Full wwPDB X-ray Structure Validation Report (i)

Mar 1, 2022 – 12:06 pm GMT

PDB ID	:	7BI4
Title	:	PI3KC2a core apo
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Deposited on	:	2021-01-12
Resolution	:	2.42 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

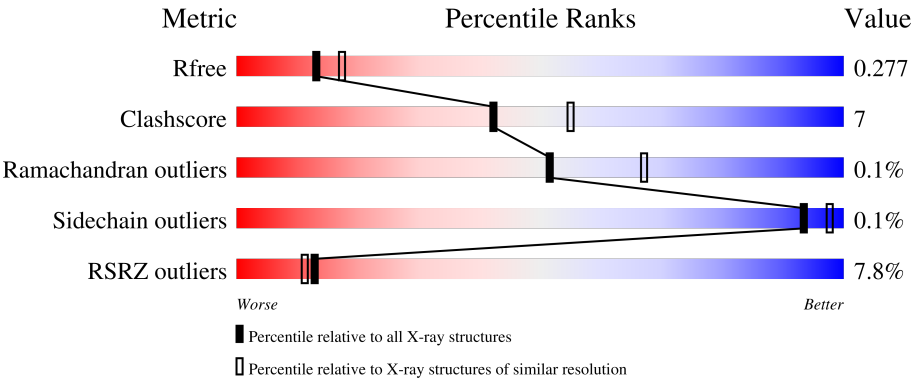
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 <=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	910	7% 77% 12% • 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6652 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.

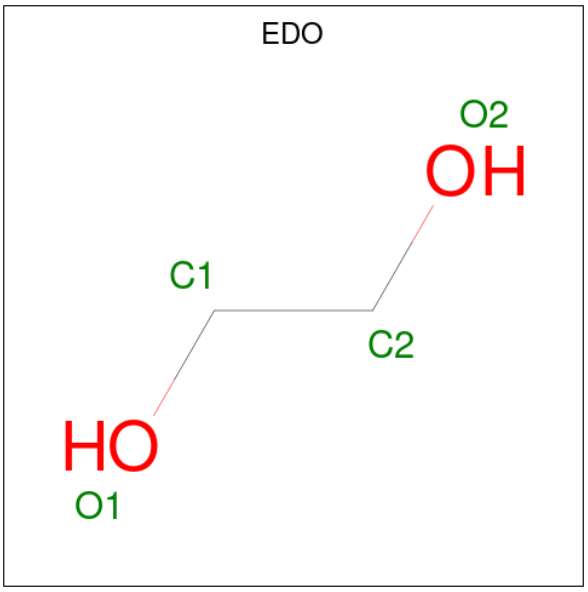
- Molecule 1 is a protein called Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit alpha,Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	822	6554	4209	1100	1204	41	0	2	0

There are 23 discrepancies between the modelled and reference sequences:

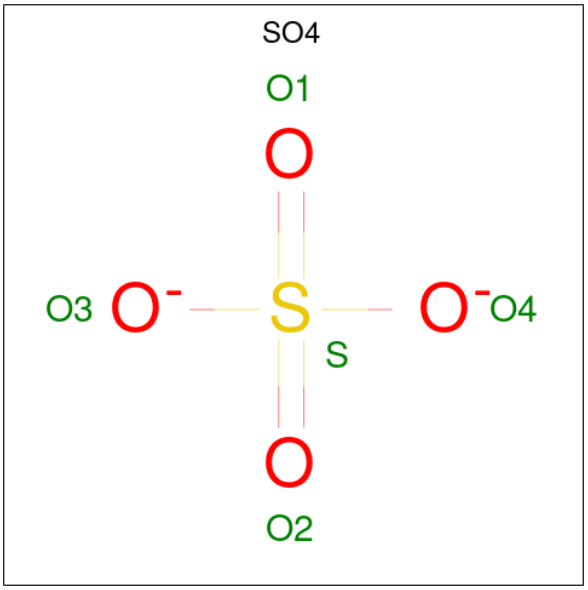
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q61194
A	2	ALA	-	expression tag	UNP Q61194
A	267	GLY	-	linker	UNP Q61194
A	268	SER	-	linker	UNP Q61194
A	269	GLY	-	linker	UNP Q61194
A	270	SER	-	linker	UNP Q61194
A	271	VAL	-	linker	UNP Q61194
A	272	MET	-	linker	UNP Q61194
A	273	THR	-	linker	UNP Q61194
A	274	ARG	-	linker	UNP Q61194
A	275	HIS	-	linker	UNP Q61194
A	276	SER	-	linker	UNP Q61194
A	277	ALA	-	linker	UNP Q61194
A	278	GLY	-	linker	UNP Q61194
A	279	ALA	-	linker	UNP Q61194
A	280	GLY	-	linker	UNP Q61194
A	281	SER	-	linker	UNP Q61194
A	282	GLY	-	linker	UNP Q61194
A	283	ALA	-	linker	UNP Q61194
A	286	GLY	ALA	conflict	UNP Q61194
A	353	ALA	PHE	engineered mutation	UNP Q61194
A	354	ALA	PHE	engineered mutation	UNP Q61194
A	427	ALA	LEU	engineered mutation	UNP Q61194

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

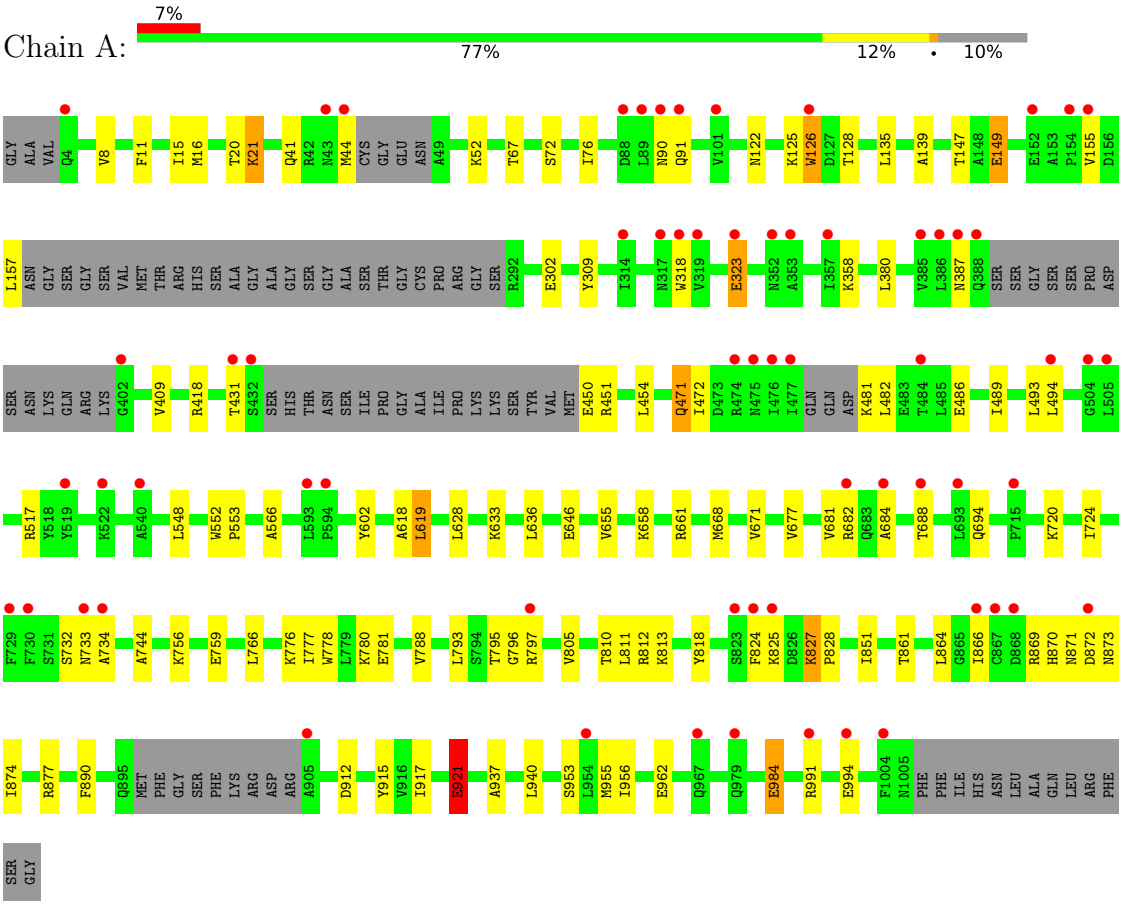
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	85	Total O 85 85	0	0

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: Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit alpha,Phosphatidylinositol 4-phosphate 3-kinase C2 domain-containing subunit alpha



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.19Å 151.57Å 56.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.06 – 2.42 45.06 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.7 (45.06-2.42) 98.7 (45.06-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.229 , 0.277 0.230 , 0.277	Depositor DCC
R_{free} test set	2100 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6652	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.42	6/6693 (0.1%)	0.74	14/9057 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	921	GLU	CD-OE2	6.46	1.32	1.25
1	A	302	GLU	CD-OE1	6.39	1.32	1.25
1	A	984	GLU	CD-OE2	5.56	1.31	1.25
1	A	149	GLU	CD-OE2	5.26	1.31	1.25
1	A	21	LYS	CE-NZ	-5.05	1.36	1.49
1	A	302	GLU	CB-CG	5.02	1.61	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	921	GLU	OE1-CD-OE2	-21.48	97.52	123.30
1	A	984	GLU	OE1-CD-OE2	-20.22	99.03	123.30
1	A	921	GLU	CG-CD-OE1	12.08	142.46	118.30
1	A	984	GLU	CG-CD-OE1	11.13	140.56	118.30
1	A	921	GLU	CG-CD-OE2	-8.85	100.61	118.30
1	A	984	GLU	CG-CD-OE2	-7.99	102.32	118.30
1	A	454	LEU	CB-CG-CD2	-7.92	97.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	450	GLU	N-CA-C	-7.53	90.67	111.00
1	A	619	LEU	CB-CG-CD2	-7.27	98.64	111.00
1	A	126	TRP	N-CA-CB	-7.01	97.99	110.60
1	A	21	LYS	CB-CG-CD	-6.81	93.88	111.60
1	A	323	GLU	CA-CB-CG	6.57	127.86	113.40
1	A	418	ARG	CB-CG-CD	5.91	126.98	111.60
1	A	471	GLN	CA-CB-CG	-5.04	102.31	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	921	GLU	Sidechain
1	A	984	GLU	Sidechain

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	6554	0	6624	91	0
2	A	8	0	12	1	0
3	A	5	0	0	0	0
4	A	85	0	0	3	0
All	All	6652	0	6636	91	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 7.

All (91) 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:658:LYS:HE2	1:A:661:ARG:HH21	1.36	0.89
1:A:52:LYS:HD3	1:A:67:THR:HG22	1.60	0.84
1:A:619:LEU:HD21	1:A:655:VAL:HG22	1.65	0.79
1:A:126:TRP:HB3	1:A:128:THR:HG23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:ARG:HB2	1:A:871:ASN:HB2	1.69	0.75
1:A:872:ASP:OD2	4:A:1201:HOH:O	2.05	0.74
1:A:16:MET:HE2	1:A:155:VAL:H	1.53	0.74
1:A:471:GLN:OE1	1:A:472:ILE:HD12	1.90	0.71
1:A:682:ARG:HH22	1:A:734:ALA:HA	1.56	0.70
1:A:471:GLN:HG3	1:A:472:ILE:N	2.07	0.68
1:A:451:ARG:O	1:A:451:ARG:HD2	1.93	0.68
1:A:962:GLU:N	1:A:962:GLU:OE1	2.30	0.64
1:A:866:ILE:HG13	1:A:869:ARG:HE	1.65	0.62
1:A:636:LEU:HD22	1:A:646:GLU:HG3	1.81	0.61
1:A:781:GLU:HG3	1:A:940:LEU:HD22	1.82	0.60
1:A:776:LYS:O	1:A:780:LYS:HG3	2.02	0.60
1:A:633:LYS:NZ	1:A:796:GLY:HA2	2.18	0.59
1:A:122:ASN:O	1:A:126:TRP:HB2	2.01	0.58
1:A:720:LYS:HD2	1:A:744:ALA:HA	1.85	0.58
1:A:866:ILE:HD11	1:A:869:ARG:HH21	1.68	0.58
1:A:126:TRP:N	1:A:126:TRP:HE3	2.01	0.58
1:A:684:ALA:HB1	1:A:688:THR:O	2.04	0.57
1:A:486:GLU:OE1	1:A:489:ILE:N	2.28	0.57
1:A:861:THR:HA	1:A:866:ILE:HG23	1.88	0.55
1:A:912:ASP:OD2	1:A:912:ASP:N	2.40	0.55
1:A:633:LYS:HE3	1:A:668:MET:HE1	1.87	0.55
1:A:323:GLU:HG2	1:A:387:ASN:HA	1.89	0.55
1:A:618:ALA:HB2	1:A:628:LEU:HD12	1.88	0.54
1:A:677:VAL:O	1:A:681:VAL:HG23	2.07	0.54
1:A:90:ASN:OD1	1:A:91:GLN:N	2.41	0.54
1:A:756:LYS:HD3	1:A:759:GLU:OE2	2.08	0.54
1:A:682:ARG:HH22	1:A:734:ALA:CA	2.21	0.53
1:A:11:PHE:O	1:A:15:ILE:HG12	2.07	0.53
1:A:126:TRP:N	1:A:126:TRP:CE3	2.77	0.53
1:A:323:GLU:HG2	1:A:387:ASN:HB3	1.91	0.53
1:A:72:SER:HB3	1:A:76:ILE:HD11	1.90	0.52
1:A:812:ARG:NH2	4:A:1201:HOH:O	2.43	0.51
1:A:818:TYR:CD2	1:A:828:PRO:HB3	2.45	0.51
1:A:451:ARG:NH1	4:A:1202:HOH:O	2.20	0.51
1:A:811:LEU:HD13	1:A:874:ILE:HG22	1.91	0.50
1:A:318:TRP:CZ2	1:A:431:THR:HG21	2.47	0.50
1:A:805:VAL:HG13	1:A:877:ARG:HH11	1.77	0.49
1:A:724:ILE:HD12	1:A:724:ILE:H	1.77	0.49
1:A:471:GLN:CG	1:A:472:ILE:N	2.76	0.49
1:A:824:PHE:O	1:A:825:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:LEU:HD23	1:A:795:THR:HG22	1.94	0.47
1:A:810:THR:HG23	1:A:813:LYS:H	1.79	0.47
1:A:658:LYS:HE2	1:A:661:ARG:NH2	2.17	0.47
1:A:125:LYS:HB3	1:A:126:TRP:CE3	2.50	0.47
1:A:471:GLN:HG3	1:A:472:ILE:H	1.77	0.47
1:A:481:LYS:HB3	1:A:482:LEU:HD12	1.96	0.46
1:A:694:GLN:OE1	1:A:724:ILE:HG22	2.16	0.46
1:A:991:ARG:NH1	1:A:994:GLU:OE2	2.48	0.46
1:A:323:GLU:HG2	1:A:387:ASN:CB	2.45	0.45
1:A:451:ARG:HD2	1:A:451:ARG:C	2.36	0.45
1:A:810:THR:HG22	1:A:813:LYS:HE3	1.97	0.45
1:A:864:LEU:HB3	1:A:890:PHE:HE1	1.82	0.45
1:A:953:SER:HA	1:A:956:ILE:HG13	1.99	0.45
1:A:493:LEU:HD23	1:A:494:LEU:HD12	1.98	0.45
1:A:827:LYS:N	1:A:828:PRO:CD	2.80	0.45
1:A:16:MET:O	1:A:20:THR:HG23	2.17	0.44
1:A:668:MET:O	1:A:671:VAL:HG22	2.17	0.44
1:A:41:GLN:O	1:A:44:MET:HG2	2.18	0.44
1:A:851:ILE:HG12	1:A:917:ILE:HG23	1.99	0.44
1:A:309:TYR:CZ	1:A:358:LYS:HE3	2.52	0.43
1:A:21:LYS:HB3	1:A:21:LYS:HE2	1.52	0.43
1:A:766:LEU:HD13	1:A:955:MET:HG3	1.99	0.43
1:A:777:ILE:HA	1:A:780:LYS:HE3	2.01	0.43
1:A:805:VAL:HB	2:A:1102:EDO:H11	2.01	0.43
1:A:126:TRP:HH2	1:A:788:VAL:HG22	1.83	0.43
1:A:517:ARG:HD2	1:A:548:LEU:HD22	2.00	0.43
1:A:824:PHE:HD2	1:A:827:LYS:HB2	1.84	0.43
1:A:732:SER:OG	1:A:733:ASN:N	2.51	0.42
1:A:861:THR:HG23	1:A:866:ILE:O	2.20	0.42
1:A:323:GLU:HG2	1:A:387:ASN:CA	2.49	0.42
1:A:915:TYR:HE2	1:A:921:GLU:HG2	1.85	0.42
1:A:869:ARG:HD3	1:A:874:ILE:HD11	2.01	0.42
1:A:8:VAL:HG13	1:A:157:LEU:HD12	2.02	0.42
1:A:778:TRP:CE2	1:A:937:ALA:HB1	2.54	0.42
1:A:147:THR:HB	1:A:149:GLU:OE1	2.20	0.41
1:A:869:ARG:NH1	1:A:873:ASN:HB3	2.35	0.41
1:A:991:ARG:HA	1:A:991:ARG:HD2	1.75	0.41
1:A:827:LYS:N	1:A:828:PRO:HD2	2.36	0.41
1:A:41:GLN:HB3	1:A:44:MET:CE	2.51	0.41
1:A:566:ALA:HB2	1:A:602:TYR:CZ	2.55	0.41
1:A:810:THR:CG2	1:A:813:LYS:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:HIS:HD2	1:A:872:ASP:H	1.69	0.41
1:A:552:TRP:HA	1:A:553:PRO:HD3	1.95	0.40
1:A:940:LEU:HD23	1:A:940:LEU:HA	1.89	0.40
1:A:380:LEU:HB2	1:A:409:VAL:HG22	2.02	0.40
1:A:135:LEU:HD12	1:A:139:ALA:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	810/910 (89%)	784 (97%)	25 (3%)	1 (0%)	51 67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	827	LYS

5.3.2 Protein sidechains (i)

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	732/800 (92%)	731 (100%)	1 (0%)	93 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	797	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	571	GLN
1	A	672	GLN
1	A	683	GLN
1	A	870	HIS
1	A	873	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 monosaccharides 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	$\#\|Z\| > 2$
3	SO4	A	1103	-	4,4,4	0.13	0	6,6,6	0.05	0
2	EDO	A	1102	-	3,3,3	0.44	0	2,2,2	0.29	0
2	EDO	A	1101	-	3,3,3	0.43	0	2,2,2	0.37	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	EDO	A	1102	-	-	0/1/1/1	-
2	EDO	A	1101	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1102	EDO	1	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, 95^{th} 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	822/910 (90%)	0.56	64 (7%)	13	11	39, 66, 112, 148	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	ILE	6.4
1	A	402	GLY	5.4
1	A	734	ALA	5.0
1	A	684	ALA	4.4
1	A	90	ASN	4.3
1	A	682	ARG	4.2
1	A	733	ASN	4.0
1	A	89	LEU	4.0
1	A	44	MET	3.9
1	A	484	THR	3.8
1	A	693	LEU	3.8
1	A	729	PHE	3.4
1	A	797	ARG	3.4
1	A	824	PHE	3.3
1	A	91	GLN	3.3
1	A	154	PRO	3.3
1	A	825	LYS	3.2
1	A	823	SER	3.1
1	A	494	LEU	3.1
1	A	323	GLU	3.1
1	A	688	THR	3.1
1	A	979	GLN	3.1
1	A	155	VAL	3.1
1	A	152	GLU	3.0
1	A	505	LEU	3.0
1	A	88	ASP	2.9
1	A	43	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	318	TRP	2.9
1	A	319	VAL	2.8
1	A	431	THR	2.8
1	A	868	ASP	2.8
1	A	314	ILE	2.8
1	A	730	PHE	2.8
1	A	474	ARG	2.8
1	A	991	ARG	2.8
1	A	905	ALA	2.7
1	A	1004	PHE	2.7
1	A	594	PRO	2.7
1	A	126	TRP	2.6
1	A	994	GLU	2.6
1	A	519	TYR	2.6
1	A	432	SER	2.5
1	A	352	ASN	2.5
1	A	475	ASN	2.5
1	A	504	GLY	2.4
1	A	4	GLN	2.4
1	A	357	ILE	2.4
1	A	867	CYS	2.4
1	A	385	VAL	2.3
1	A	522	LYS	2.3
1	A	387	ASN	2.3
1	A	593	LEU	2.3
1	A	967	GLN	2.3
1	A	866	ILE	2.3
1	A	101	VAL	2.2
1	A	954	LEU	2.2
1	A	388	GLN	2.1
1	A	477	ILE	2.1
1	A	715	PRO	2.1
1	A	386	LEU	2.1
1	A	353	ALA	2.0
1	A	872	ASP	2.0
1	A	540	ALA	2.0
1	A	317	ASN	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 monosaccharides 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, 95^{th} 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	EDO	A	1101	4/4	0.84	0.41	68,70,77,82	0
2	EDO	A	1102	4/4	0.84	0.53	95,96,105,111	0
3	SO4	A	1103	5/5	0.85	0.37	117,118,126,128	0

6.5 Other polymers (i)

There are no such residues in this entry.