Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 06:47 am GMT

PDB ID	:	1GZE
Title	:	Structure of the Clostridium botulinum C3 exoenzyme (L177C mutant)
Authors	:	Menetrey, J.; Flatau, G.; Stura, E.A.; Charbonnier, J.B.; Gas, F.; Teulon, J.M.; Le Du, M.H.; Boquet, P.; Menez, A.
Deposited on	:	2002-05-21
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

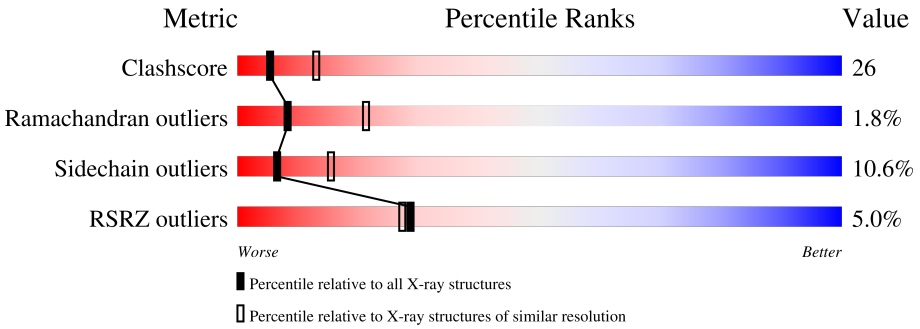
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	211	7%, 55%, 37%
1	B	211	3%, 54%, 35%, 7%
1	C	211	7%, 46%, 46%, 7%
1	D	211	3%, 56%, 35%, 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6511 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 MONO-ADP-RIBOSYLTRANSFERASE C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1623	1029	276	310	8			
1	B	203	Total	C	N	O	S	0	0	0
			1595	1011	272	304	8			
1	C	210	Total	C	N	O	S	0	0	0
			1651	1047	281	315	8			
1	D	203	Total	C	N	O	S	0	0	0
			1595	1011	272	304	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	CYS	LEU	engineered mutation	UNP P15879
B	177	CYS	LEU	engineered mutation	UNP P15879
C	177	CYS	LEU	engineered mutation	UNP P15879
D	177	CYS	LEU	engineered mutation	UNP P15879

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Hg	0	0
			1	1		
2	B	1	Total	Hg	0	0
			1	1		
2	C	1	Total	Hg	0	0
			1	1		
2	D	1	Total	Hg	0	0
			1	1		

- Molecule 3 is water.

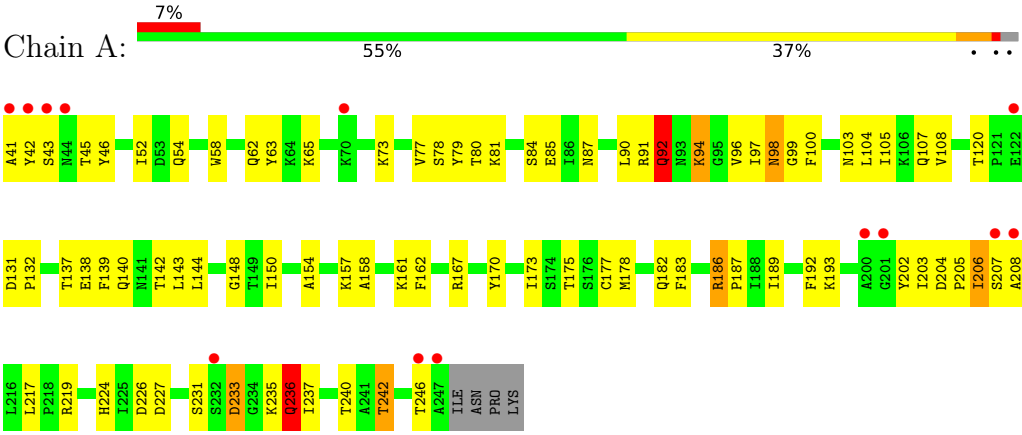
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	11	Total O 11 11	0	0
3	C	11	Total O 11 11	0	0
3	D	14	Total O 14 14	0	0

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.

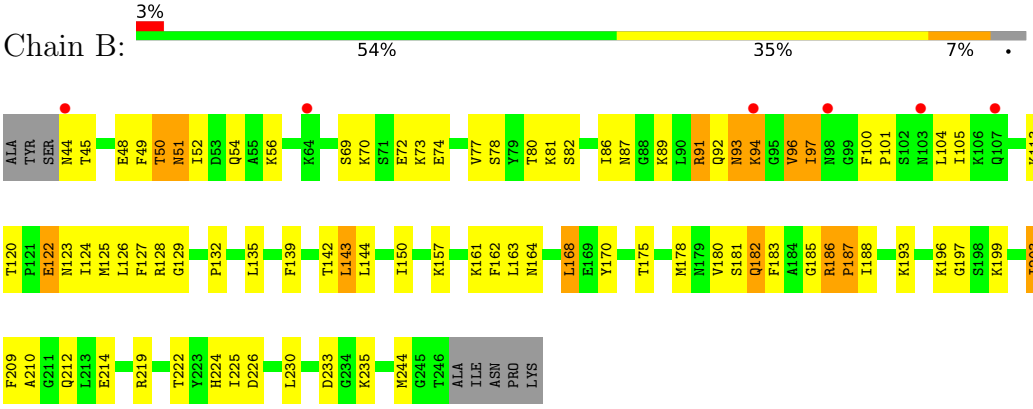
• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3

Chain A:



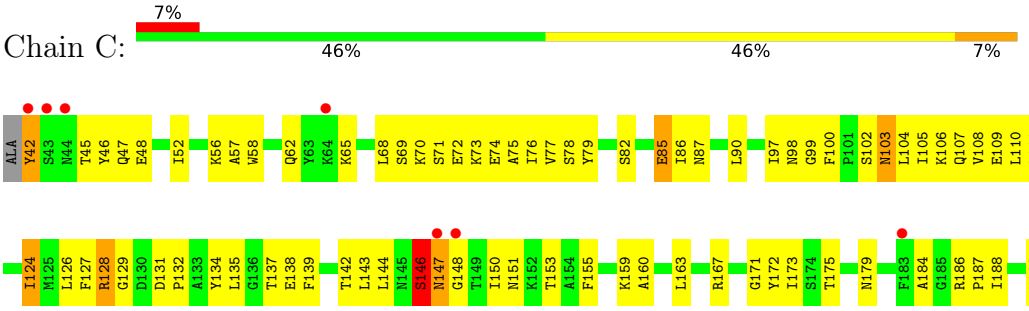
• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3

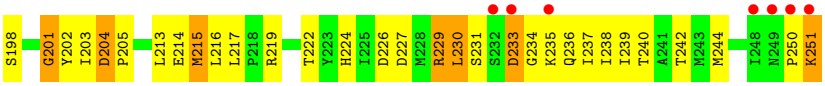
Chain B:



• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3

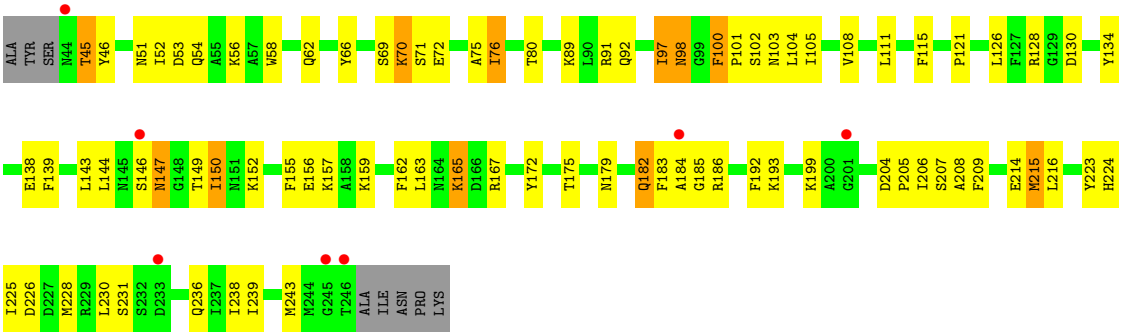
Chain C:





• Molecule 1: MONO-ADP-RIBOSYLTRANSFERASE C3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	109.00Å 75.60Å 123.47Å 90.00° 102.37° 90.00°	Depositor
Resolution (Å)	18.12 – 2.70 19.85 – 2.71	Depositor EDS
% Data completeness (in resolution range)	93.1 (18.12-2.70) 89.9 (19.85-2.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.71Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.290 0.255 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6511	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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: HG

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	0.78	3/1652 (0.2%)	1.55	10/2219 (0.5%)
1	B	0.64	0/1623	0.81	1/2179 (0.0%)
1	C	0.51	0/1681	0.76	2/2257 (0.1%)
1	D	0.57	0/1623	0.79	2/2179 (0.1%)
All	All	0.63	3/6579 (0.0%)	1.03	15/8834 (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	1
1	B	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	ARG	CD-NE	-10.92	1.27	1.46
1	A	186	ARG	NE-CZ	-9.54	1.20	1.33
1	A	186	ARG	CG-CD	5.38	1.65	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	ARG	NE-CZ-NH1	36.97	138.78	120.30
1	A	186	ARG	NE-CZ-NH2	-33.10	103.75	120.30
1	A	186	ARG	CD-NE-CZ	31.86	168.20	123.60
1	A	186	ARG	CG-CD-NE	-8.71	93.51	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	183	PHE	N-CA-C	-8.14	89.01	111.00
1	A	236	GLN	O-C-N	7.78	135.14	122.70
1	A	236	GLN	CA-C-N	-7.09	101.60	117.20
1	B	186	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	C	186	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	A	236	GLN	N-CA-CB	6.51	122.32	110.60
1	A	128	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	A	206	ILE	CB-CA-C	-6.13	99.34	111.60
1	D	91	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	C	234	GLY	N-CA-C	-5.13	100.27	113.10
1	D	76	ILE	CB-CA-C	-5.09	101.43	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	ARG	Sidechain
1	B	187	PRO	Mainchain
1	B	96	VAL	Mainchain

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	1623	0	1633	84	0
1	B	1595	0	1609	84	0
1	C	1651	0	1665	95	0
1	D	1595	0	1609	89	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	7	0	0	0	0
3	B	11	0	0	1	0
3	C	11	0	0	0	0
3	D	14	0	0	0	0
All	All	6511	0	6516	339	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (339) 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:D:150:ILE:HD13	1:D:150:ILE:O	1.48	1.12
1:C:251:LYS:HG3	1:C:251:LYS:O	1.52	1.07
1:B:91:ARG:HG3	1:B:91:ARG:HH11	1.23	1.02
1:D:70:LYS:HD3	1:D:70:LYS:N	1.77	0.99
1:C:251:LYS:O	1:C:251:LYS:CG	2.13	0.97
1:D:182:GLN:HE21	1:D:182:GLN:HA	1.29	0.96
1:A:128:ARG:HH11	1:A:128:ARG:HG3	1.30	0.94
1:A:128:ARG:HH11	1:A:128:ARG:CG	1.82	0.92
1:D:97:ILE:HD13	1:D:97:ILE:H	1.37	0.90
1:C:230:LEU:HD12	1:C:235:LYS:HG2	1.52	0.90
1:B:97:ILE:HD13	1:B:97:ILE:H	1.36	0.89
1:A:203:ILE:HA	1:A:206:ILE:HD13	1.58	0.84
1:B:93:ASN:O	1:B:96:VAL:HG22	1.78	0.83
1:D:101:PRO:O	1:D:105:ILE:HG13	1.79	0.82
1:B:91:ARG:HH11	1:B:91:ARG:CG	1.92	0.81
1:C:150:ILE:HD11	1:C:230:LEU:HD11	1.63	0.80
1:C:128:ARG:HG2	1:C:128:ARG:HH21	1.45	0.80
1:D:102:SER:HA	1:D:105:ILE:HD12	1.64	0.79
1:A:97:ILE:HG22	1:A:105:ILE:HG12	1.64	0.79
1:D:89:LYS:HB3	1:D:100:PHE:HZ	1.48	0.79
1:D:150:ILE:HD12	1:D:150:ILE:H	1.46	0.79
1:C:128:ARG:HH21	1:C:128:ARG:CG	1.96	0.79
1:D:97:ILE:O	1:D:100:PHE:HB2	1.82	0.79
1:D:70:LYS:HD3	1:D:70:LYS:H	1.47	0.78
1:D:89:LYS:HB3	1:D:100:PHE:CZ	2.18	0.78
1:D:152:LYS:O	1:D:156:GLU:HG2	1.84	0.78
1:D:58:TRP:O	1:D:62:GLN:HG2	1.84	0.77
1:A:94:LYS:HG2	1:A:170:TYR:CE2	2.22	0.75
1:A:80:THR:HB	1:A:209:PHE:O	1.86	0.75
1:C:47:GLN:HG3	1:C:48:GLU:N	2.03	0.74
1:A:41:ALA:C	1:A:42:TYR:HD2	1.91	0.73
1:B:128:ARG:HA	1:B:183:PHE:CZ	2.23	0.73
1:B:233:ASP:OD2	1:B:235:LYS:HG2	1.90	0.72
1:B:91:ARG:HG3	1:B:91:ARG:NH1	1.96	0.71
1:D:182:GLN:HE21	1:D:182:GLN:CA	2.01	0.70
1:B:80:THR:HG21	1:B:210:ALA:N	2.06	0.70
1:D:80:THR:HG22	1:D:209:PHE:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LYS:O	1:B:74:GLU:HG3	1.91	0.70
1:A:54:GLN:HG3	1:D:45:THR:HG22	1.72	0.70
1:D:100:PHE:O	1:D:105:ILE:HD11	1.91	0.70
1:C:150:ILE:HD11	1:C:230:LEU:CD1	2.22	0.70
1:A:231:SER:OG	1:A:233:ASP:HB2	1.91	0.69
1:B:183:PHE:O	1:B:186:ARG:HB2	1.93	0.69
1:C:179:ASN:ND2	1:C:184:ALA:HB2	2.07	0.69
1:A:52:ILE:HG12	1:A:178:MET:CE	2.22	0.68
1:A:235:LYS:O	1:A:235:LYS:HG2	1.92	0.68
1:B:80:THR:HG22	1:B:209:PHE:CB	2.23	0.68
1:D:76:ILE:HD13	1:D:111:LEU:CD1	2.24	0.68
1:D:89:LYS:CB	1:D:100:PHE:HZ	2.06	0.68
1:A:81:LYS:NZ	1:A:81:LYS:HB2	2.09	0.68
1:C:104:LEU:HD12	1:C:107:GLN:HB2	1.75	0.68
1:D:150:ILE:HD11	1:D:230:LEU:HD13	1.76	0.67
1:A:97:ILE:HG23	1:A:100:PHE:CD1	2.30	0.67
1:A:97:ILE:HD11	1:A:219:ARG:NH2	2.10	0.67
1:A:207:SER:OG	1:A:210:ALA:HB2	1.95	0.67
1:D:150:ILE:H	1:D:150:ILE:CD1	2.09	0.66
1:A:208:ALA:HB1	1:C:251:LYS:OXT	1.94	0.66
1:C:126:LEU:HD13	1:C:175:THR:OG1	1.94	0.66
1:D:51:ASN:ND2	1:D:54:GLN:H	1.93	0.66
1:D:182:GLN:HA	1:D:182:GLN:NE2	2.09	0.66
1:C:124:ILE:H	1:C:124:ILE:HD13	1.60	0.66
1:D:143:LEU:HD12	1:D:144:LEU:HD12	1.77	0.66
1:B:115:PHE:HB3	1:B:199:LYS:HD3	1.78	0.65
1:A:52:ILE:HG12	1:A:178:MET:HE1	1.77	0.65
1:C:69:SER:O	1:C:73:LYS:HG3	1.97	0.65
1:C:87:ASN:ND2	1:C:172:TYR:H	1.94	0.65
1:D:80:THR:HG22	1:D:209:PHE:CB	2.28	0.64
1:B:80:THR:HG22	1:B:209:PHE:HB3	1.80	0.64
1:C:146:SER:O	1:C:147:ASN:HB2	1.98	0.64
1:C:227:ASP:OD1	1:C:229:ARG:HD2	1.97	0.64
1:D:150:ILE:CD1	1:D:150:ILE:N	2.61	0.64
1:B:168:LEU:HD12	1:B:222:THR:OG1	1.97	0.64
1:C:104:LEU:O	1:C:108:VAL:HG23	1.98	0.63
1:A:128:ARG:HG3	1:A:128:ARG:NH1	2.07	0.63
1:D:128:ARG:HG3	1:D:128:ARG:HH11	1.64	0.63
1:B:86:ILE:HG13	1:B:104:LEU:HD11	1.80	0.63
1:A:227:ASP:HB3	1:A:240:THR:HB	1.81	0.62
1:B:204:ASP:N	1:B:205:PRO:HD2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ASN:N	1:D:98:ASN:HD22	1.97	0.62
1:D:231:SER:HB3	1:D:236:GLN:HG3	1.81	0.62
1:C:144:LEU:HG	1:C:150:ILE:HG22	1.81	0.62
1:B:163:LEU:HD21	1:C:163:LEU:HD21	1.81	0.62
1:B:150:ILE:O	1:B:150:ILE:HD12	2.00	0.61
1:C:251:LYS:O	1:C:251:LYS:HD2	2.01	0.61
1:B:50:THR:HA	1:B:178:MET:HE3	1.81	0.61
1:C:250:PRO:O	1:C:251:LYS:HB3	2.00	0.61
1:C:251:LYS:O	1:C:251:LYS:CD	2.48	0.61
1:C:58:TRP:O	1:C:62:GLN:HG2	2.01	0.61
1:A:54:GLN:NE2	1:D:45:THR:HG23	2.15	0.60
1:C:87:ASN:HD21	1:C:172:TYR:H	1.49	0.60
1:B:162:PHE:HB3	1:B:225:ILE:HD12	1.81	0.60
1:B:182:GLN:HG3	1:B:182:GLN:O	2.00	0.60
1:A:58:TRP:O	1:A:62:GLN:HG2	2.00	0.60
1:B:94:LYS:HG3	1:B:170:TYR:CE1	2.36	0.60
1:B:73:LYS:O	1:B:77:VAL:HG23	2.01	0.60
1:A:144:LEU:CD2	1:A:235:LYS:HE3	2.31	0.60
1:C:103:ASN:C	1:C:103:ASN:HD22	2.03	0.60
1:A:104:LEU:O	1:A:108:VAL:HG23	2.01	0.59
1:A:42:TYR:N	1:A:42:TYR:CD2	2.67	0.59
1:B:128:ARG:HA	1:B:183:PHE:CE2	2.36	0.59
1:B:180:VAL:HG11	1:B:212:GLN:HB3	1.83	0.59
1:B:97:ILE:O	1:B:100:PHE:HB2	2.03	0.59
1:C:238:ILE:HG22	1:C:238:ILE:O	2.01	0.59
1:B:51:ASN:CB	1:B:54:GLN:HG2	2.31	0.59
1:B:80:THR:HG21	1:B:209:PHE:C	2.23	0.59
1:B:82:SER:O	1:B:86:ILE:HD13	2.02	0.58
1:C:128:ARG:CG	1:C:128:ARG:NH2	2.61	0.58
1:B:122:GLU:O	1:B:124:ILE:HG23	2.03	0.58
1:D:80:THR:CG2	1:D:209:PHE:HB2	2.34	0.58
1:D:238:ILE:O	1:D:238:ILE:HG22	2.02	0.58
1:B:80:THR:CG2	1:B:209:PHE:C	2.73	0.57
1:D:97:ILE:HD13	1:D:97:ILE:N	2.13	0.57
1:C:231:SER:C	1:C:233:ASP:H	2.07	0.57
1:D:128:ARG:HG3	1:D:128:ARG:NH1	2.19	0.57
1:C:187:PRO:HB2	1:C:188:ILE:HD12	1.86	0.57
1:A:54:GLN:HE21	1:D:45:THR:HG23	1.70	0.57
1:A:85:GLU:HB2	1:C:98:ASN:HD22	1.69	0.57
1:D:70:LYS:H	1:D:70:LYS:CD	2.13	0.57
1:C:230:LEU:CD1	1:C:235:LYS:HG2	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ASP:N	1:C:205:PRO:HD2	2.20	0.56
1:B:89:LYS:HG2	1:B:100:PHE:CE1	2.40	0.56
1:C:135:LEU:HD12	1:C:143:LEU:HD11	1.86	0.56
1:D:146:SER:O	1:D:147:ASN:HB3	2.06	0.56
1:B:113:LYS:O	1:B:116:ASN:HB2	2.05	0.56
1:D:80:THR:CG2	1:D:209:PHE:CB	2.84	0.56
1:D:204:ASP:N	1:D:205:PRO:HD2	2.21	0.56
1:C:138:GLU:HG3	1:C:139:PHE:CD1	2.41	0.56
1:B:196:LYS:O	1:B:196:LYS:HG3	2.06	0.56
1:C:188:ILE:HD12	1:C:188:ILE:N	2.21	0.55
1:D:206:ILE:HG22	1:D:206:ILE:O	2.06	0.55
1:A:206:ILE:H	1:A:206:ILE:HD12	1.71	0.55
1:D:46:TYR:CE1	1:D:193:LYS:HB3	2.41	0.55
1:B:69:SER:HB2	1:B:72:GLU:HG3	1.88	0.55
1:D:192:PHE:CD1	1:D:243:MET:HE1	2.42	0.55
1:A:81:LYS:HD3	1:A:209:PHE:CD1	2.42	0.55
1:B:132:PRO:HD3	1:B:187:PRO:HG2	1.88	0.55
1:A:150:ILE:CD1	1:A:237:ILE:HG13	2.38	0.54
1:D:51:ASN:HD22	1:D:54:GLN:H	1.54	0.54
1:B:94:LYS:HG3	1:B:170:TYR:CZ	2.42	0.54
1:D:162:PHE:O	1:D:165:LYS:HB2	2.08	0.54
1:B:127:PHE:O	1:B:128:ARG:HB3	2.07	0.54
1:B:161:LYS:HD3	1:B:162:PHE:CE2	2.42	0.54
1:C:104:LEU:HG	1:C:108:VAL:HG23	1.89	0.54
1:A:78:SER:HB3	1:A:107:GLN:OE1	2.08	0.53
1:B:144:LEU:CD1	1:B:150:ILE:HG22	2.38	0.53
1:D:231:SER:CB	1:D:236:GLN:HG3	2.38	0.53
1:A:139:PHE:CE2	1:A:158:ALA:HB2	2.44	0.53
1:C:230:LEU:HD12	1:C:235:LYS:CG	2.32	0.53
1:A:41:ALA:C	1:A:42:TYR:CD2	2.77	0.53
1:B:164:ASN:HD21	1:C:160:ALA:HA	1.74	0.53
1:B:144:LEU:HD12	1:B:150:ILE:HG22	1.90	0.53
1:C:144:LEU:HD23	1:C:148:GLY:O	2.09	0.52
1:B:97:ILE:HD13	1:B:97:ILE:N	2.16	0.52
1:D:134:TYR:CE1	1:D:167:ARG:NH1	2.78	0.52
1:D:70:LYS:N	1:D:70:LYS:CD	2.55	0.52
1:A:144:LEU:HD21	1:A:235:LYS:HE3	1.92	0.52
1:C:124:ILE:CD1	1:C:194:VAL:HB	2.40	0.52
1:D:98:ASN:C	1:D:100:PHE:H	2.13	0.52
1:D:115:PHE:CZ	1:D:216:LEU:HD23	2.45	0.52
1:A:78:SER:HA	1:A:81:LYS:NZ	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLY:O	1:A:235:LYS:HD2	2.10	0.52
1:B:80:THR:CG2	1:B:209:PHE:HB2	2.40	0.52
1:B:206:ILE:O	1:B:206:ILE:HG22	2.09	0.52
1:C:155:PHE:CZ	1:C:159:LYS:HE3	2.45	0.52
1:C:201:GLY:O	1:C:203:ILE:HG23	2.09	0.52
1:B:51:ASN:HB3	1:B:54:GLN:HG2	1.92	0.52
1:C:144:LEU:HD12	1:C:144:LEU:N	2.25	0.52
1:A:131:ASP:HB3	1:A:132:PRO:HD2	1.92	0.51
1:D:80:THR:HG22	1:D:80:THR:O	2.10	0.51
1:D:80:THR:HG21	1:D:209:PHE:HB2	1.92	0.51
1:C:103:ASN:C	1:C:103:ASN:ND2	2.63	0.51
1:A:81:LYS:HB2	1:A:81:LYS:HZ2	1.74	0.51
1:A:42:TYR:HD2	1:A:42:TYR:N	2.07	0.51
1:C:42:TYR:HB3	1:C:193:LYS:NZ	2.25	0.51
1:C:69:SER:OG	1:C:72:GLU:HG3	2.11	0.51
1:D:143:LEU:HD13	1:D:143:LEU:O	2.11	0.51
1:B:126:LEU:HD13	1:B:175:THR:OG1	2.11	0.50
1:D:192:PHE:CD1	1:D:243:MET:CE	2.94	0.50
1:A:128:ARG:CG	1:A:128:ARG:NH1	2.51	0.50
1:B:135:LEU:HD12	1:B:143:LEU:CD1	2.41	0.50
1:C:173:ILE:HB	1:C:217:LEU:HB2	1.93	0.50
1:C:222:THR:O	1:C:244:MET:HB2	2.11	0.50
1:D:155:PHE:O	1:D:159:LYS:HG3	2.11	0.50
1:A:142:THR:HG22	1:A:154:ALA:HB2	1.94	0.50
1:A:242:THR:O	1:A:242:THR:HG22	2.11	0.50
1:C:120:THR:HG22	1:C:198:SER:O	2.12	0.50
1:C:79:TYR:CE2	1:C:216:LEU:HD11	2.47	0.50
1:A:138:GLU:HG2	1:A:139:PHE:CD1	2.47	0.50
1:B:91:ARG:CG	1:B:91:ARG:NH1	2.62	0.50
1:D:150:ILE:HD13	1:D:150:ILE:C	2.14	0.50
1:D:150:ILE:O	1:D:150:ILE:CD1	2.39	0.50
1:B:204:ASP:N	1:B:205:PRO:CD	2.74	0.50
1:B:80:THR:HG22	1:B:209:PHE:HB2	1.94	0.49
1:B:150:ILE:HD11	1:B:230:LEU:CD1	2.42	0.49
1:B:150:ILE:HD11	1:B:230:LEU:CD2	2.42	0.49
1:B:203:ILE:HD11	1:B:214:GLU:OE2	2.13	0.49
1:A:73:LYS:O	1:A:77:VAL:HG23	2.13	0.49
1:A:81:LYS:HD3	1:A:209:PHE:HD1	1.78	0.49
1:A:52:ILE:HG12	1:A:178:MET:HE2	1.94	0.49
1:C:151:ASN:OD1	1:C:153:THR:HB	2.13	0.49
1:A:91:ARG:HA	1:A:170:TYR:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:PHE:O	1:B:178:MET:HE3	2.13	0.49
1:C:47:GLN:HG3	1:C:48:GLU:H	1.74	0.49
1:C:171:GLY:O	1:C:219:ARG:HA	2.12	0.49
1:C:73:LYS:O	1:C:77:VAL:HG23	2.12	0.49
1:D:108:VAL:HG13	1:D:172:TYR:OH	2.13	0.49
1:A:161:LYS:HE2	1:A:162:PHE:CZ	2.48	0.49
1:B:97:ILE:H	1:B:97:ILE:CD1	2.17	0.48
1:D:228:MET:HG2	1:D:239:ILE:HG13	1.95	0.48
1:A:79:TYR:O	1:A:79:TYR:CG	2.67	0.48
1:C:128:ARG:HG2	1:C:129:GLY:N	2.29	0.48
1:D:182:GLN:CA	1:D:182:GLN:NE2	2.67	0.48
1:B:123:ASN:OD1	1:B:196:LYS:HB3	2.14	0.48
1:C:72:GLU:O	1:C:76:ILE:HD13	2.14	0.48
1:A:173:ILE:HB	1:A:217:LEU:HB2	1.95	0.48
1:B:51:ASN:CB	1:B:54:GLN:CG	2.92	0.48
1:C:82:SER:O	1:C:86:ILE:HG13	2.13	0.47
1:D:115:PHE:HZ	1:D:216:LEU:HD23	1.79	0.47
1:D:51:ASN:HD21	1:D:53:ASP:HB2	1.79	0.47
1:C:100:PHE:N	1:C:100:PHE:CD2	2.82	0.47
1:C:202:TYR:CE2	1:C:205:PRO:HD3	2.49	0.47
1:D:98:ASN:N	1:D:98:ASN:ND2	2.62	0.47
1:B:139:PHE:HA	1:B:142:THR:HB	1.97	0.47
1:C:52:ILE:O	1:C:56:LYS:HG3	2.15	0.47
1:D:150:ILE:HD11	1:D:230:LEU:CD1	2.41	0.47
1:C:134:TYR:CZ	1:C:167:ARG:NH1	2.83	0.47
1:A:52:ILE:CG1	1:A:178:MET:HE1	2.44	0.47
1:A:150:ILE:HG13	1:A:235:LYS:HA	1.95	0.47
1:A:204:ASP:HB3	1:A:205:PRO:HD3	1.97	0.47
1:A:78:SER:HA	1:A:81:LYS:HZ2	1.79	0.46
1:B:80:THR:CG2	1:B:209:PHE:CB	2.90	0.46
1:D:103:ASN:CG	1:D:104:LEU:H	2.18	0.46
1:B:51:ASN:CG	1:B:54:GLN:HG2	2.36	0.46
1:B:170:TYR:O	1:B:219:ARG:HB2	2.15	0.46
1:C:142:THR:O	1:C:142:THR:HG22	2.14	0.46
1:B:87:ASN:O	1:B:91:ARG:HG2	2.15	0.46
1:B:52:ILE:HG22	1:B:56:LYS:HE3	1.98	0.46
1:C:196:LYS:HB3	1:C:196:LYS:HE3	1.76	0.46
1:A:144:LEU:HD21	1:A:187:PRO:HB3	1.96	0.46
1:A:177:CYS:SG	1:A:215:MET:SD	3.12	0.46
1:C:224:HIS:HD2	1:C:226:ASP:OD1	1.99	0.46
1:C:214:GLU:CG	1:C:215:MET:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLU:HA	3:B:2009:HOH:O	2.15	0.46
1:B:203:ILE:HD11	1:B:214:GLU:CD	2.37	0.45
1:A:128:ARG:HH11	1:A:128:ARG:HG2	1.74	0.45
1:A:125:MET:HA	1:A:192:PHE:O	2.16	0.45
1:A:150:ILE:HD13	1:A:237:ILE:HG13	1.97	0.45
1:C:75:ALA:O	1:C:78:SER:HB3	2.17	0.45
1:D:192:PHE:HD1	1:D:243:MET:CE	2.30	0.45
1:D:97:ILE:H	1:D:97:ILE:CD1	2.18	0.45
1:D:207:SER:OG	1:D:209:PHE:HB2	2.16	0.45
1:D:51:ASN:HD22	1:D:54:GLN:HG3	1.81	0.45
1:D:115:PHE:HB3	1:D:199:LYS:HD3	1.99	0.45
1:A:54:GLN:HG3	1:D:45:THR:CG2	2.43	0.45
1:A:214:GLU:HG3	1:A:215:MET:N	2.32	0.45
1:D:159:LYS:O	1:D:163:LEU:HB2	2.17	0.45
1:C:124:ILE:HD11	1:C:194:VAL:HB	1.98	0.45
1:A:80:THR:HG21	1:A:207:SER:OG	2.17	0.44
1:B:224:HIS:HD2	1:B:226:ASP:OD1	2.00	0.44
1:A:173:ILE:HG22	1:A:175:THR:CG2	2.47	0.44
1:A:63:TYR:CE1	1:A:206:ILE:HD11	2.52	0.44
1:A:81:LYS:HB2	1:A:81:LYS:HZ3	1.82	0.44
1:C:97:ILE:C	1:C:99:GLY:H	2.21	0.44
1:C:124:ILE:HD13	1:C:124:ILE:N	2.29	0.44
1:C:214:GLU:HG3	1:C:215:MET:H	1.81	0.44
1:C:242:THR:HG22	1:C:242:THR:O	2.18	0.44
1:D:89:LYS:CB	1:D:100:PHE:CZ	2.89	0.44
1:B:120:THR:HG23	1:B:197:GLY:H	1.82	0.44
1:C:72:GLU:O	1:C:75:ALA:HB3	2.17	0.44
1:D:97:ILE:N	1:D:97:ILE:CD1	2.80	0.44
1:C:131:ASP:HB3	1:C:132:PRO:CD	2.48	0.44
1:C:150:ILE:CD1	1:C:237:ILE:HG12	2.48	0.44
1:C:239:ILE:HG22	1:C:240:THR:N	2.33	0.44
1:A:202:TYR:CE2	1:A:204:ASP:HB3	2.52	0.43
1:C:106:LYS:O	1:C:110:LEU:HG	2.18	0.43
1:C:65:LYS:HD2	1:D:147:ASN:HA	2.00	0.43
1:B:203:ILE:HD13	1:B:214:GLU:O	2.18	0.43
1:C:90:LEU:HD21	1:C:219:ARG:HH11	1.84	0.43
1:B:164:ASN:ND2	1:C:160:ALA:HA	2.33	0.43
1:D:204:ASP:N	1:D:205:PRO:CD	2.81	0.43
1:B:129:GLY:HA2	1:B:188:ILE:O	2.18	0.43
1:C:231:SER:OG	1:C:235:LYS:HA	2.19	0.43
1:A:98:ASN:OD1	1:A:98:ASN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:GLN:CG	1:C:48:GLU:N	2.77	0.43
1:D:225:ILE:HD12	1:D:225:ILE:N	2.32	0.43
1:C:85:GLU:HG3	1:C:86:ILE:N	2.29	0.43
1:C:138:GLU:HG3	1:C:139:PHE:CE1	2.53	0.43
1:D:224:HIS:HD2	1:D:226:ASP:OD1	2.01	0.43
1:A:140:GLN:HE21	1:A:140:GLN:HB2	1.60	0.43
1:D:138:GLU:HG2	1:D:139:PHE:N	2.33	0.43
1:A:46:TYR:CE2	1:A:193:LYS:HB3	2.54	0.42
1:D:138:GLU:HG2	1:D:139:PHE:H	1.84	0.42
1:B:80:THR:HG22	1:B:80:THR:O	2.19	0.42
1:A:224:HIS:CD2	1:A:226:ASP:OD2	2.72	0.42
1:B:81:LYS:HE2	1:B:209:PHE:CE2	2.55	0.42
1:C:127:PHE:CD1	1:C:127:PHE:N	2.87	0.42
1:B:203:ILE:HD13	1:B:203:ILE:H	1.85	0.42
1:A:96:VAL:HG13	1:A:98:ASN:CG	2.40	0.42
1:A:132:PRO:HD3	1:A:187:PRO:HG2	2.02	0.42
1:A:54:GLN:HE21	1:D:45:THR:CG2	2.33	0.42
1:A:87:ASN:HA	1:A:90:LEU:HD12	2.00	0.42
1:A:235:LYS:O	1:A:236:GLN:HG3	2.19	0.42
1:C:100:PHE:N	1:C:100:PHE:HD2	2.18	0.42
1:A:41:ALA:O	1:A:42:TYR:HD2	2.02	0.42
1:B:150:ILE:HD12	1:B:150:ILE:C	2.39	0.42
1:C:131:ASP:HB3	1:C:132:PRO:HD2	2.02	0.42
1:D:126:LEU:HD13	1:D:175:THR:OG1	2.19	0.42
1:C:131:ASP:O	1:C:134:TYR:HB3	2.19	0.42
1:B:51:ASN:HB3	1:B:54:GLN:H	1.83	0.41
1:C:179:ASN:HD22	1:C:184:ALA:HB2	1.82	0.41
1:A:77:VAL:HA	1:A:207:SER:HB3	2.01	0.41
1:D:214:GLU:HG2	1:D:215:MET:N	2.35	0.41
1:B:101:PRO:O	1:B:105:ILE:HG13	2.21	0.41
1:B:125:MET:CE	1:B:193:LYS:HG2	2.50	0.41
1:D:183:PHE:C	1:D:185:GLY:H	2.23	0.41
1:A:92:GLN:C	1:A:94:LYS:H	2.23	0.41
1:B:97:ILE:HG22	1:B:100:PHE:CE2	2.56	0.41
1:B:185:GLY:O	1:B:186:ARG:HG3	2.21	0.41
1:A:189:ILE:HD13	1:A:189:ILE:HA	1.91	0.41
1:B:50:THR:O	1:B:50:THR:OG1	2.37	0.41
1:B:157:LYS:HE2	1:D:208:ALA:O	2.21	0.41
1:C:70:LYS:O	1:C:74:GLU:HG2	2.21	0.41
1:C:105:ILE:O	1:C:109:GLU:HG3	2.21	0.41
1:D:231:SER:HB3	1:D:238:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLU:OE1	1:C:98:ASN:HB3	2.21	0.41
1:D:72:GLU:O	1:D:75:ALA:HB3	2.21	0.41
1:D:192:PHE:HD1	1:D:243:MET:HE2	1.86	0.41
1:B:186:ARG:HA	1:B:187:PRO:HD3	1.97	0.40
1:A:81:LYS:NZ	1:A:81:LYS:CB	2.82	0.40
1:C:46:TYR:CE1	1:C:193:LYS:HB3	2.56	0.40
1:D:179:ASN:ND2	1:D:184:ALA:HB2	2.37	0.40
1:C:76:ILE:HD12	1:C:76:ILE:H	1.86	0.40
1:A:100:PHE:HB2	1:A:105:ILE:HG12	2.03	0.40
1:A:150:ILE:HD11	1:A:236:GLN:HA	2.04	0.40
1:A:231:SER:C	1:A:233:ASP:H	2.24	0.40
1:B:50:THR:CA	1:B:178:MET:HE3	2.46	0.40
1:C:76:ILE:HD12	1:C:76:ILE:N	2.35	0.40
1:D:159:LYS:O	1:D:163:LEU:CB	2.69	0.40
1:A:94:LYS:HG2	1:A:170:TYR:CZ	2.55	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	205/211 (97%)	175 (85%)	26 (13%)	4 (2%)	7 19
1	B	201/211 (95%)	181 (90%)	17 (8%)	3 (2%)	10 26
1	C	208/211 (99%)	175 (84%)	28 (14%)	5 (2%)	6 15
1	D	201/211 (95%)	173 (86%)	25 (12%)	3 (2%)	10 26
All	All	815/844 (97%)	704 (86%)	96 (12%)	15 (2%)	8 21

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	147	ASN
1	D	147	ASN
1	B	181	SER
1	D	66	TYR
1	A	65	LYS
1	A	92	GLN
1	A	236	GLN
1	B	94	LYS
1	C	146	SER
1	C	57	ALA
1	B	92	GLN
1	D	69	SER
1	C	213	LEU
1	A	99	GLY
1	C	201	GLY

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	175/179 (98%)	156 (89%)	19 (11%)	6 14
1	B	173/179 (97%)	158 (91%)	15 (9%)	10 23
1	C	179/179 (100%)	158 (88%)	21 (12%)	5 12
1	D	173/179 (97%)	154 (89%)	19 (11%)	6 14
All	All	700/716 (98%)	626 (89%)	74 (11%)	6 15

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	A	45	THR
1	A	84	SER
1	A	92	GLN
1	A	94	LYS
1	A	98	ASN
1	A	103	ASN

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Mol	Chain	Res	Type
1	A	120	THR
1	A	125	MET
1	A	128	ARG
1	A	137	THR
1	A	143	LEU
1	A	157	LYS
1	A	182	GLN
1	A	186	ARG
1	A	215	MET
1	A	233	ASP
1	A	242	THR
1	A	246	THR
1	B	44	ASN
1	B	45	THR
1	B	50	THR
1	B	51	ASN
1	B	78	SER
1	B	91	ARG
1	B	93	ASN
1	B	97	ILE
1	B	116	ASN
1	B	122	GLU
1	B	143	LEU
1	B	168	LEU
1	B	182	GLN
1	B	203	ILE
1	B	244	MET
1	C	42	TYR
1	C	45	THR
1	C	68	LEU
1	C	71	SER
1	C	85	GLU
1	C	102	SER
1	C	103	ASN
1	C	111	LEU
1	C	114	SER
1	C	124	ILE
1	C	128	ARG
1	C	137	THR
1	C	146	SER
1	C	196	LYS
1	C	204	ASP

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Mol	Chain	Res	Type
1	C	215	MET
1	C	229	ARG
1	C	230	LEU
1	C	233	ASP
1	C	236	GLN
1	C	251	LYS
1	D	45	THR
1	D	52	ILE
1	D	56	LYS
1	D	70	LYS
1	D	71	SER
1	D	92	GLN
1	D	97	ILE
1	D	98	ASN
1	D	100	PHE
1	D	121	PRO
1	D	130	ASP
1	D	149	THR
1	D	150	ILE
1	D	157	LYS
1	D	165	LYS
1	D	182	GLN
1	D	186	ARG
1	D	215	MET
1	D	223	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	47	GLN
1	A	54	GLN
1	A	92	GLN
1	A	140	GLN
1	A	164	ASN
1	A	182	GLN
1	B	54	GLN
1	B	60	ASN
1	B	92	GLN
1	B	93	ASN
1	B	140	GLN
1	B	141	ASN

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Mol	Chain	Res	Type
1	B	164	ASN
1	B	182	GLN
1	B	224	HIS
1	C	47	GLN
1	C	54	GLN
1	C	60	ASN
1	C	87	ASN
1	C	103	ASN
1	C	140	GLN
1	C	179	ASN
1	C	182	GLN
1	C	220	HIS
1	C	236	GLN
1	D	44	ASN
1	D	47	GLN
1	D	51	ASN
1	D	54	GLN
1	D	60	ASN
1	D	98	ASN
1	D	140	GLN
1	D	179	ASN
1	D	182	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	207/211 (98%)	0.32	14 (6%)	17	15	38, 63, 86, 99	0
1	B	203/211 (96%)	0.08	6 (2%)	50	51	27, 58, 84, 91	0
1	C	210/211 (99%)	0.31	14 (6%)	17	16	39, 64, 89, 96	0
1	D	203/211 (96%)	0.04	7 (3%)	45	45	25, 52, 79, 91	0
All	All	823/844 (97%)	0.19	41 (4%)	28	27	25, 60, 86, 99	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	43	SER	7.6
1	A	41	ALA	7.5
1	A	42	TYR	6.6
1	C	42	TYR	6.2
1	A	43	SER	5.4
1	C	147	ASN	4.6
1	D	44	ASN	4.1
1	A	208	ALA	4.0
1	A	247	ALA	3.8
1	A	209	PHE	3.8
1	A	44	ASN	3.6
1	C	44	ASN	3.3
1	B	44	ASN	3.0
1	D	245	GLY	2.9
1	A	201	GLY	2.8
1	C	148	GLY	2.8
1	C	249	ASN	2.8
1	B	94	LYS	2.7
1	B	98	ASN	2.6
1	C	251	LYS	2.6
1	C	233	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	246	THR	2.5
1	D	201	GLY	2.4
1	D	246	THR	2.4
1	C	232	SER	2.4
1	C	250	PRO	2.4
1	A	70	LYS	2.4
1	D	233	ASP	2.3
1	D	184	ALA	2.3
1	B	64	LYS	2.3
1	A	232	SER	2.2
1	A	200	ALA	2.2
1	C	235	LYS	2.2
1	C	183	PHE	2.2
1	D	146	SER	2.2
1	C	248	ILE	2.1
1	B	103	ASN	2.1
1	B	107	GLN	2.1
1	A	122	GLU	2.0
1	C	64	LYS	2.0
1	A	207	SER	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	HG	A	1248	1/1	0.98	0.06	62,62,62,62	0
2	HG	B	1247	1/1	0.98	0.11	81,81,81,81	0
2	HG	C	1252	1/1	0.99	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HG	D	1247	1/1	0.99	0.10	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.