



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:32 PM GMT

PDB ID : 1G44
Title : CRYSTAL STRUCTURE OF A COMPLEMENT CONTROL PROTEIN THAT REGULATES BOTH PATHWAYS OF COMPLEMENT ACTIVATION AND BINDS HEPARAN SULFATE PROTEOGLYCANS
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Deposited on : 2000-10-26
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

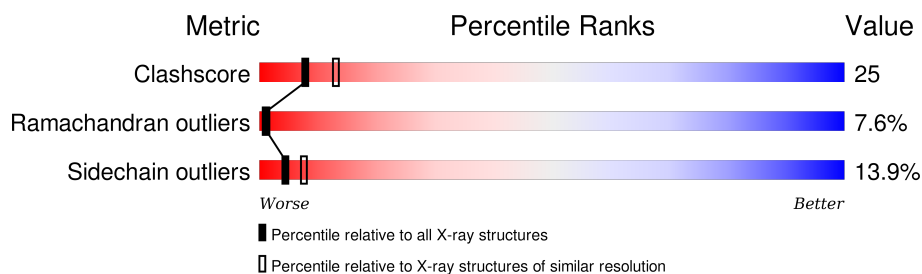
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	244	
1	B	244	
1	C	244	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5191 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 COMPLEMENT CONTROL PROTEIN.

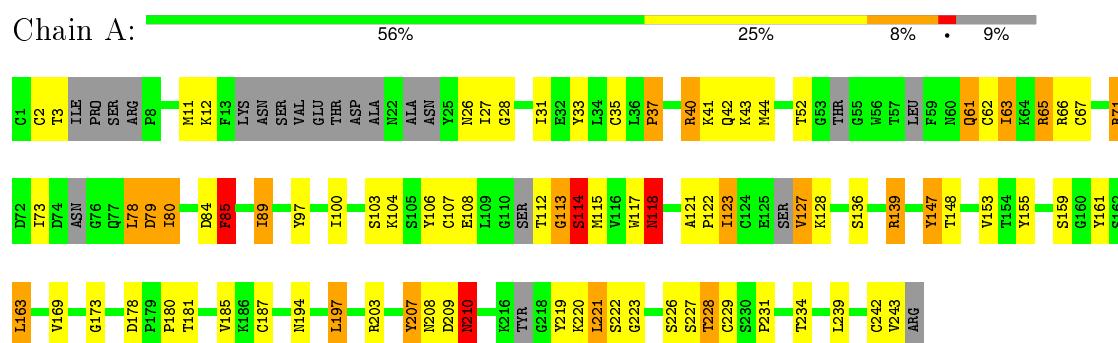
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1698	1060	284	334	20			
1	B	231	Total	C	N	O	S	0	0	0
			1752	1087	295	350	20			
1	C	228	Total	C	N	O	S	0	0	0
			1741	1082	293	346	20			

3 Residue-property plots [i](#)

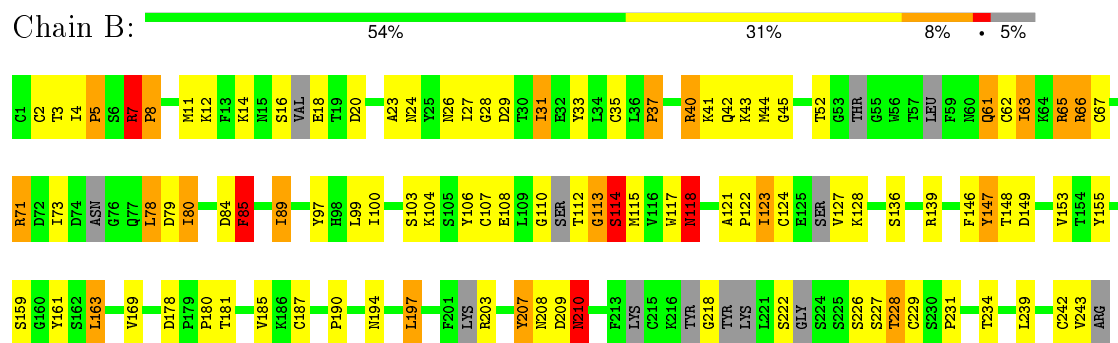
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

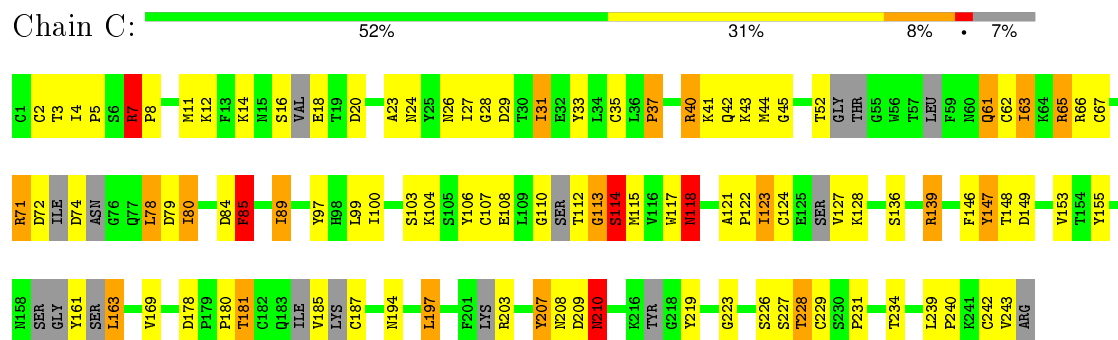
• Molecule 1: COMPLEMENT CONTROL PROTEIN



• Molecule 1: COMPLEMENT CONTROL PROTEIN



• Molecule 1: COMPLEMENT CONTROL PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	99.20 Å 110.30 Å 268.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	93.0 (8.00-2.60)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5191	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.46	0/1736	1.57	37/2338 (1.6%)
1	B	0.45	0/1788	1.56	40/2410 (1.7%)
1	C	0.46	0/1776	1.56	41/2390 (1.7%)
All	All	0.46	0/5300	1.57	118/7138 (1.7%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	TYR	CA-CB-CG	8.02	128.64	113.40
1	C	97	TYR	CA-CB-CG	7.67	127.96	113.40
1	A	219	TYR	CA-CB-CG	7.61	127.86	113.40
1	B	118	ASN	CB-CA-C	7.51	125.43	110.40
1	A	148	THR	C-N-CA	7.49	140.42	121.70
1	A	118	ASN	CB-CA-C	7.49	125.37	110.40
1	C	118	ASN	CB-CA-C	7.42	125.25	110.40
1	B	197	LEU	CA-CB-CG	7.39	132.30	115.30
1	C	197	LEU	CA-CB-CG	7.39	132.29	115.30
1	A	197	LEU	CA-CB-CG	7.36	132.22	115.30
1	A	40	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	C	40	ARG	NE-CZ-NH1	7.24	123.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	C	147	TYR	CA-CB-CG	7.12	126.94	113.40
1	A	97	TYR	CA-CB-CG	7.11	126.91	113.40
1	B	7	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	147	TYR	CA-CB-CG	7.02	126.73	113.40
1	B	147	TYR	CA-CB-CG	7.00	126.71	113.40
1	B	148	THR	C-N-CA	6.96	139.09	121.70
1	C	148	THR	C-N-CA	6.83	138.77	121.70
1	B	65	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	85	PHE	CA-CB-CG	6.77	130.15	113.90
1	C	85	PHE	CA-CB-CG	6.75	130.09	113.90
1	A	203	ARG	CD-NE-CZ	6.74	133.04	123.60
1	C	7	ARG	CD-NE-CZ	6.70	132.98	123.60
1	B	85	PHE	CA-CB-CG	6.70	129.97	113.90
1	B	97	TYR	CA-CB-CG	6.60	125.94	113.40
1	A	65	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	C	65	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	66	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	C	40	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	40	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	78	LEU	CA-CB-CG	6.46	130.15	115.30
1	A	66	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	78	LEU	CA-CB-CG	6.43	130.09	115.30
1	C	79	ASP	C-N-CA	6.41	137.72	121.70
1	C	66	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	C	78	LEU	CA-CB-CG	6.36	129.93	115.30
1	B	79	ASP	C-N-CA	6.26	137.36	121.70
1	C	80	ILE	CA-CB-CG1	6.25	122.87	111.00
1	B	80	ILE	CA-CB-CG1	6.25	122.86	111.00
1	B	40	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	106	TYR	CA-CB-CG	6.16	125.11	113.40
1	C	106	TYR	CA-CB-CG	6.16	125.10	113.40
1	A	106	TYR	CA-CB-CG	6.14	125.07	113.40
1	C	207	TYR	CA-CB-CG	6.13	125.04	113.40
1	B	207	TYR	CA-CB-CG	6.08	124.96	113.40
1	A	207	TYR	CA-CB-CG	6.06	124.92	113.40
1	A	80	ILE	CA-CB-CG1	6.06	122.51	111.00
1	C	71	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	203	ARG	CD-NE-CZ	5.92	131.89	123.60
1	B	163	LEU	CA-CB-CG	5.91	128.88	115.30
1	A	163	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	139	ARG	CD-NE-CZ	5.90	131.86	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	LEU	CA-CB-CG	5.90	128.86	115.30
1	A	221	LEU	CA-CB-CG	5.90	128.86	115.30
1	B	139	ARG	CD-NE-CZ	5.89	131.85	123.60
1	C	139	ARG	CD-NE-CZ	5.87	131.81	123.60
1	B	127	VAL	CA-CB-CG1	5.86	119.69	110.90
1	B	203	ARG	CD-NE-CZ	5.85	131.79	123.60
1	B	114	SER	N-CA-CB	5.79	119.18	110.50
1	C	127	VAL	CA-CB-CG1	5.77	119.55	110.90
1	B	80	ILE	N-CA-CB	5.76	124.05	110.80
1	B	71	ARG	CD-NE-CZ	5.75	131.66	123.60
1	C	114	SER	N-CA-CB	5.74	119.10	110.50
1	A	71	ARG	CD-NE-CZ	5.73	131.62	123.60
1	C	80	ILE	N-CA-CB	5.72	123.97	110.80
1	C	97	TYR	CB-CG-CD1	5.71	124.42	121.00
1	C	161	TYR	CA-CB-CG	5.69	124.20	113.40
1	B	161	TYR	CA-CB-CG	5.68	124.20	113.40
1	B	71	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	114	SER	N-CA-CB	5.68	119.01	110.50
1	A	161	TYR	CA-CB-CG	5.67	124.17	113.40
1	B	127	VAL	CB-CA-C	5.63	122.10	111.40
1	C	40	ARG	CD-NE-CZ	5.63	131.48	123.60
1	C	71	ARG	CD-NE-CZ	5.63	131.49	123.60
1	A	71	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	40	ARG	CD-NE-CZ	5.58	131.42	123.60
1	C	127	VAL	CB-CA-C	5.54	121.92	111.40
1	B	40	ARG	CD-NE-CZ	5.52	131.33	123.60
1	B	210	ASN	O-C-N	-5.51	113.88	122.70
1	B	139	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	210	ASN	O-C-N	-5.46	113.97	122.70
1	A	79	ASP	CB-CG-OD1	5.46	123.21	118.30
1	C	210	ASN	O-C-N	-5.44	113.99	122.70
1	A	97	TYR	CB-CG-CD1	5.43	124.26	121.00
1	C	79	ASP	O-C-N	-5.42	114.03	122.70
1	B	79	ASP	O-C-N	-5.41	114.04	122.70
1	C	139	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	80	ILE	N-CA-CB	5.38	123.18	110.80
1	A	79	ASP	C-N-CA	5.38	135.14	121.70
1	A	66	ARG	CD-NE-CZ	5.35	131.09	123.60
1	A	139	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	C	66	ARG	CD-NE-CZ	5.33	131.07	123.60
1	B	203	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	203	ARG	NE-CZ-NH1	5.31	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ARG	CD-NE-CZ	5.28	130.99	123.60
1	C	79	ASP	CA-C-O	5.23	131.09	120.10
1	C	103	SER	C-N-CA	5.22	134.75	121.70
1	A	65	ARG	CD-NE-CZ	5.21	130.90	123.60
1	A	239	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	103	SER	C-N-CA	5.21	134.72	121.70
1	C	65	ARG	CD-NE-CZ	5.21	130.89	123.60
1	B	239	LEU	CA-CB-CG	5.20	127.26	115.30
1	C	239	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	103	SER	C-N-CA	5.19	134.67	121.70
1	B	79	ASP	CA-C-O	5.18	130.99	120.10
1	A	127	VAL	CB-CA-C	5.18	121.23	111.40
1	C	40	ARG	CA-CB-CG	5.17	124.78	113.40
1	A	40	ARG	CA-CB-CG	5.16	124.75	113.40
1	B	65	ARG	CD-NE-CZ	5.13	130.78	123.60
1	B	80	ILE	CA-C-N	5.07	126.33	116.20
1	A	80	ILE	CA-C-N	5.06	126.33	116.20
1	C	80	ILE	CA-C-N	5.06	126.33	116.20
1	B	40	ARG	CA-CB-CG	5.06	124.53	113.40
1	B	149	ASP	CA-C-N	5.02	126.25	116.20
1	C	149	ASP	CA-C-N	5.01	126.23	116.20
1	B	5	PRO	N-CD-CG	5.01	110.71	103.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	ASN	Mainchain
1	B	210	ASN	Mainchain
1	C	210	ASN	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1698	0	1586	92	0
1	B	1752	0	1625	81	18

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1741	0	1610	99	8
All	All	5191	0	4821	250	18

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 25.

All (250) 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:B:43:LYS:HE2	1:B:115:MET:CG	1.17	1.61
1:C:43:LYS:HE2	1:C:115:MET:CG	1.23	1.61
1:A:43:LYS:HE2	1:A:115:MET:CG	1.20	1.58
1:A:42:GLN:CG	1:A:63:ILE:HG12	1.29	1.55
1:A:163:LEU:HB2	1:A:207:TYR:CE2	1.45	1.51
1:B:42:GLN:CG	1:B:63:ILE:HG12	1.29	1.50
1:C:42:GLN:CG	1:C:63:ILE:HG12	1.29	1.49
1:C:163:LEU:HB2	1:C:207:TYR:CE2	1.45	1.49
1:B:42:GLN:HG2	1:B:63:ILE:CG1	1.26	1.47
1:B:163:LEU:HB2	1:B:207:TYR:CE2	1.45	1.45
1:C:7:ARG:HG2	1:C:8:PRO:CD	1.42	1.45
1:C:7:ARG:CG	1:C:8:PRO:HD3	1.49	1.40
1:A:42:GLN:HG2	1:A:63:ILE:CG1	1.27	1.39
1:C:42:GLN:HG2	1:C:63:ILE:CG1	1.27	1.39
1:C:100:ILE:O	1:C:122:PRO:HB2	1.20	1.38
1:A:100:ILE:O	1:A:122:PRO:HB2	1.28	1.30
1:A:43:LYS:CE	1:A:115:MET:CG	2.12	1.28
1:B:100:ILE:O	1:B:122:PRO:HB2	1.27	1.28
1:B:43:LYS:CE	1:B:115:MET:CG	2.10	1.27
1:C:43:LYS:CE	1:C:115:MET:CG	2.16	1.22
1:B:100:ILE:O	1:B:122:PRO:CB	1.90	1.19
1:A:163:LEU:CB	1:A:207:TYR:CE2	2.27	1.18
1:C:163:LEU:CB	1:C:207:TYR:CE2	2.26	1.17
1:B:163:LEU:CB	1:B:207:TYR:CE2	2.26	1.17
1:A:100:ILE:O	1:A:122:PRO:CB	1.91	1.17
1:A:43:LYS:HE2	1:A:115:MET:HG2	1.27	1.16
1:C:100:ILE:O	1:C:122:PRO:CB	1.94	1.16
1:B:43:LYS:HE2	1:B:115:MET:SD	1.87	1.14
1:C:43:LYS:HE2	1:C:115:MET:HG3	1.20	1.14
1:A:43:LYS:HE2	1:A:115:MET:SD	1.87	1.14
1:C:43:LYS:HE2	1:C:115:MET:HG2	1.27	1.13
1:C:43:LYS:HE2	1:C:115:MET:SD	1.88	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LYS:HE2	1:B:115:MET:HG3	1.13	1.10
1:A:43:LYS:CE	1:A:115:MET:SD	2.41	1.08
1:B:43:LYS:CE	1:B:115:MET:SD	2.40	1.08
1:B:43:LYS:HE2	1:B:115:MET:HG2	1.24	1.06
1:B:43:LYS:NZ	1:B:115:MET:SD	2.28	1.05
1:A:43:LYS:HE2	1:A:115:MET:HG3	1.14	1.05
1:A:223:GLY:HA2	1:C:121:ALA:CB	1.87	1.04
1:A:43:LYS:NZ	1:A:115:MET:SD	2.31	1.04
1:C:43:LYS:CE	1:C:115:MET:SD	2.44	1.03
1:A:222:SER:OG	1:C:123:ILE:HD11	1.61	1.00
1:C:43:LYS:NZ	1:C:115:MET:SD	2.35	0.98
1:B:163:LEU:HB2	1:B:207:TYR:CZ	2.00	0.97
1:C:85:PHE:CD1	1:C:112:THR:O	2.16	0.97
1:B:85:PHE:CD1	1:B:112:THR:O	2.17	0.97
1:A:85:PHE:CD1	1:A:112:THR:O	2.16	0.97
1:C:163:LEU:HB2	1:C:207:TYR:CZ	2.00	0.97
1:A:163:LEU:HB2	1:A:207:TYR:CZ	2.00	0.96
1:C:43:LYS:CE	1:C:115:MET:HG2	1.87	0.95
1:A:43:LYS:CE	1:A:115:MET:HG2	1.86	0.94
1:B:194:ASN:O	1:B:242:CYS:HB3	1.69	0.93
1:B:73:ILE:HG12	1:B:123:ILE:HG23	1.50	0.93
1:B:43:LYS:CE	1:B:115:MET:HG2	1.83	0.93
1:C:194:ASN:O	1:C:242:CYS:HB3	1.69	0.92
1:A:194:ASN:O	1:A:242:CYS:HB3	1.70	0.91
1:A:223:GLY:N	1:C:121:ALA:HA	1.85	0.91
1:C:163:LEU:CG	1:C:207:TYR:CE2	2.56	0.89
1:B:163:LEU:CG	1:B:207:TYR:CE2	2.56	0.88
1:C:163:LEU:CB	1:C:207:TYR:CZ	2.56	0.87
1:A:163:LEU:CB	1:A:207:TYR:CZ	2.56	0.87
1:B:163:LEU:CB	1:B:207:TYR:CZ	2.56	0.87
1:A:163:LEU:CG	1:A:207:TYR:CE2	2.57	0.87
1:A:222:SER:OG	1:C:123:ILE:CG1	2.23	0.86
1:A:222:SER:OG	1:C:123:ILE:CD1	2.23	0.85
1:B:163:LEU:HD23	1:B:207:TYR:HE2	1.41	0.84
1:A:163:LEU:HD23	1:A:207:TYR:HE2	1.41	0.84
1:C:163:LEU:HD23	1:C:207:TYR:HE2	1.41	0.84
1:B:163:LEU:HB2	1:B:207:TYR:CD2	2.12	0.84
1:C:163:LEU:HB2	1:C:207:TYR:CD2	2.12	0.84
1:A:89:ILE:HD11	1:A:117:TRP:CZ3	2.15	0.82
1:A:163:LEU:HB2	1:A:207:TYR:CD2	2.13	0.82
1:A:163:LEU:CG	1:A:207:TYR:HE2	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LEU:CG	1:C:207:TYR:HE2	1.93	0.81
1:C:163:LEU:CD2	1:C:207:TYR:HE2	1.95	0.80
1:A:163:LEU:CD2	1:A:207:TYR:HE2	1.95	0.80
1:A:222:SER:CB	1:C:123:ILE:HD11	2.12	0.80
1:A:223:GLY:HA2	1:C:121:ALA:HB1	1.62	0.80
1:B:163:LEU:CD2	1:B:207:TYR:HE2	1.95	0.79
1:C:89:ILE:HD11	1:C:117:TRP:CZ3	2.18	0.79
1:B:163:LEU:CG	1:B:207:TYR:HE2	1.93	0.78
1:B:42:GLN:HG3	1:B:63:ILE:HG12	1.60	0.78
1:A:223:GLY:HA2	1:C:121:ALA:HB2	1.66	0.77
1:A:89:ILE:CD1	1:A:117:TRP:CZ3	2.67	0.77
1:A:85:PHE:HB2	1:A:114:SER:OG	1.85	0.77
1:C:89:ILE:CD1	1:C:117:TRP:CZ3	2.67	0.77
1:A:42:GLN:CG	1:A:63:ILE:CG1	2.10	0.76
1:C:85:PHE:HB2	1:C:114:SER:OG	1.85	0.76
1:A:163:LEU:HD23	1:A:207:TYR:CE2	2.22	0.75
1:B:89:ILE:CD1	1:B:117:TRP:CZ3	2.69	0.75
1:A:89:ILE:CD1	1:A:117:TRP:HZ3	2.00	0.74
1:B:42:GLN:CG	1:B:63:ILE:CG1	2.09	0.73
1:C:89:ILE:CD1	1:C:117:TRP:HZ3	2.02	0.73
1:B:85:PHE:HB2	1:B:114:SER:OG	1.88	0.73
1:C:163:LEU:HD23	1:C:207:TYR:CE2	2.22	0.73
1:B:163:LEU:HD23	1:B:207:TYR:CE2	2.22	0.73
1:B:89:ILE:HD11	1:B:117:TRP:CZ3	2.24	0.73
1:A:127:VAL:HG11	1:C:7:ARG:HG3	1.72	0.71
1:B:20:ASP:HB2	1:B:23:ALA:HB2	1.74	0.70
1:C:20:ASP:HB2	1:C:23:ALA:HB2	1.73	0.70
1:B:73:ILE:HG12	1:B:123:ILE:CG2	2.22	0.70
1:A:42:GLN:HG3	1:A:63:ILE:HG12	1.61	0.70
1:C:42:GLN:HG3	1:C:63:ILE:HG12	1.61	0.69
1:B:153:VAL:HB	1:B:169:VAL:HB	1.74	0.69
1:B:12:LYS:NZ	1:B:41:LYS:HD3	2.08	0.69
1:C:153:VAL:HB	1:C:169:VAL:HB	1.74	0.69
1:A:73:ILE:HG12	1:A:123:ILE:HG23	1.73	0.69
1:B:89:ILE:CD1	1:B:117:TRP:HZ3	2.06	0.68
1:B:208:ASN:HA	1:B:229:CYS:CB	2.24	0.68
1:C:85:PHE:CE1	1:C:112:THR:O	2.47	0.68
1:C:42:GLN:CG	1:C:63:ILE:CG1	2.10	0.67
1:B:43:LYS:CE	1:B:115:MET:HG3	2.02	0.67
1:C:208:ASN:HA	1:C:229:CYS:CB	2.24	0.67
1:A:208:ASN:HA	1:A:229:CYS:CB	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LYS:HE3	1:B:115:MET:HG2	1.73	0.66
1:A:85:PHE:CE1	1:A:112:THR:O	2.47	0.66
1:C:43:LYS:HE3	1:C:115:MET:HG2	1.77	0.65
1:B:208:ASN:HA	1:B:229:CYS:HB3	1.79	0.65
1:C:121:ALA:N	1:C:122:PRO:HD2	2.12	0.65
1:A:43:LYS:HE3	1:A:115:MET:HG2	1.74	0.64
1:A:121:ALA:N	1:A:122:PRO:HD2	2.12	0.64
1:A:208:ASN:HA	1:A:229:CYS:HB3	1.80	0.64
1:C:7:ARG:CG	1:C:8:PRO:CD	2.35	0.64
1:A:153:VAL:HB	1:A:169:VAL:HB	1.80	0.64
1:A:121:ALA:N	1:A:122:PRO:CD	2.61	0.63
1:C:208:ASN:HA	1:C:229:CYS:HB3	1.79	0.63
1:A:163:LEU:HG	1:A:207:TYR:CE2	2.34	0.62
1:C:121:ALA:N	1:C:122:PRO:CD	2.62	0.62
1:B:121:ALA:N	1:B:122:PRO:HD2	2.14	0.62
1:B:121:ALA:N	1:B:122:PRO:CD	2.63	0.62
1:B:85:PHE:CE1	1:B:112:THR:O	2.51	0.62
1:A:223:GLY:CA	1:C:121:ALA:HA	2.29	0.62
1:B:12:LYS:HZ3	1:B:41:LYS:HD3	1.65	0.62
1:A:222:SER:CA	1:C:121:ALA:O	2.48	0.61
1:C:185:VAL:HG11	1:C:231:PRO:HA	1.82	0.61
1:A:185:VAL:HG11	1:A:231:PRO:HA	1.81	0.61
1:B:185:VAL:HG11	1:B:231:PRO:HA	1.82	0.61
1:C:40:ARG:HG3	1:C:65:ARG:H	1.67	0.60
1:B:163:LEU:HG	1:B:207:TYR:CE2	2.33	0.60
1:C:163:LEU:HG	1:C:207:TYR:CE2	2.33	0.59
1:C:163:LEU:CD2	1:C:207:TYR:CE2	2.80	0.59
1:C:43:LYS:CE	1:C:115:MET:HG3	2.09	0.59
1:B:11:MET:HA	1:B:62:CYS:HB3	1.85	0.59
1:A:127:VAL:HG13	1:A:173:GLY:HA2	1.84	0.59
1:A:222:SER:OG	1:C:123:ILE:HG13	2.02	0.59
1:A:40:ARG:HH22	1:A:84:ASP:HB3	1.68	0.59
1:C:163:LEU:HB3	1:C:207:TYR:CZ	2.38	0.59
1:A:40:ARG:HG3	1:A:65:ARG:H	1.67	0.58
1:A:43:LYS:CE	1:A:115:MET:HG3	2.03	0.58
1:B:100:ILE:O	1:B:122:PRO:HB3	1.96	0.58
1:C:40:ARG:HH22	1:C:84:ASP:HB3	1.68	0.58
1:A:163:LEU:HB3	1:A:207:TYR:CZ	2.38	0.58
1:A:100:ILE:O	1:A:122:PRO:HB3	1.95	0.58
1:B:163:LEU:HB3	1:B:207:TYR:CZ	2.38	0.58
1:A:12:LYS:NZ	1:A:41:LYS:HD3	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:HG23	1:B:169:VAL:O	2.04	0.57
1:C:153:VAL:HG23	1:C:169:VAL:O	2.04	0.57
1:C:12:LYS:NZ	1:C:41:LYS:HD3	2.20	0.57
1:B:40:ARG:HG3	1:B:65:ARG:H	1.67	0.57
1:A:221:LEU:HD13	1:A:242:CYS:HB2	1.88	0.55
1:C:108:GLU:HG2	1:C:118:ASN:HB2	1.89	0.55
1:A:108:GLU:HG2	1:A:118:ASN:HB2	1.89	0.54
1:B:40:ARG:HH22	1:B:84:ASP:HB3	1.72	0.54
1:B:208:ASN:HA	1:B:229:CYS:HB2	1.90	0.54
1:A:163:LEU:CD2	1:A:207:TYR:CE2	2.80	0.53
1:A:153:VAL:HG23	1:A:169:VAL:O	2.08	0.53
1:A:208:ASN:HA	1:A:229:CYS:HB2	1.91	0.53
1:B:163:LEU:HG	1:B:207:TYR:OH	2.08	0.53
1:C:24:ASN:OD1	1:C:29:ASP:OD1	2.27	0.53
1:A:11:MET:HA	1:A:62:CYS:HB3	1.90	0.53
1:A:163:LEU:HG	1:A:207:TYR:OH	2.09	0.53
1:C:11:MET:HA	1:C:62:CYS:HB3	1.90	0.53
1:C:163:LEU:HG	1:C:207:TYR:OH	2.08	0.52
1:A:107:CYS:HA	1:A:117:TRP:HA	1.91	0.52
1:C:208:ASN:HA	1:C:229:CYS:HB2	1.90	0.52
1:B:24:ASN:OD1	1:B:29:ASP:OD1	2.26	0.52
1:B:12:LYS:HB2	1:B:33:TYR:HB3	1.92	0.52
1:A:223:GLY:CA	1:C:121:ALA:CB	2.75	0.52
1:B:108:GLU:HG2	1:B:118:ASN:HB2	1.91	0.52
1:A:222:SER:HB3	1:C:121:ALA:O	2.10	0.51
1:C:107:CYS:HA	1:C:117:TRP:HA	1.92	0.51
1:A:208:ASN:HB2	1:A:229:CYS:H	1.76	0.51
1:A:222:SER:HA	1:C:121:ALA:O	2.10	0.51
1:B:89:ILE:HD12	1:B:117:TRP:CZ3	2.45	0.51
1:A:73:ILE:HG12	1:A:123:ILE:CG2	2.41	0.51
1:A:12:LYS:HB2	1:A:33:TYR:HB3	1.93	0.51
1:B:16:SER:O	1:B:18:GLU:N	2.44	0.51
1:B:163:LEU:CD2	1:B:207:TYR:CE2	2.80	0.51
1:C:16:SER:O	1:C:18:GLU:N	2.44	0.51
1:C:89:ILE:HD12	1:C:117:TRP:CZ3	2.45	0.51
1:C:12:LYS:HB2	1:C:33:TYR:HB3	1.92	0.51
1:B:107:CYS:HA	1:B:117:TRP:HA	1.93	0.50
1:B:208:ASN:HB2	1:B:229:CYS:H	1.76	0.50
1:A:208:ASN:OD1	1:A:228:THR:CG2	2.60	0.50
1:C:12:LYS:HZ3	1:C:41:LYS:HD3	1.76	0.50
1:A:89:ILE:HD12	1:A:117:TRP:CZ3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:SER:CB	1:C:123:ILE:CD1	2.87	0.49
1:C:100:ILE:O	1:C:122:PRO:HB3	2.04	0.49
1:C:208:ASN:HB2	1:C:229:CYS:H	1.76	0.49
1:A:42:GLN:HB2	1:A:61:GLN:HB3	1.95	0.49
1:B:100:ILE:O	1:B:122:PRO:CG	2.59	0.48
1:B:7:ARG:HB3	1:B:8:PRO:HD3	1.95	0.48
1:C:208:ASN:OD1	1:C:228:THR:CG2	2.62	0.48
1:C:155:TYR:CD1	1:C:180:PRO:HG3	2.49	0.48
1:B:208:ASN:OD1	1:B:228:THR:CG2	2.62	0.47
1:B:155:TYR:CD1	1:B:180:PRO:HG3	2.49	0.47
1:C:42:GLN:HB2	1:C:61:GLN:HB3	1.96	0.47
1:B:12:LYS:HZ2	1:B:41:LYS:HD3	1.81	0.46
1:B:42:GLN:HB2	1:B:61:GLN:HB3	1.97	0.46
1:A:223:GLY:HA2	1:C:121:ALA:CA	2.46	0.46
1:B:73:ILE:CG1	1:B:123:ILE:CG2	2.93	0.46
1:A:223:GLY:H	1:C:121:ALA:HA	1.77	0.46
1:A:155:TYR:CD1	1:A:180:PRO:HG3	2.51	0.45
1:A:223:GLY:CA	1:C:121:ALA:CA	2.94	0.45
1:A:12:LYS:HZ3	1:A:41:LYS:HD3	1.80	0.45
1:A:222:SER:C	1:C:121:ALA:O	2.54	0.45
1:B:40:ARG:HB3	1:B:113:GLY:HA2	1.99	0.45
1:A:208:ASN:CA	1:A:229:CYS:HB3	2.46	0.44
1:B:208:ASN:CA	1:B:229:CYS:HB3	2.46	0.44
1:C:4:ILE:HB	1:C:5:PRO:HD2	2.00	0.44
1:B:163:LEU:HG	1:B:207:TYR:CZ	2.53	0.44
1:C:163:LEU:HG	1:C:207:TYR:CZ	2.53	0.43
1:A:223:GLY:N	1:C:121:ALA:CA	2.70	0.43
1:B:208:ASN:CB	1:B:229:CYS:HB3	2.49	0.43
1:C:99:LEU:HA	1:C:124:CYS:HA	2.01	0.43
1:C:40:ARG:HB3	1:C:113:GLY:HA2	1.99	0.43
1:A:163:LEU:HG	1:A:207:TYR:CZ	2.53	0.43
1:C:223:GLY:HA3	1:C:240:PRO:HB3	2.00	0.43
1:A:40:ARG:HB3	1:A:113:GLY:HA2	2.00	0.43
1:C:12:LYS:HB3	1:C:35:CYS:SG	2.59	0.43
1:B:14:LYS:HD3	1:B:31:ILE:HD13	2.01	0.43
1:B:12:LYS:HB3	1:B:35:CYS:SG	2.59	0.43
1:A:208:ASN:CB	1:A:229:CYS:HB3	2.49	0.42
1:A:12:LYS:HB3	1:A:35:CYS:SG	2.59	0.42
1:A:222:SER:CB	1:C:121:ALA:O	2.68	0.42
1:C:208:ASN:CA	1:C:229:CYS:HB3	2.46	0.42
1:C:14:LYS:HD3	1:C:31:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLN:HG3	1:A:63:ILE:CG2	2.50	0.42
1:C:208:ASN:CB	1:C:229:CYS:HB3	2.49	0.42
1:A:194:ASN:O	1:A:242:CYS:CB	2.56	0.42
1:B:14:LYS:HD3	1:B:31:ILE:HG21	2.01	0.42
1:B:4:ILE:HB	1:B:5:PRO:HD2	2.01	0.41
1:C:42:GLN:HG2	1:C:63:ILE:HG12	0.46	0.41
1:B:73:ILE:CG1	1:B:123:ILE:HG23	2.36	0.41
1:B:45:GLY:O	1:B:110:GLY:O	2.39	0.41
1:B:42:GLN:HG3	1:B:63:ILE:CG1	2.33	0.40
1:C:42:GLN:HG3	1:C:63:ILE:CG2	2.51	0.40
1:B:99:LEU:HA	1:B:124:CYS:HA	2.03	0.40
1:C:45:GLY:O	1:C:110:GLY:O	2.40	0.40
1:B:42:GLN:HG3	1:B:63:ILE:CG2	2.52	0.40

All (18) 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)
1:B:222:SER:CA	1:B:222:SER:CB[4_566]	0.59	1.61
1:B:218:GLY:CA	1:C:181:THR:OG1[3_656]	0.88	1.32
1:B:222:SER:C	1:B:222:SER:CB[4_566]	0.98	1.22
1:B:222:SER:CA	1:B:222:SER:CA[4_566]	1.17	1.03
1:B:218:GLY:CA	1:C:181:THR:CB[3_656]	1.35	0.85
1:B:222:SER:C	1:B:222:SER:OG[4_566]	1.35	0.85
1:B:218:GLY:O	1:C:181:THR:CG2[3_656]	1.42	0.78
1:B:222:SER:N	1:B:222:SER:OG[4_566]	1.48	0.72
1:B:218:GLY:N	1:C:181:THR:OG1[3_656]	1.49	0.71
1:B:222:SER:CA	1:B:222:SER:OG[4_566]	1.50	0.70
1:B:218:GLY:C	1:C:181:THR:CB[3_656]	1.63	0.57
1:B:218:GLY:O	1:C:181:THR:CB[3_656]	1.77	0.43
1:B:218:GLY:C	1:C:181:THR:CG2[3_656]	1.80	0.40
1:B:222:SER:CB	1:B:222:SER:CB[4_566]	1.84	0.36
1:B:222:SER:N	1:B:222:SER:CB[4_566]	1.85	0.35
1:B:222:SER:O	1:B:222:SER:OG[4_566]	1.92	0.28
1:B:222:SER:O	1:B:222:SER:CB[4_566]	2.00	0.20
1:B:218:GLY:CA	1:C:181:THR:CG2[3_656]	2.16	0.04

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	204/244 (84%)	145 (71%)	44 (22%)	15 (7%)	1	1
1	B	208/244 (85%)	145 (70%)	46 (22%)	17 (8%)	1	1
1	C	203/244 (83%)	143 (70%)	45 (22%)	15 (7%)	1	1
All	All	615/732 (84%)	433 (70%)	135 (22%)	47 (8%)	1	1

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	118	ASN
1	A	210	ASN
1	B	104	LYS
1	B	118	ASN
1	B	210	ASN
1	C	104	LYS
1	C	118	ASN
1	C	210	ASN
1	A	44	MET
1	A	113	GLY
1	A	159	SER
1	B	44	MET
1	B	113	GLY
1	B	159	SER
1	C	44	MET
1	C	113	GLY
1	A	37	PRO
1	A	178	ASP
1	B	37	PRO
1	B	178	ASP
1	C	37	PRO
1	C	178	ASP
1	A	114	SER

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Mol	Chain	Res	Type
1	A	226	SER
1	B	80	ILE
1	B	114	SER
1	B	226	SER
1	C	7	ARG
1	C	80	ILE
1	C	114	SER
1	C	226	SER
1	A	80	ILE
1	A	136	SER
1	B	136	SER
1	C	136	SER
1	A	28	GLY
1	B	28	GLY
1	C	28	GLY
1	A	63	ILE
1	B	63	ILE
1	C	63	ILE
1	A	27	ILE
1	B	8	PRO
1	B	27	ILE
1	C	27	ILE
1	B	7	ARG

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	195/214 (91%)	168 (86%)	27 (14%)	4	7
1	B	202/214 (94%)	175 (87%)	27 (13%)	5	8
1	C	200/214 (94%)	171 (86%)	29 (14%)	4	6
All	All	597/642 (93%)	514 (86%)	83 (14%)	4	7

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	CYS
1	A	3	THR
1	A	26	ASN
1	A	31	ILE
1	A	37	PRO
1	A	52	THR
1	A	61	GLN
1	A	67	CYS
1	A	71	ARG
1	A	78	LEU
1	A	79	ASP
1	A	85	PHE
1	A	89	ILE
1	A	114	SER
1	A	123	ILE
1	A	128	LYS
1	A	139	ARG
1	A	147	TYR
1	A	181	THR
1	A	187	CYS
1	A	197	LEU
1	A	209	ASP
1	A	220	LYS
1	A	227	SER
1	A	228	THR
1	A	234	THR
1	A	243	VAL
1	B	2	CYS
1	B	3	THR
1	B	26	ASN
1	B	31	ILE
1	B	37	PRO
1	B	52	THR
1	B	61	GLN
1	B	66	ARG
1	B	67	CYS
1	B	71	ARG
1	B	78	LEU
1	B	85	PHE
1	B	89	ILE
1	B	114	SER
1	B	123	ILE
1	B	128	LYS

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Mol	Chain	Res	Type
1	B	146	PHE
1	B	147	TYR
1	B	181	THR
1	B	187	CYS
1	B	190	PRO
1	B	197	LEU
1	B	209	ASP
1	B	227	SER
1	B	228	THR
1	B	234	THR
1	B	243	VAL
1	C	2	CYS
1	C	3	THR
1	C	7	ARG
1	C	26	ASN
1	C	31	ILE
1	C	37	PRO
1	C	52	THR
1	C	61	GLN
1	C	67	CYS
1	C	71	ARG
1	C	72	ASP
1	C	74	ASP
1	C	78	LEU
1	C	85	PHE
1	C	89	ILE
1	C	114	SER
1	C	123	ILE
1	C	128	LYS
1	C	139	ARG
1	C	146	PHE
1	C	147	TYR
1	C	181	THR
1	C	187	CYS
1	C	197	LEU
1	C	209	ASP
1	C	227	SER
1	C	228	THR
1	C	234	THR
1	C	243	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	60	ASN
1	A	130	GLN
1	B	26	ASN
1	B	60	ASN
1	C	26	ASN
1	C	60	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.