL:C	4:X:517:HOH:O	2.51	0.49
1:X:312:GLN:NE2	4:X:552:HOH:O	2.45	0.49
1:X:241:ASP:O	1:X:245:ARG:HG2	2.13	0.48
1:B:309:ASP:HB3	4:B:531:HOH:O	2.12	0.48
1:B:52:SER:OG	4:B:502:HOH:O	2.02	0.48
1:X:130:THR:HG23	1:X:132:PHE:N	2.29	0.48
1:B:186:ALA:HA	1:B:209:MET:HE3	1.96	0.48
1:B:121:ASP:HB3	4:B:541:HOH:O	2.14	0.47
1:B:171[B]:LYS:HE2	4:B:513:HOH:O	2.14	0.47
1:X:44:ARG:HG3	1:X:56:GLU:HB2	1.97	0.47
1:B:210:TYR:HB2	4:B:701:HOH:O	2.15	0.46
1:X:271:ASN:N	1:X:271:ASN:HD22	2.14	0.46
1:X:208:GLN:CD	1:B:75:LYS:HZ2	2.20	0.46
1:B:179:LEU:HD21	4:B:961:HOH:O	2.17	0.45
1:B:71:LEU:HD13	1:B:79:ILE:HG12	1.98	0.45
1:B:266:LEU:HD22	1:B:267:ASP:H	1.81	0.45
1:B:267:ASP:OD2	1:B:269:HIS:HB3	2.15	0.45
1:B:138:MET:SD	1:B:219[B]:LEU:HD11	2.57	0.45
1:B:135:ARG:NH1	4:B:581:HOH:O	2.50	0.45
1:B:267:ASP:HA	1:B:268:PRO:HD3	1.85	0.45
1:B:90:ARG:NH2	1:B:98:LEU:O	2.50	0.44
1:B:43:VAL:HG13	4:B:562:HOH:O	2.17	0.44
1:B:291:ARG:NH2	4:B:580:HOH:O	2.50	0.44
1:B:44:ARG:HG3	1:B:56:GLU:HB2	2.00	0.44
1:B:16:VAL:O	1:B:20:ARG:HG2	2.18	0.44
1:B:317:LYS:O	1:B:321:GLU:HG3	2.17	0.44
1:X:73:PRO:HD2	4:B:727:HOH:O	2.17	0.44
1:B:317:LYS:HE3	1:B:317:LYS:HB2	1.79	0.44
1:B:286:ILE:HG12	1:B:294:VAL:HG11	1.99	0.43
1:B:290:ASN:O	1:B:294:VAL:HG23	2.18	0.43
1:X:163:VAL:HG11	4:X:922:HOH:O	2.18	0.43
1:X:203:LEU:HD23	4:X:541:HOH:O	2.19	0.43
1:B:152:GLY:HA2	4:B:533:HOH:O	2.19	0.43
1:B:34:TRP:CD1	1:B:103:LYS:HE3	2.53	0.43
1:B:121:ASP:CG	4:B:541:HOH:O	2.57	0.43
1:B:129:LEU:HD22	1:B:133:ASP:HB3	2.01	0.43
1:X:140:GLU:CD	4:X:529:HOH:O	2.56	0.43
1:B:213:SER:OG	1:B:310:HIS:HB2	2.18	0.42
1:X:138:MET:HG3	1:X:223:LEU:HD13	2.01	0.42
1:B:244:VAL:HG22	1:B:274:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLN:O	4:B:519:HOH:O	2.21	0.42
1:B:269:HIS:O	1:B:269:HIS:ND1	2.53	0.42
1:B:119:ASN:HB2	1:B:164:MET:CE	2.47	0.41
1:X:222:MET:HE1	4:X:813:HOH:O	2.20	0.41
1:B:141:LEU:HD23	1:B:219[B]:LEU:HD13	2.01	0.41
1:B:86:LEU:HA	1:B:86:LEU:HD23	1.84	0.41
1:X:179:LEU:O	4:X:515:HOH:O	2.22	0.41
1:X:56:GLU:CD	1:X:65:ARG:HH11	2.19	0.41
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.87	0.40
1:B:78:LYS:NZ	4:B:585:HOH:O	2.52	0.40
1:X:244:VAL:HG12	1:X:248:LYS:HZ3	1.87	0.40
1:X:255:LEU:O	1:X:259:LEU:HG	2.21	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:815:HOH:O	4:B:680:HOH:O[1_554]	1.82	0.38
4:X:930:HOH:O	4:B:874:HOH:O[1_554]	1.99	0.21
4:X:569:HOH:O	4:X:571:HOH:O[2_655]	2.00	0.20
4:X:569:HOH:O	4:X:631:HOH:O[2_655]	2.02	0.18
4:X:530:HOH:O	4:X:833:HOH:O[2_645]	2.03	0.17
4:X:611:HOH:O	4:B:679:HOH:O[2_645]	2.07	0.13
4:B:755:HOH:O	4:B:808:HOH:O[2_646]	2.09	0.11
4:X:966:HOH:O	4:B:842:HOH:O[2_646]	2.10	0.10
4:B:573:HOH:O	4:B:717:HOH:O[2_656]	2.17	0.03
4:B:589:HOH:O	4:B:901:HOH:O[2_656]	2.17	0.03

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	B	317/339 (94%)	306 (96%)	10 (3%)	1 (0%)	41	31
1	X	318/339 (94%)	307 (96%)	8 (2%)	3 (1%)	17	7
All	All	635/678 (94%)	613 (96%)	18 (3%)	4 (1%)	25	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	75	LYS
1	X	76	LYS
1	X	176	ASP
1	B	273	ILE

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	B	294/306 (96%)	288 (98%)	6 (2%)	55	51
1	X	294/306 (96%)	288 (98%)	6 (2%)	55	51
All	All	588/612 (96%)	576 (98%)	12 (2%)	53	51

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	44	ARG
1	X	76	LYS
1	X	181	GLU
1	X	271	ASN
1	X	276	GLN
1	X	329	VAL
1	B	18	SER
1	B	74	VAL
1	B	95	ILE
1	B	117	ILE
1	B	266	LEU
1	B	329	VAL

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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	X	404	-	4,4,4	0.14	0	6,6,6	0.11	0
3	SO4	B	402	-	4,4,4	0.12	0	6,6,6	0.27	0
3	SO4	X	406	-	4,4,4	0.14	0	6,6,6	0.15	0
3	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.25	0
3	SO4	X	402	-	4,4,4	0.24	0	6,6,6	0.20	0
3	SO4	X	405	-	4,4,4	0.16	0	6,6,6	0.14	0
2	NIO	B	401	-	7,9,9	3.81	1 (14%)	8,11,11	0.76	0
3	SO4	B	404	-	4,4,4	0.21	0	6,6,6	0.10	0
2	NIO	X	401	-	7,9,9	1.37	1 (14%)	8,11,11	0.97	0
3	SO4	X	403	-	4,4,4	0.16	0	6,6,6	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NIO	B	401	-	-	0/0/4/4	0/1/1/1
2	NIO	X	401	-	-	0/0/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NIO	C2-C6	9.90	1.57	1.47
2	X	401	NIO	C2-C6	3.31	1.50	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	SO4	1	0
3	X	406	SO4	1	0
3	X	402	SO4	2	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	B	319/339 (94%)	1.24	63 (19%) 1 1	8, 17, 34, 57	0
1	X	319/339 (94%)	0.91	29 (9%) 9 10	5, 12, 28, 44	0
All	All	638/678 (94%)	1.07	92 (14%) 2 2	5, 15, 32, 57	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	VAL	6.5
1	B	52	SER	5.7
1	X	74	VAL	5.0
1	B	272	ASP	4.5
1	X	6	ALA	4.5
1	B	21	SER	4.4
1	B	61	THR	4.2
1	B	90	ARG	4.2
1	X	270	PHE	4.2
1	B	237	GLN	4.0
1	B	71	LEU	3.9
1	B	270	PHE	3.9
1	B	195	SER	3.9
1	B	271	ASN	3.7
1	B	7	GLY	3.6
1	B	23	GLU	3.5
1	B	264	ILE	3.5
1	X	266	LEU	3.5
1	X	91	GLY	3.4
1	B	91	GLY	3.3
1	X	61	THR	3.3
1	X	7	GLY	3.3
1	X	90	ARG	3.2
1	X	105	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	X	271	ASN	3.1
1	B	63	ASN	3.1
1	B	265	ASP	3.0
1	X	55	PHE	3.0
1	X	36	ASN	3.0
1	B	12	VAL	3.0
1	B	269	HIS	2.9
1	B	16	VAL	2.9
1	B	273	ILE	2.9
1	B	282	TRP	2.9
1	B	22	ARG	2.8
1	B	329	VAL	2.7
1	B	6	ALA	2.7
1	B	205	VAL	2.7
1	X	73	PRO	2.7
1	B	301	LEU	2.7
1	B	262	TYR	2.6
1	B	255	LEU	2.6
1	B	260	LYS	2.6
1	B	268	PRO	2.6
1	X	47	GLY	2.6
1	X	281[A]	ARG	2.5
1	B	235	HIS	2.5
1	X	71	LEU	2.5
1	B	60	ILE	2.5
1	B	45	LYS	2.5
1	B	119	ASN	2.5
1	B	99	ILE	2.5
1	B	120	THR	2.4
1	X	35	GLY	2.4
1	B	249	VAL	2.4
1	B	266	LEU	2.4
1	B	93	THR	2.4
1	B	36	ASN	2.4
1	X	240	TYR	2.4
1	B	276	GLN	2.4
1	X	145	LEU	2.4
1	X	274	LEU	2.3
1	B	116	TYR	2.3
1	X	46	LEU	2.3
1	B	106	VAL	2.3
1	X	63	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	87	GLU	2.2
1	B	145	LEU	2.2
1	B	247	ALA	2.2
1	X	106	VAL	2.2
1	X	269	HIS	2.2
1	B	244	VAL	2.2
1	B	117	ILE	2.1
1	B	315	THR	2.1
1	X	62	ASN	2.1
1	B	95	ILE	2.1
1	B	172	LEU	2.1
1	B	24	TYR	2.1
1	B	328	VAL	2.1
1	B	46	LEU	2.1
1	X	15	GLU	2.1
1	B	236	GLY	2.1
1	X	117	ILE	2.1
1	B	9	ARG	2.0
1	B	34	TRP	2.0
1	B	224	ALA	2.0
1	B	175	ILE	2.0
1	B	274	LEU	2.0
1	B	151	LYS	2.0
1	X	258	TYR	2.0
1	B	234	PHE	2.0
1	X	120	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	SO4	X	402	5/5	0.80	0.25	23,25,33,39	0
3	SO4	X	405	5/5	0.85	0.33	21,28,41,49	0
2	NIO	B	401	9/9	0.85	0.18	13,16,21,21	0
3	SO4	B	402	5/5	0.87	0.23	30,32,36,39	0
2	NIO	X	401	9/9	0.88	0.18	9,14,18,19	0
3	SO4	X	404	5/5	0.90	0.27	34,40,46,50	0
3	SO4	B	404	5/5	0.91	0.20	23,26,30,37	0
3	SO4	X	403	5/5	0.92	0.27	20,23,25,31	0
3	SO4	X	406	5/5	0.93	0.17	19,23,28,34	0
3	SO4	B	403	5/5	0.95	0.25	25,25,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.