



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 09:08 PM EDT

PDB ID : 7KYS  
Title : Crystal structure of human BCCIP beta (Native2)  
Authors : Choi, W.S.; Liu, B.; Shen, Z.; Yang, W.  
Deposited on : 2020-12-08  
Resolution : 2.20 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](mailto: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>.

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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 : 2.35.1  
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) : 2.35.1

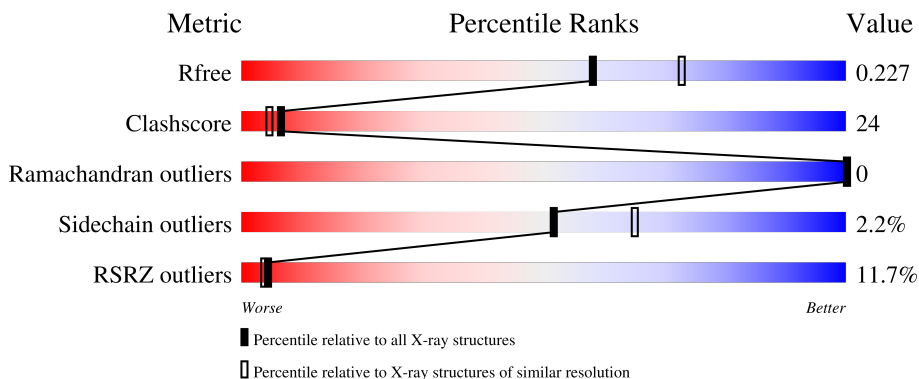
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	256	
1	B	256	
1	C	256	

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
2	EDO	A	401	-	-	X	-
2	EDO	A	402	-	-	X	-
2	EDO	A	403	-	-	X	-
2	EDO	A	405	-	-	X	-
2	EDO	A	406	-	-	X	-
2	EDO	C	402	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5767 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 BRCA2 and CDKN1A-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	230	1836	1182	295	346	13	0	0	0
1	B	230	1821	1172	295	341	13	0	2	0
1	C	230	1833	1184	294	343	12	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	HIS	-	expression tag	UNP Q9P287
A	60	HIS	-	expression tag	UNP Q9P287
B	59	HIS	-	expression tag	UNP Q9P287
B	60	HIS	-	expression tag	UNP Q9P287
C	59	HIS	-	expression tag	UNP Q9P287
C	60	HIS	-	expression tag	UNP Q9P287

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	C O	0	0
			7	4 3		

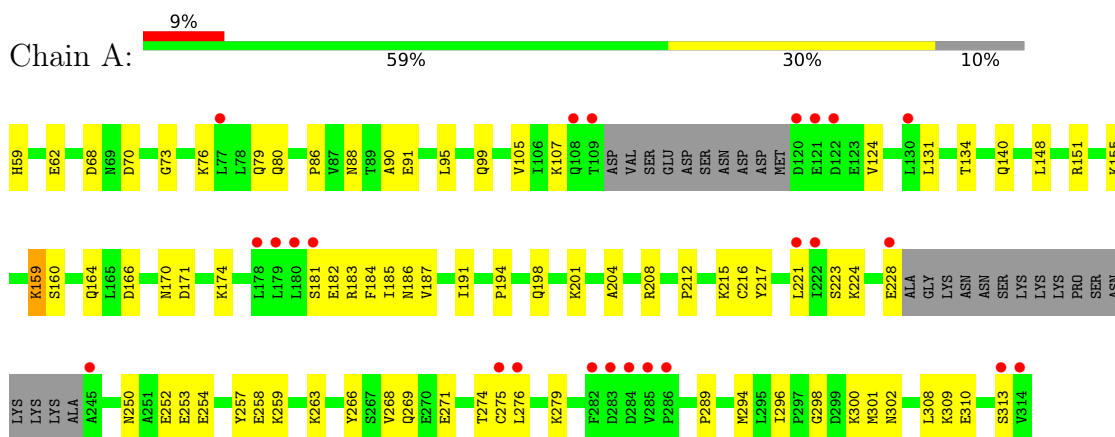
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total	O	0	0
			120	120		
4	B	80	Total	O	0	0
			80	80		
4	C	38	Total	O	0	0
			38	38		

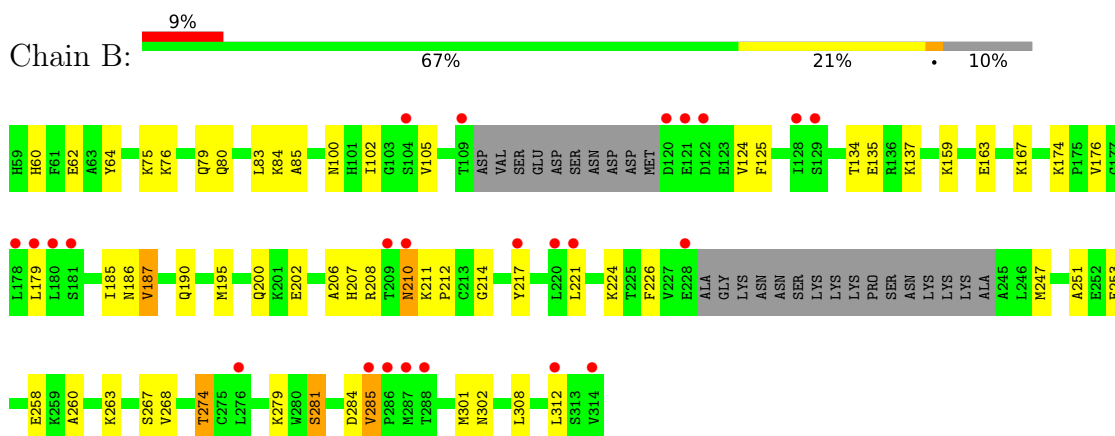
### 3 Residue-property plots [i](#)

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.

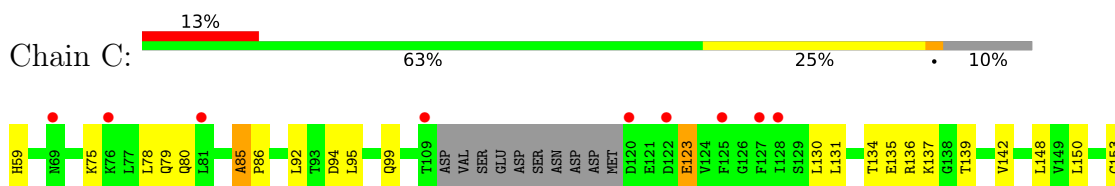
- Molecule 1: BRCA2 and CDKN1A-interacting protein

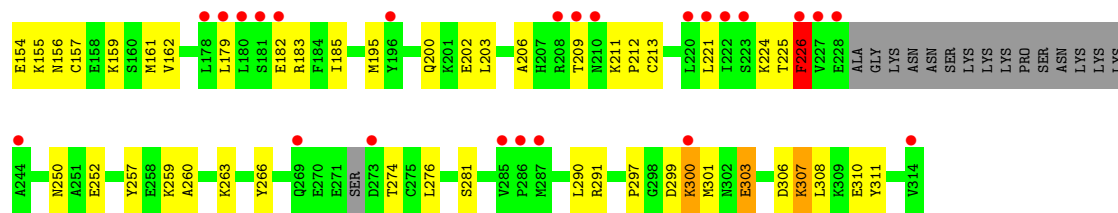


- Molecule 1: BRCA2 and CDKN1A-interacting protein



- Molecule 1: BRCA2 and CDKN1A-interacting protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.04Å 67.00Å 99.53Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	29.73 – 2.20 29.73 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.73-2.20) 98.8 (29.73-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.205 , 0.227 0.205 , 0.227	Depositor DCC
$R_{free}$ test set	1023 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.8	Xtrriage
Anisotropy	0.329	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5767	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, PEG

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	0/1869	0.61	0/2521
1	B	0.51	2/1853 (0.1%)	0.70	3/2503 (0.1%)
1	C	0.48	4/1865 (0.2%)	0.70	5/2517 (0.2%)
All	All	0.47	6/5587 (0.1%)	0.67	8/7541 (0.1%)

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	C	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	307	LYS	CE-NZ	6.18	1.64	1.49
1	C	307	LYS	CD-CE	5.95	1.66	1.51
1	B	208	ARG	CZ-NH1	5.85	1.40	1.33
1	B	208	ARG	CD-NE	5.64	1.56	1.46
1	C	86	PRO	N-CD	5.35	1.55	1.47
1	C	303	GLU	CD-OE2	5.10	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	ARG	CA-CB-CG	9.37	134.01	113.40
1	C	300	LYS	CA-CB-CG	7.37	129.62	113.40
1	C	300	LYS	CB-CG-CD	7.06	129.95	111.60
1	B	85	ALA	C-N-CD	6.03	141.05	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	ASN	C-N-CA	5.94	136.54	121.70
1	C	85	ALA	C-N-CD	5.50	139.94	128.40
1	C	307	LYS	CD-CE-NZ	5.34	123.99	111.70
1	C	226	PHE	CB-CG-CD2	-5.07	117.25	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	226	PHE	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	1836	0	1827	99	3
1	B	1821	0	1795	57	3
1	C	1833	0	1815	89	2
2	A	24	0	36	28	0
2	C	8	0	12	10	0
3	B	7	0	10	1	0
4	A	120	0	0	74	1
4	B	80	0	0	33	1
4	C	38	0	0	20	0
All	All	5767	0	5495	263	5

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 24.

All (263) 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:C:75:LYS:HZ3	1:C:79:GLN:NE2	1.07	1.51
1:C:75:LYS:NZ	1:C:79:GLN:NE2	1.67	1.37
1:C:179:LEU:HB3	1:C:221[B]:LEU:CD2	1.51	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:LYS:HE3	2:C:402:EDO:C1	1.68	1.23
1:C:203:LEU:HD21	4:C:534:HOH:O	1.36	1.19
1:A:88:ASN:OD1	4:A:501:HOH:O	1.63	1.17
1:A:134:THR:HG23	4:A:556:HOH:O	1.41	1.17
1:C:307:LYS:CE	2:C:402:EDO:H11	1.74	1.17
1:A:271:GLU:HA	4:A:551:HOH:O	1.41	1.17
1:B:84:LYS:HE2	1:B:84:LYS:HA	1.18	1.15
2:A:401:EDO:C1	2:A:402:EDO:H21	1.76	1.15
1:A:224:LYS:HD2	4:A:613:HOH:O	1.46	1.14
2:A:406:EDO:H21	4:A:575:HOH:O	1.46	1.13
1:B:134:THR:OG1	4:B:502:HOH:O	1.69	1.11
1:C:276:LEU:HB2	4:C:503:HOH:O	1.49	1.10
1:A:140:GLN:HG3	4:A:532:HOH:O	1.53	1.09
2:A:401:EDO:H11	2:A:402:EDO:C2	1.82	1.09
1:B:179:LEU:HD22	4:B:577:HOH:O	1.52	1.08
1:B:251:ALA:N	4:B:501:HOH:O	1.68	1.07
2:A:406:EDO:H11	4:A:504:HOH:O	1.55	1.06
1:C:136:ARG:O	1:C:139[B]:THR:HG22	1.53	1.06
1:C:179:LEU:HB3	1:C:221[B]:LEU:HD23	1.30	1.06
1:A:95:LEU:HG	4:A:554:HOH:O	1.57	1.05
1:C:179:LEU:HB3	1:C:221[B]:LEU:HD21	1.22	1.05
1:A:131:LEU:HD21	4:A:554:HOH:O	1.58	1.02
1:A:90:ALA:N	4:A:501:HOH:O	1.90	1.02
1:A:76:LYS:HE3	4:A:580:HOH:O	1.59	1.01
2:A:406:EDO:O1	4:A:502:HOH:O	1.78	1.01
1:C:307:LYS:CE	2:C:402:EDO:C1	2.35	1.00
2:A:403:EDO:H11	4:A:552:HOH:O	1.63	0.99
1:A:252:GLU:OE1	4:A:503:HOH:O	1.81	0.98
1:C:195:MET:HE1	4:C:526:HOH:O	1.61	0.98
1:C:134:THR:HG23	4:C:525:HOH:O	1.63	0.98
1:B:137:LYS:HE3	4:B:559:HOH:O	1.61	0.97
1:C:179:LEU:CB	1:C:221[B]:LEU:HD21	1.95	0.97
1:B:187:VAL:HG22	4:B:556:HOH:O	1.64	0.97
1:A:221:LEU:HD23	4:A:550:HOH:O	1.66	0.96
1:A:254:GLU:CG	4:A:506:HOH:O	2.16	0.94
2:A:406:EDO:C2	4:A:575:HOH:O	2.04	0.94
1:C:75:LYS:NZ	1:C:79:GLN:HE22	1.46	0.94
1:C:75:LYS:NZ	1:C:79:GLN:HE21	1.54	0.94
1:C:179:LEU:CB	1:C:221[B]:LEU:CD2	2.44	0.93
1:C:134:THR:HG22	4:C:516:HOH:O	1.69	0.93
2:A:401:EDO:H11	2:A:402:EDO:H21	0.93	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:403:EDO:C2	4:A:552:HOH:O	2.19	0.91
1:A:140:GLN:HB3	4:A:561:HOH:O	1.71	0.91
1:B:207:HIS:HB2	4:B:509:HOH:O	1.72	0.90
1:A:271:GLU:HG2	1:A:289:PRO:HG3	1.52	0.89
1:A:276:LEU:HA	4:A:588:HOH:O	1.70	0.89
2:A:406:EDO:C1	4:A:504:HOH:O	2.15	0.88
1:A:254:GLU:HG3	4:A:506:HOH:O	1.70	0.88
1:C:179:LEU:HD23	1:C:221[B]:LEU:HD21	1.58	0.85
4:A:514:HOH:O	1:B:258:GLU:HG2	1.76	0.85
1:B:210:ASN:O	4:B:503:HOH:O	1.95	0.85
1:A:187:VAL:HG23	4:A:528:HOH:O	1.74	0.85
1:C:130:LEU:HB3	4:C:534:HOH:O	1.77	0.84
2:A:403:EDO:H22	4:A:552:HOH:O	1.76	0.84
1:C:213:CYS:HB2	4:C:506:HOH:O	1.75	0.84
1:C:139[B]:THR:CG2	1:C:142:VAL:HG13	2.09	0.83
1:B:80:GLN:HB3	4:B:538:HOH:O	1.77	0.82
1:B:84:LYS:HE2	1:B:84:LYS:CA	2.04	0.82
1:C:307:LYS:HE3	2:C:402:EDO:H11	0.86	0.82
1:A:198:GLN:HB2	2:A:404:EDO:H21	1.62	0.82
1:B:221:LEU:HD21	1:B:253:GLU:HG2	1.63	0.81
1:A:174:LYS:HE3	4:A:604:HOH:O	1.81	0.80
1:C:179:LEU:CD2	1:C:221[B]:LEU:HD21	2.13	0.78
2:A:406:EDO:O2	4:A:504:HOH:O	2.02	0.78
1:C:183:ARG:NH1	4:C:502:HOH:O	2.17	0.77
1:A:174:LYS:CE	4:A:604:HOH:O	2.31	0.77
1:A:221:LEU:CD2	4:A:550:HOH:O	2.27	0.77
1:C:75:LYS:HZ1	1:C:79:GLN:HE21	1.30	0.77
1:C:307:LYS:CE	2:C:402:EDO:H12	2.15	0.77
1:A:204:ALA:HB3	4:A:511:HOH:O	1.85	0.76
2:A:403:EDO:C1	4:A:552:HOH:O	2.21	0.76
1:B:100:ASN:O	4:B:504:HOH:O	2.04	0.75
1:B:301:MET:HE2	4:B:511:HOH:O	1.85	0.75
1:C:179:LEU:CB	1:C:221[B]:LEU:HD23	2.15	0.74
1:C:259:LYS:HD2	1:C:300:LYS:HD2	1.69	0.74
1:A:212:PRO:HD3	4:A:522:HOH:O	1.87	0.73
1:A:91:GLU:N	4:A:501:HOH:O	2.11	0.73
1:B:301:MET:HE1	4:B:577:HOH:O	1.88	0.73
1:A:59:HIS:N	4:A:512:HOH:O	2.23	0.72
1:A:187:VAL:CG2	4:A:528:HOH:O	2.33	0.72
1:B:224:LYS:HD3	4:B:538:HOH:O	1.89	0.72
1:B:137:LYS:CE	4:B:559:HOH:O	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:NH1	4:A:510:HOH:O	2.20	0.71
1:C:75:LYS:HZ1	1:C:79:GLN:NE2	1.81	0.71
1:C:75:LYS:HZ2	1:C:79:GLN:HE22	1.38	0.71
1:B:75:LYS:O	1:B:79:GLN:HG2	1.91	0.70
1:B:302:ASN:OD1	4:B:505:HOH:O	2.09	0.70
1:B:84:LYS:HA	1:B:84:LYS:CE	2.08	0.70
1:C:59:HIS:CB	4:C:528:HOH:O	2.41	0.69
1:B:163[B]:GLU:OE1	4:B:506:HOH:O	2.11	0.68
1:B:187:VAL:CG2	4:B:556:HOH:O	2.27	0.68
1:A:271:GLU:CA	4:A:551:HOH:O	2.17	0.68
1:C:200:GLN:HB2	2:C:401:EDO:H11	1.77	0.66
1:B:214:GLY:CA	4:B:509:HOH:O	2.42	0.66
1:C:259:LYS:HD2	1:C:300:LYS:CD	2.26	0.66
1:B:76:LYS:HA	1:B:79:GLN:HG3	1.78	0.66
1:B:200:GLN:HG3	3:B:401:PEG:H11	1.77	0.66
1:A:313:SER:N	4:A:516:HOH:O	2.28	0.66
1:C:139[B]:THR:HG21	1:C:142:VAL:HG13	1.78	0.66
1:A:105:VAL:HG13	1:A:124:VAL:HG13	1.77	0.66
1:A:298:GLY:O	4:A:505:HOH:O	2.14	0.65
1:A:216:CYS:O	4:A:507:HOH:O	2.15	0.64
1:A:258:GLU:OE1	4:A:506:HOH:O	2.14	0.64
1:A:90:ALA:CA	4:A:501:HOH:O	2.37	0.64
1:A:212:PRO:CD	4:A:522:HOH:O	2.45	0.64
1:B:284:ASP:N	4:B:508:HOH:O	2.22	0.64
1:A:257:TYR:CE1	1:A:263:LYS:HD3	2.32	0.64
1:C:139[B]:THR:HG23	1:C:142:VAL:HG13	1.80	0.64
1:B:260:ALA:HB3	1:B:263:LYS:HE2	1.80	0.63
1:B:105:VAL:HG13	1:B:124:VAL:HG13	1.80	0.63
2:A:401:EDO:H21	4:A:603:HOH:O	1.97	0.63
1:B:224:LYS:NZ	4:B:507:HOH:O	2.16	0.63
1:C:307:LYS:NZ	2:C:402:EDO:C1	2.61	0.63
1:C:139[B]:THR:CG2	1:C:142:VAL:CG1	2.78	0.62
1:B:176:VAL:HB	4:B:502:HOH:O	2.00	0.62
1:C:213:CYS:N	4:C:506:HOH:O	2.30	0.62
1:A:279:LYS:NZ	4:A:519:HOH:O	2.29	0.62
1:B:176:VAL:N	4:B:502:HOH:O	2.24	0.62
1:C:260:ALA:HB3	1:C:263:LYS:HE2	1.81	0.62
1:A:198:GLN:HB3	4:A:544:HOH:O	2.00	0.62
1:C:182:GLU:OE1	4:C:501:HOH:O	2.16	0.61
1:B:214:GLY:HA2	4:B:509:HOH:O	1.99	0.61
1:C:307:LYS:NZ	2:C:402:EDO:H12	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:406:EDO:H21	4:A:542:HOH:O	2.02	0.60
1:A:250:ASN:HA	4:A:541:HOH:O	2.02	0.60
1:B:308:LEU:O	1:B:312:LEU:HB2	2.03	0.58
1:A:274:THR:HG23	1:A:276:LEU:HD22	1.84	0.58
1:B:185:ILE:HD11	1:B:274:THR:HB	1.86	0.58
1:A:198:GLN:CG	4:A:544:HOH:O	2.52	0.57
1:B:285:VAL:HG23	4:B:558:HOH:O	2.04	0.57
1:A:259:LYS:HE3	1:A:300:LYS:HD2	1.86	0.57
1:B:190:GLN:HA	1:B:312:LEU:HD12	1.85	0.57
1:C:159:LYS:HA	1:C:162:VAL:HG12	1.86	0.57
1:C:209:THR:OG1	1:C:211:LYS:HG2	2.05	0.57
1:A:276:LEU:CA	4:A:588:HOH:O	2.42	0.56
1:A:221:LEU:HG	4:A:550:HOH:O	2.04	0.56
1:B:179:LEU:CD2	4:B:577:HOH:O	2.27	0.56
1:C:206:ALA:HB1	1:C:211:LYS:HB2	1.88	0.56
1:A:80:GLN:NE2	1:A:275:CYS:H	2.04	0.56
1:A:254:GLU:HG2	4:A:506:HOH:O	1.91	0.55
1:C:153:CYS:O	1:C:157:CYS:HB2	2.07	0.54
1:B:224:LYS:CE	4:B:538:HOH:O	2.55	0.54
1:A:185:ILE:CG1	1:A:274:THR:HG21	2.38	0.54
1:A:294:MET:HG3	1:A:296:ILE:HD11	1.88	0.54
1:C:299:ASP:OD1	1:C:299:ASP:N	2.41	0.53
1:A:86:PRO:HD2	1:A:148:LEU:HD13	1.90	0.53
1:A:99:GLN:NE2	4:A:523:HOH:O	2.34	0.53
1:A:159:LYS:HG3	4:A:617:HOH:O	2.08	0.53
1:B:76:LYS:O	1:B:79:GLN:HB2	2.08	0.53
1:B:125:PHE:CB	4:B:556:HOH:O	2.56	0.53
1:B:224:LYS:CD	4:B:538:HOH:O	2.52	0.53
1:C:139[A]:THR:O	1:C:142:VAL:HG22	2.09	0.53
1:C:135:GLU:OE2	1:C:212:PRO:HB2	2.10	0.52
1:B:100:ASN:N	4:B:504:HOH:O	2.35	0.52
1:A:171:ASP:HB3	4:A:547:HOH:O	2.09	0.52
1:C:150:LEU:O	1:C:154:GLU:HG3	2.10	0.52
1:C:303:GLU:HA	1:C:306:ASP:OD2	2.10	0.52
1:A:266:TYR:CE1	2:A:405:EDO:H21	2.45	0.52
1:C:134:THR:CG2	4:C:525:HOH:O	2.38	0.52
1:A:184:PHE:O	1:A:187:VAL:HG22	2.10	0.51
1:A:68:ASP:OD2	1:C:159:LYS:HE3	2.09	0.51
1:C:179:LEU:CG	1:C:221[B]:LEU:HD21	2.40	0.51
1:A:263:LYS:NZ	4:A:531:HOH:O	2.43	0.51
1:B:80:GLN:OE1	1:B:274:THR:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LYS:HA	1:C:291:ARG:HE	1.75	0.51
1:A:186:ASN:N	1:A:186:ASN:OD1	2.44	0.51
1:C:297:PRO:HB2	1:C:299:ASP:OD1	2.11	0.51
1:A:228:GLU:CG	1:A:228:GLU:O	2.58	0.51
1:B:226:PHE:O	1:B:247:MET:HB2	2.10	0.51
1:B:195:MET:HE1	4:B:525:HOH:O	2.11	0.51
1:B:176:VAL:CB	4:B:502:HOH:O	2.58	0.51
1:A:79:GLN:HG2	4:A:571:HOH:O	2.11	0.50
1:B:62:GLU:HG2	1:B:64:TYR:CZ	2.47	0.50
1:A:228:GLU:O	1:A:228:GLU:HG3	2.11	0.50
1:A:310:GLU:HB2	4:A:596:HOH:O	2.11	0.49
1:C:154:GLU:HG2	1:C:162:VAL:HG21	1.93	0.49
1:C:80:GLN:NE2	1:C:274:THR:CB	2.76	0.49
1:A:185:ILE:HG12	1:A:274:THR:HG21	1.93	0.49
1:A:221:LEU:HD22	1:A:223:SER:OG	2.12	0.49
2:A:405:EDO:O1	4:A:509:HOH:O	2.19	0.49
1:B:76:LYS:HA	1:B:79:GLN:CG	2.42	0.49
2:A:406:EDO:H22	4:A:575:HOH:O	1.91	0.49
1:A:224:LYS:NZ	4:A:521:HOH:O	2.31	0.49
1:A:302:ASN:ND2	4:A:534:HOH:O	2.44	0.48
1:C:250:ASN:ND2	4:C:512:HOH:O	2.43	0.48
1:A:266:TYR:HE1	2:A:405:EDO:H21	1.78	0.48
1:C:307:LYS:HZ1	2:C:402:EDO:H12	1.79	0.48
1:C:137:LYS:NZ	4:C:509:HOH:O	2.38	0.48
1:C:310:GLU:HG3	1:C:311:TYR:HD1	1.78	0.48
1:A:90:ALA:HB3	4:A:501:HOH:O	2.13	0.48
1:C:155:LYS:HG3	1:C:156:ASN:OD1	2.14	0.48
1:C:139[B]:THR:O	1:C:142:VAL:HG22	2.14	0.47
1:C:257:TYR:CE1	1:C:263:LYS:HD3	2.49	0.47
1:B:206:ALA:HB1	1:B:211:LYS:HB2	1.96	0.47
1:C:211:LYS:HB3	4:C:506:HOH:O	2.13	0.47
1:B:212:PRO:HB2	4:B:567:HOH:O	2.14	0.47
1:C:225:THR:OG1	1:C:290:LEU:HD12	2.15	0.47
1:B:190:GLN:HA	1:B:312:LEU:CD1	2.45	0.47
1:C:259:LYS:HB3	1:C:300:LYS:HG3	1.96	0.47
1:A:174:LYS:HA	1:A:217:TYR:CD1	2.50	0.47
1:A:201:LYS:O	4:A:511:HOH:O	2.21	0.46
1:A:257:TYR:CZ	1:A:263:LYS:HD3	2.51	0.46
1:A:252:GLU:HB2	1:A:308:LEU:HD21	1.97	0.46
1:B:102:ILE:HD13	1:B:202:GLU:HB3	1.97	0.46
1:C:85:ALA:HB1	1:C:148:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLU:OE1	1:C:136:ARG:NE	2.49	0.46
1:A:215:LYS:CE	4:A:522:HOH:O	2.64	0.46
1:B:159:LYS:O	1:B:163[A]:GLU:HG2	2.16	0.46
1:B:174:LYS:HG2	1:B:217:TYR:CD2	2.51	0.45
1:B:83:LEU:O	1:B:84:LYS:HE2	2.16	0.45
1:A:181:SER:C	1:A:182:GLU:HG2	2.36	0.45
1:C:99:GLN:HB2	4:C:513:HOH:O	2.17	0.45
1:C:185:ILE:HD12	1:C:185:ILE:H	1.80	0.45
1:A:140:GLN:CB	4:A:561:HOH:O	2.47	0.45
1:A:191:ILE:O	1:A:194:PRO:HD2	2.16	0.45
1:C:78:LEU:HD13	1:C:92:LEU:HD23	1.97	0.45
1:A:151:ARG:HD3	1:A:155:LYS:HE3	1.99	0.45
1:C:137:LYS:CE	4:C:516:HOH:O	2.65	0.45
1:A:70:ASP:OD1	1:A:107:LYS:HE3	2.17	0.45
1:A:250:ASN:HB2	1:A:253:GLU:HG3	1.99	0.45
1:A:73:GLY:HA3	1:A:124:VAL:HB	1.99	0.44
2:A:402:EDO:H12	4:A:502:HOH:O	2.17	0.44
1:A:90:ALA:CB	4:A:501:HOH:O	2.64	0.44
1:A:268:VAL:HG12	2:A:405:EDO:H12	1.98	0.44
1:C:310:GLU:HG3	1:C:311:TYR:CD1	2.53	0.44
1:A:174:LYS:HE2	4:A:604:HOH:O	2.06	0.44
1:A:309:LYS:O	1:A:313:SER:HB2	2.18	0.44
1:A:166:ASP:OD1	1:A:170:ASN:ND2	2.51	0.44
1:B:167:LYS:NZ	4:B:506:HOH:O	2.41	0.43
1:A:160:SER:O	1:A:164:GLN:HG2	2.17	0.43
1:A:212:PRO:N	4:A:522:HOH:O	2.50	0.43
1:C:156:ASN:ND2	1:C:266:TYR:HA	2.33	0.43
1:A:263:LYS:NZ	4:A:543:HOH:O	2.50	0.43
2:A:406:EDO:C2	4:A:542:HOH:O	2.62	0.43
1:A:276:LEU:H	1:A:276:LEU:HD23	1.84	0.42
1:A:301:MET:CB	2:A:406:EDO:H12	2.49	0.42
1:C:157:CYS:HB3	1:C:161:MET:HE2	2.00	0.42
1:B:124:VAL:HG23	4:B:546:HOH:O	2.18	0.42
1:C:130:LEU:CB	4:C:534:HOH:O	2.52	0.42
1:C:80:GLN:HE22	1:C:274:THR:CB	2.33	0.42
1:C:301:MET:HB3	2:C:401:EDO:O2	2.20	0.42
1:A:268:VAL:CG1	2:A:405:EDO:H12	2.49	0.42
1:C:211:LYS:CB	4:C:506:HOH:O	2.68	0.42
1:C:131:LEU:HD23	1:C:131:LEU:HA	1.94	0.42
1:A:159:LYS:HE2	1:A:159:LYS:HB3	1.58	0.42
1:C:136:ARG:O	1:C:142:VAL:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:GLU:HB2	1:C:308:LEU:CD2	2.50	0.41
1:C:135:GLU:HG2	1:C:136:ARG:HD3	2.01	0.41
1:C:179:LEU:O	1:C:221[A]:LEU:HD12	2.19	0.41
1:A:266:TYR:OH	2:A:405:EDO:H21	2.21	0.41
1:A:221:LEU:CG	4:A:550:HOH:O	2.58	0.41
1:C:226:PHE:CD1	1:C:226:PHE:N	2.89	0.41
1:C:252:GLU:HB2	1:C:308:LEU:HD21	2.03	0.41
1:C:123:GLU:CD	4:C:510:HOH:O	2.58	0.41
1:A:301:MET:HG3	2:A:406:EDO:H12	2.03	0.41
1:A:183:ARG:HD2	1:A:187:VAL:HG21	2.03	0.41
1:A:252:GLU:HB3	4:A:503:HOH:O	2.21	0.41
1:A:259:LYS:HD2	1:A:259:LYS:HA	1.75	0.40
1:A:269:GLN:OE1	1:A:269:GLN:N	2.50	0.40
1:A:198:GLN:OE1	2:A:404:EDO:C2	2.69	0.40

All (5) 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:A:615:HOH:O	4:B:572:HOH:O[2_656]	0.25	1.95
1:B:60:HIS:NE2	1:C:281:SER:OG[2_545]	1.88	0.32
1:A:208:ARG:NH1	1:B:135:GLU:O[2_556]	2.12	0.08
1:A:62:GLU:OE2	1:B:281[B]:SER:OG[1_565]	2.15	0.05
1:A:279:LYS:NZ	1:C:202:GLU:OE2[2_655]	2.15	0.05

## 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	224/256 (88%)	223 (100%)	1 (0%)	0	100 100
1	B	226/256 (88%)	224 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	224/256 (88%)	223 (100%)	1 (0%)	0	100	100
All	All	674/768 (88%)	670 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	204/233 (88%)	203 (100%)	1 (0%)	88	94
1	B	198/233 (85%)	189 (96%)	9 (4%)	27	34
1	C	200/233 (86%)	196 (98%)	4 (2%)	55	69
All	All	602/699 (86%)	588 (98%)	14 (2%)	52	63

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	LYS
1	B	186	ASN
1	B	187	VAL
1	B	267	SER
1	B	268	VAL
1	B	274	THR
1	B	279	LYS
1	B	281[A]	SER
1	B	281[B]	SER
1	B	285	VAL
1	C	94	ASP
1	C	95	LEU
1	C	123	GLU
1	C	226	PHE

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	80	GLN
1	A	99	GLN
1	C	79	GLN
1	C	80	GLN
1	C	100	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](#)

9 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	EDO	A	401	-	3,3,3	0.67	0	2,2,2	0.79	0
2	EDO	A	406	-	3,3,3	0.67	0	2,2,2	0.78	0
3	PEG	B	401	-	6,6,6	0.68	0	5,5,5	0.63	0
2	EDO	A	403	-	3,3,3	0.67	0	2,2,2	0.78	0
2	EDO	C	402	-	3,3,3	0.68	0	2,2,2	0.77	0
2	EDO	A	404	-	3,3,3	0.66	0	2,2,2	0.82	0
2	EDO	A	402	-	3,3,3	0.67	0	2,2,2	0.78	0
2	EDO	C	401	-	3,3,3	0.66	0	2,2,2	0.80	0
2	EDO	A	405	-	3,3,3	0.68	0	2,2,2	0.78	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	401	-	-	1/1/1/1	-
2	EDO	A	406	-	-	1/1/1/1	-
3	PEG	B	401	-	-	1/4/4/4	-
2	EDO	A	403	-	-	1/1/1/1	-
2	EDO	C	402	-	-	1/1/1/1	-
2	EDO	A	404	-	-	1/1/1/1	-
2	EDO	A	402	-	-	1/1/1/1	-
2	EDO	C	401	-	-	1/1/1/1	-
2	EDO	A	405	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	EDO	O1-C1-C2-O2
2	A	402	EDO	O1-C1-C2-O2
2	A	403	EDO	O1-C1-C2-O2
2	C	402	EDO	O1-C1-C2-O2
2	A	404	EDO	O1-C1-C2-O2
2	C	401	EDO	O1-C1-C2-O2
2	A	406	EDO	O1-C1-C2-O2
2	A	405	EDO	O1-C1-C2-O2
3	B	401	PEG	O2-C3-C4-O4

There are no ring outliers.

9 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	EDO	4	0
2	A	406	EDO	11	0
3	B	401	PEG	1	0
2	A	403	EDO	4	0
2	C	402	EDO	8	0
2	A	404	EDO	2	0
2	A	402	EDO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	EDO	2	0
2	A	405	EDO	6	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	230/256 (89%)	0.53	24 (10%) 6 5	41, 58, 113, 178	0
1	B	230/256 (89%)	0.46	24 (10%) 6 5	43, 64, 109, 138	0
1	C	230/256 (89%)	0.85	33 (14%) 2 2	56, 83, 113, 140	0
All	All	690/768 (89%)	0.61	81 (11%) 4 4	41, 68, 113, 178	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	285	VAL	8.5
1	B	314	VAL	8.1
1	C	314	VAL	7.7
1	A	314	VAL	7.5
1	C	221[A]	LEU	6.4
1	C	181	SER	6.0
1	C	244	ALA	5.9
1	A	121	GLU	5.6
1	C	180	LEU	5.2
1	C	120	ASP	5.0
1	A	275	CYS	5.0
1	B	179	LEU	5.0
1	C	128	ILE	4.9
1	C	179	LEU	4.7
1	A	282	PHE	4.6
1	B	180	LEU	4.6
1	A	286	PRO	4.4
1	C	286	PRO	4.3
1	C	127	PHE	4.2
1	B	109	THR	4.1
1	B	128	ILE	4.1
1	B	221	LEU	4.1
1	A	120	ASP	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	285	VAL	3.6
1	C	222	ILE	3.6
1	B	217	TYR	3.6
1	A	179	LEU	3.5
1	B	287	MET	3.4
1	A	180	LEU	3.4
1	A	109	THR	3.3
1	C	178	LEU	3.3
1	A	245	ALA	3.3
1	C	208	ARG	3.3
1	A	221	LEU	3.2
1	B	121	GLU	3.2
1	A	283	ASP	3.1
1	B	209	THR	3.1
1	B	286	PRO	2.9
1	A	108	GLN	2.9
1	C	220	LEU	2.9
1	C	223	SER	2.9
1	C	81	LEU	2.9
1	B	181	SER	2.8
1	C	209	THR	2.8
1	C	273	ASP	2.8
1	B	122	ASP	2.8
1	B	210	ASN	2.8
1	B	120	ASP	2.8
1	B	288	THR	2.8
1	A	181	SER	2.8
1	C	227	VAL	2.7
1	A	77	LEU	2.7
1	B	129	SER	2.7
1	B	220	LEU	2.7
1	B	285	VAL	2.7
1	C	228	GLU	2.6
1	A	222	ILE	2.6
1	C	287	MET	2.5
1	B	178	LEU	2.5
1	B	228	GLU	2.5
1	C	69	ASN	2.5
1	B	276	LEU	2.5
1	C	76	LYS	2.4
1	A	122	ASP	2.4
1	C	182	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	210	ASN	2.4
1	A	228	GLU	2.3
1	C	122	ASP	2.3
1	B	104	SER	2.3
1	A	130	LEU	2.2
1	A	178	LEU	2.2
1	A	276	LEU	2.2
1	C	226	PHE	2.2
1	C	196	TYR	2.2
1	C	300	LYS	2.1
1	C	269	GLN	2.1
1	B	312	LEU	2.1
1	C	109	THR	2.1
1	A	284	ASP	2.1
1	A	313	SER	2.1
1	C	125	PHE	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	EDO	C	402	4/4	0.65	0.33	83,89,90,91	0
3	PEG	B	401	7/7	0.74	0.18	76,79,83,87	0
2	EDO	A	403	4/4	0.78	0.23	75,76,77,80	0
2	EDO	A	402	4/4	0.85	0.19	64,66,70,71	0
2	EDO	C	401	4/4	0.85	0.27	80,81,82,89	0
2	EDO	A	406	4/4	0.88	0.18	105,105,111,121	0
2	EDO	A	405	4/4	0.89	0.22	62,63,65,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	A	401	4/4	0.90	0.10	73,74,74,79	0
2	EDO	A	404	4/4	0.93	0.18	54,60,68,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.