Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 03:54 PM EDT

PDB ID	:	6UBN
Title	:	Crystal structure of D678E GoxA bound to glycine
Authors	:	Yukl, E.T.
Deposited on	:	2019-09-12
Resolution	:	2.15 Å(reported)

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

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

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

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

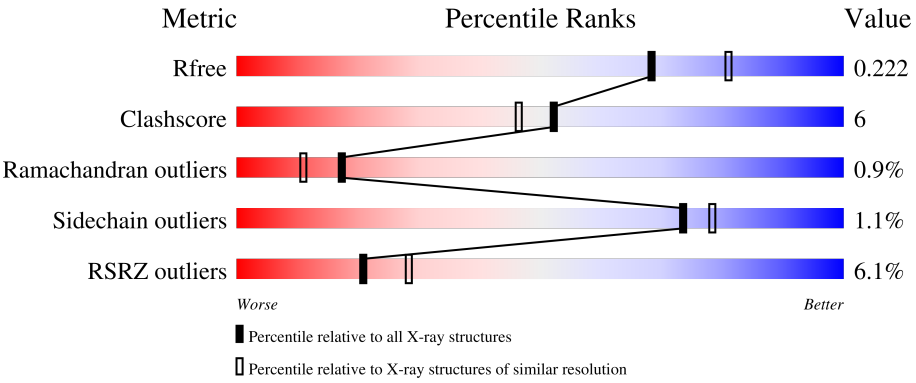
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	816	4% 84% 11% ·
1	B	816	6% 84% 12% · ·
1	C	816	5% 85% 9% 6%
1	D	816	8% 82% 13% · ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26439 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 Quinoprotein glycine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	784	Total	C	N	O	S	0	1	0
			6211	3929	1055	1207	20			
1	B	791	Total	C	N	O	S	0	1	0
			6268	3961	1066	1221	20			
1	C	771	Total	C	N	O	S	0	1	0
			6097	3855	1037	1185	20			
1	D	787	Total	C	N	O	S	0	1	0
			6234	3938	1062	1214	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	678	GLU	ASP	engineered mutation	UNP A0A161XU12
B	678	GLU	ASP	engineered mutation	UNP A0A161XU12
C	678	GLU	ASP	engineered mutation	UNP A0A161XU12
D	678	GLU	ASP	engineered mutation	UNP A0A161XU12

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0

- Molecule 4 is water.

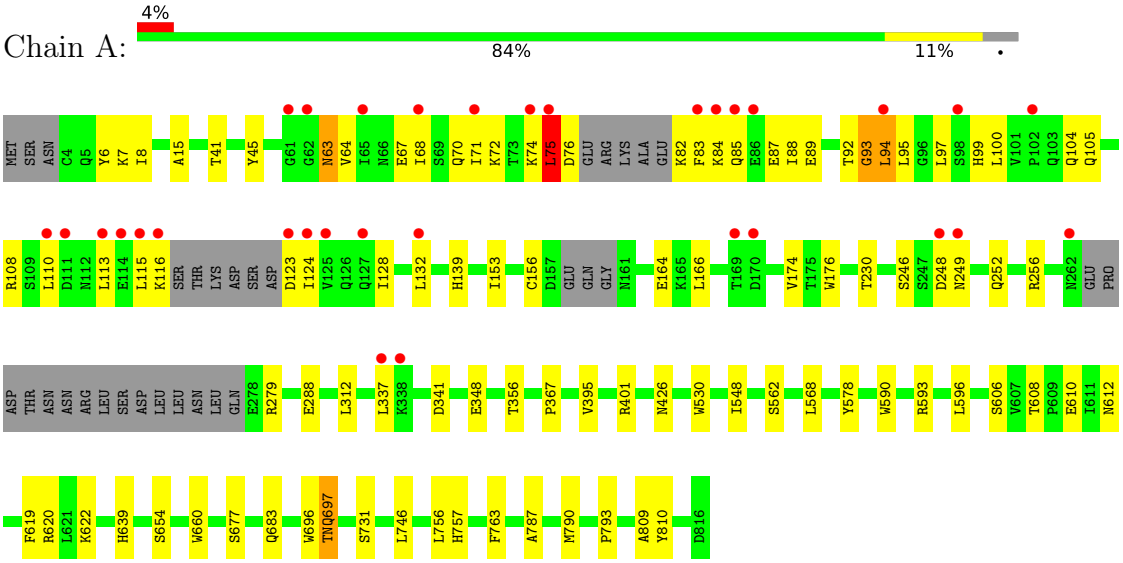
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	436	Total O 436 436	0	0
4	B	422	Total O 422 422	0	0
4	C	411	Total O 411 411	0	0
4	D	355	Total O 355 355	0	0

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.

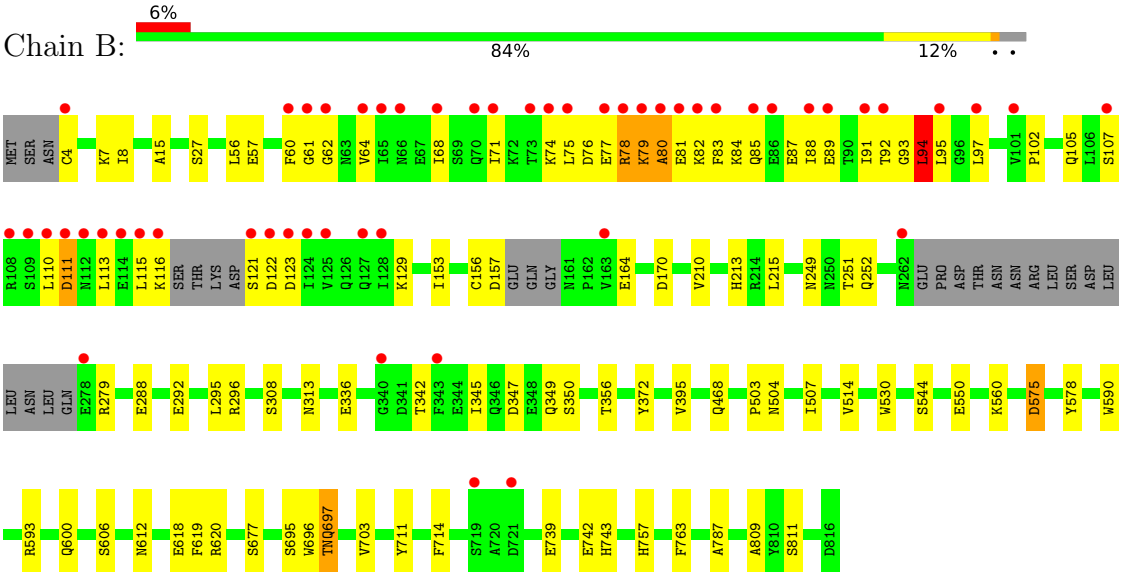
• Molecule 1: Quinoprotein glycine oxidase

Chain A:



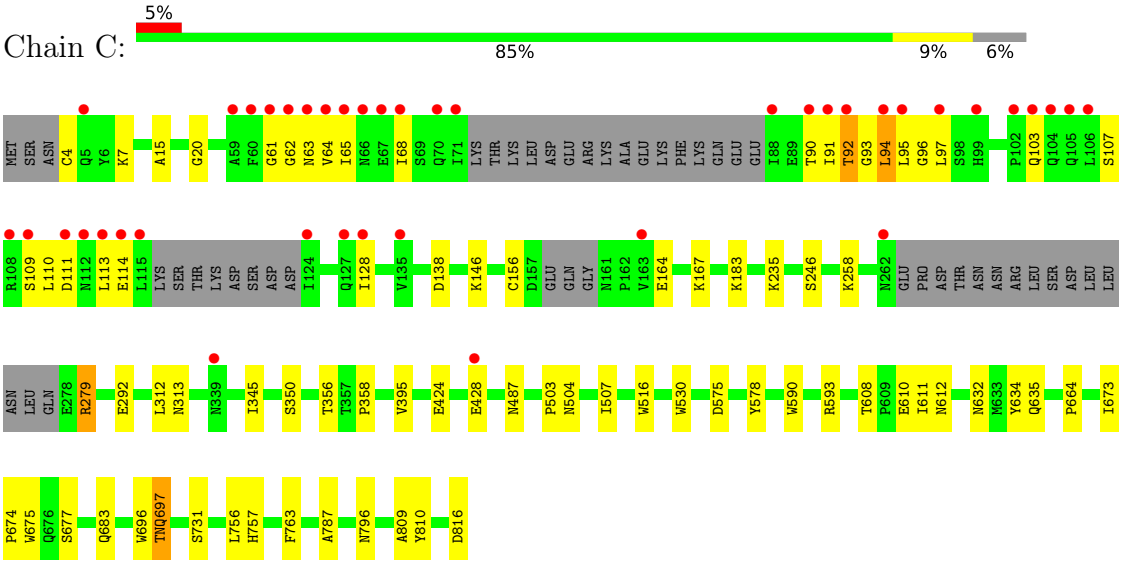
• Molecule 1: Quinoprotein glycine oxidase

Chain B:



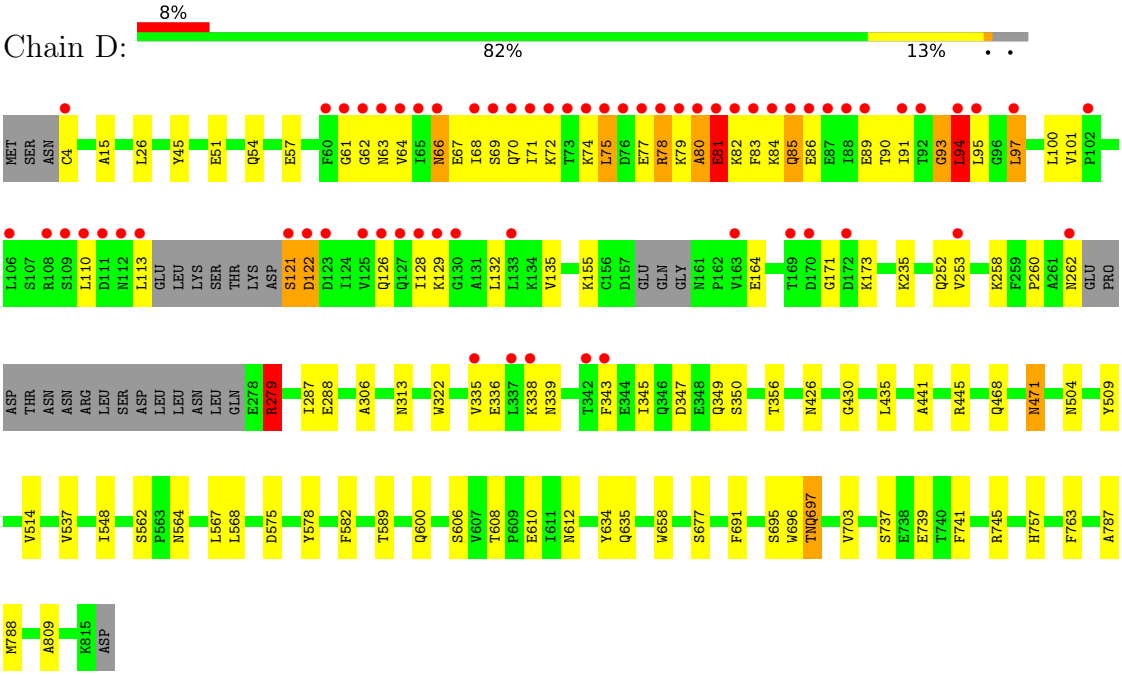
• Molecule 1: Quinoprotein glycine oxidase

Chain C:



• Molecule 1: Quinoprotein glycine oxidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	110.24Å 92.13Å 178.44Å 90.00° 91.16° 90.00°	Depositor
Resolution (Å)	47.31 – 2.15 47.31 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.7 (47.31-2.15) 95.7 (47.31-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.170 , 0.222 0.170 , 0.222	Depositor DCC
R_{free} test set	9338 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.789	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26439	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TNQ, MG, NA

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	0.30	0/6338	0.53	1/8625 (0.0%)
1	B	0.34	2/6396 (0.0%)	0.52	2/8703 (0.0%)
1	C	0.30	0/6223	0.51	0/8475
1	D	0.29	0/6362	0.53	3/8658 (0.0%)
All	All	0.31	2/25319 (0.0%)	0.52	6/34461 (0.0%)

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	3
1	B	0	2
1	C	0	2
1	D	0	4
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	ARG	CB-CG	-8.84	1.28	1.52
1	B	78	ARG	CD-NE	-5.46	1.37	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	75	LEU	CA-CB-CG	11.37	141.44	115.30
1	B	78	ARG	CG-CD-NE	-7.13	96.83	111.80
1	D	81	GLU	CA-CB-CG	6.83	128.42	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	75	LEU	CB-CG-CD1	-5.58	101.52	111.00
1	D	80	ALA	C-N-CA	5.35	135.09	121.70
1	B	80	ALA	C-N-CA	5.34	135.06	121.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	ASN	Peptide
1	A	75	LEU	Peptide
1	A	93	GLY	Peptide
1	B	79	LYS	Peptide
1	B	94	LEU	Peptide
1	C	111	ASP	Peptide
1	C	91	ILE	Peptide
1	D	81	GLU	Peptide
1	D	93	GLY	Peptide
1	D	94	LEU	Peptide
1	D	97	LEU	Peptide

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	6211	0	5976	67	0
1	B	6268	0	6028	75	0
1	C	6097	0	5851	47	0
1	D	6234	0	5990	84	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	B	1	0	0	0	0
4	A	436	0	0	2	0
4	B	422	0	0	4	0
4	C	411	0	0	2	0
4	D	355	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	26439	0	23845	268	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 6.

All (268) 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:80:ALA:HB1	1:D:81:GLU:HB2	1.42	1.01
1:D:80:ALA:CB	1:D:81:GLU:HB2	2.00	0.91
1:D:75:LEU:HD11	1:D:80:ALA:HB3	1.54	0.90
1:B:336:GLU:HG2	1:B:342:THR:HG22	1.54	0.90
1:C:92:THR:HG22	1:C:103:GLN:HE22	1.39	0.88
1:B:349:GLN:HE22	1:B:600:GLN:HB2	1.42	0.84
1:B:88:ILE:HD12	1:B:107:SER:HB2	1.61	0.82
1:B:83:PHE:HB3	1:B:87:GLU:HG3	1.63	0.79
1:B:71:ILE:HD11	1:B:87:GLU:HB2	1.65	0.78
1:C:65:ILE:HA	1:C:68:ILE:HD12	1.64	0.78
1:D:86:GLU:HA	1:D:89:GLU:HB2	1.67	0.77
1:D:70:GLN:OE1	1:D:74:LYS:NZ	2.15	0.77
1:D:75:LEU:C	1:D:75:LEU:HD13	2.07	0.76
1:C:612:ASN:ND2	4:C:1002:HOH:O	2.20	0.74
1:B:503:PRO:HB3	1:B:507:ILE:HD12	1.69	0.74
1:A:71:ILE:HA	1:A:74:LYS:HB2	1.71	0.73
1:A:312:LEU:HD11	1:C:312:LEU:HD11	1.69	0.73
1:B:71:ILE:HD11	1:B:87:GLU:CB	2.19	0.73
1:A:596:LEU:HD23	1:A:660:TRP:CE2	2.23	0.73
1:B:74:LYS:HA	1:B:77:GLU:HG3	1.71	0.73
1:B:68:ILE:HA	1:B:71:ILE:HG22	1.72	0.72
1:B:116:LYS:O	4:B:1001:HOH:O	2.08	0.72
1:D:84:LYS:HG3	1:D:85:GLN:H	1.54	0.71
1:C:95:LEU:O	1:C:97:LEU:N	2.23	0.71
1:A:608:THR:HG22	1:A:610:GLU:H	1.54	0.70
1:D:80:ALA:CA	1:D:81:GLU:HB2	2.22	0.69
1:A:71:ILE:O	1:A:75:LEU:HB2	1.94	0.68
1:C:167:LYS:NZ	1:C:292:GLU:OE1	2.27	0.67
1:D:430:GLY:HA2	4:D:1312:HOH:O	1.94	0.67
1:D:75:LEU:HD21	1:D:80:ALA:HB2	1.77	0.67
1:A:63:ASN:N	1:A:63:ASN:OD1	2.28	0.66
1:C:138:ASP:OD2	4:C:1001:HOH:O	2.12	0.66
1:A:67:GLU:O	1:A:71:ILE:HG13	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:ILE:HG23	1:C:350:SER:HB3	1.77	0.65
1:B:80:ALA:HA	1:B:81:GLU:HB2	1.80	0.63
1:A:93:GLY:O	1:A:94:LEU:HB2	1.98	0.62
1:D:128:ILE:O	1:D:132:LEU:HG	1.99	0.62
1:B:347:ASP:OD1	4:B:1002:HOH:O	2.15	0.62
1:D:345:ILE:HG23	1:D:350:SER:OG	1.99	0.62
1:C:279:ARG:HH11	1:C:279:ARG:HB2	1.65	0.61
1:B:95:LEU:HD12	1:B:97:LEU:HG	1.83	0.61
1:C:608:THR:HG22	1:C:610:GLU:H	1.67	0.60
1:C:113:LEU:HD12	1:C:114:GLU:H	1.65	0.60
1:A:115:LEU:HD12	1:A:124:ILE:HD11	1.84	0.59
1:C:95:LEU:O	1:C:97:LEU:HG	2.02	0.59
1:B:313:ASN:ND2	1:B:677:SER:OG	2.32	0.59
1:A:63:ASN:ND2	1:A:94:LEU:HG	2.17	0.59
1:D:606:SER:HB3	1:D:612:ASN:HA	1.85	0.59
1:D:787:ALA:HB1	1:D:809:ALA:HB1	1.84	0.59
1:C:816:ASP:OD2	1:D:691:PHE:N	2.22	0.59
1:B:742:GLU:OE2	4:B:1003:HOH:O	2.17	0.59
1:A:75:LEU:HD13	1:A:76:ASP:HA	1.85	0.58
1:B:8:ILE:O	1:B:620:ARG:NH2	2.37	0.58
1:D:75:LEU:CD1	1:D:80:ALA:HB3	2.31	0.58
1:D:91:ILE:HD11	1:D:110:LEU:HD13	1.86	0.58
1:C:395:VAL:HG21	1:C:530:TRP:HB2	1.86	0.57
1:D:64:VAL:O	1:D:68:ILE:HG12	2.05	0.57
1:D:349:GLN:HE22	1:D:600:GLN:HB2	1.68	0.57
1:A:15:ALA:O	1:A:356:THR:HA	2.05	0.57
1:D:15:ALA:O	1:D:356:THR:HA	2.04	0.56
1:D:95:LEU:HB3	1:D:97:LEU:HD12	1.86	0.56
1:B:102:PRO:HB2	1:B:105:GLN:HG3	1.88	0.56
1:C:608:THR:HB	1:C:611:ILE:HB	1.88	0.56
1:A:68:ILE:O	1:A:72:LYS:N	2.39	0.55
1:D:739:GLU:H	1:D:739:GLU:CD	2.09	0.55
1:B:395:VAL:HG21	1:B:530:TRP:HB2	1.89	0.55
1:D:347:ASP:OD1	1:D:350:SER:HB3	2.05	0.55
1:D:737:SER:HB2	1:D:739:GLU:OE1	2.06	0.55
1:C:787:ALA:HB1	1:C:809:ALA:HB1	1.88	0.55
1:A:104:GLN:O	1:A:108:ARG:HG2	2.06	0.55
1:C:62:GLY:O	1:C:65:ILE:N	2.25	0.55
1:D:171:GLY:H	1:D:338:LYS:CD	2.19	0.55
1:D:75:LEU:HD21	1:D:80:ALA:CB	2.35	0.54
1:B:64:VAL:O	1:B:68:ILE:HG13	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ASP:OD1	1:B:350:SER:HB3	2.07	0.54
1:C:313:ASN:HD22	1:C:677:SER:HG	1.50	0.54
1:A:252:GLN:HG3	1:A:288:GLU:HG2	1.90	0.54
1:B:8:ILE:HG12	1:B:153:ILE:HD13	1.90	0.54
1:A:249:ASN:HB3	4:A:1005:HOH:O	2.06	0.54
1:B:110:LEU:HA	1:B:113:LEU:HD13	1.89	0.54
1:C:62:GLY:O	1:C:65:ILE:HG22	2.07	0.54
1:B:606:SER:HB2	1:B:612:ASN:HA	1.90	0.53
1:B:85:GLN:HA	1:B:88:ILE:HG12	1.90	0.53
1:B:468:GLN:NE2	1:C:635:GLN:OE1	2.34	0.53
1:A:787:ALA:HB1	1:A:809:ALA:HB1	1.90	0.53
1:C:279:ARG:HB2	1:C:279:ARG:NH1	2.23	0.53
1:C:424:GLU:HG2	1:C:428:GLU:OE1	2.09	0.53
1:D:75:LEU:C	1:D:77:GLU:H	2.10	0.53
1:C:683:GLN:HG3	1:C:756:LEU:HD11	1.89	0.53
1:D:75:LEU:HD13	1:D:75:LEU:O	2.09	0.53
1:A:110:LEU:HD23	1:A:113:LEU:HD12	1.91	0.53
1:B:210:VAL:HA	1:B:215:LEU:HD22	1.91	0.53
1:D:468:GLN:O	1:D:471[B]:ASN:ND2	2.27	0.52
1:B:696:TRP:HB3	1:B:697:TNQ:CE3	2.39	0.52
1:B:15:ALA:O	1:B:356:THR:HA	2.10	0.52
1:B:88:ILE:O	1:B:92:THR:HG23	2.10	0.52
1:A:70:GLN:HB3	1:A:74:LYS:NZ	2.24	0.52
1:D:608:THR:HG22	1:D:610:GLU:H	1.75	0.52
1:D:696:TRP:HB3	1:D:697:TNQ:CE3	2.39	0.52
1:A:110:LEU:HD21	1:A:128:ILE:HG23	1.92	0.51
1:B:81:GLU:H	1:B:115:LEU:HG	1.75	0.51
1:D:252:GLN:HG3	1:D:288:GLU:HG3	1.92	0.51
1:C:15:ALA:O	1:C:356:THR:HA	2.10	0.51
1:D:91:ILE:O	1:D:95:LEU:HG	2.11	0.50
1:A:83:PHE:HB2	1:A:88:ILE:HD11	1.94	0.50
1:D:75:LEU:C	1:D:77:GLU:N	2.64	0.50
1:B:85:GLN:HA	1:B:88:ILE:CD1	2.42	0.49
1:A:41:THR:HB	1:A:793:PRO:HD3	1.94	0.49
1:A:696:TRP:HB3	1:A:697:TNQ:CE3	2.42	0.49
1:B:349:GLN:NE2	1:B:600:GLN:HB2	2.20	0.49
1:A:6:TYR:CE1	1:A:166:LEU:HD13	2.47	0.49
1:D:85:GLN:O	1:D:89:GLU:N	2.35	0.49
1:A:426:ASN:HD21	1:A:548:ILE:HG22	1.78	0.49
1:B:739:GLU:HG2	1:B:743:HIS:CE1	2.48	0.49
1:B:80:ALA:HB1	1:B:82:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:ALA:HA	1:B:811:SER:HB3	1.94	0.49
1:C:62:GLY:O	1:C:64:VAL:N	2.46	0.49
1:B:107:SER:O	1:B:111:ASP:N	2.29	0.49
1:A:84:LYS:O	1:A:87:GLU:N	2.45	0.49
1:A:395:VAL:HG21	1:A:530:TRP:HB2	1.94	0.49
1:B:292:GLU:OE2	4:B:1004:HOH:O	2.20	0.48
1:B:71:ILE:HD11	1:B:87:GLU:HB3	1.95	0.48
1:B:81:GLU:N	1:B:81:GLU:OE1	2.47	0.48
1:D:564:ASN:ND2	1:D:567:LEU:HD22	2.29	0.48
1:B:345:ILE:HG23	1:B:350:SER:OG	2.13	0.48
1:A:348:GLU:O	1:A:620:ARG:HD3	2.13	0.48
1:D:110:LEU:HA	1:D:113:LEU:HD12	1.96	0.48
1:D:173:LYS:HG3	1:D:336:GLU:HB2	1.96	0.48
1:A:71:ILE:O	1:A:75:LEU:CB	2.62	0.48
1:B:213:HIS:HB2	1:B:215:LEU:HD11	1.95	0.48
1:B:308:SER:HB2	1:C:487:ASN:OD1	2.13	0.48
1:A:128:ILE:O	1:A:132:LEU:HG	2.14	0.48
1:A:63:ASN:HD22	1:A:94:LEU:HG	1.78	0.47
1:D:80:ALA:HA	1:D:81:GLU:HB2	1.94	0.47
1:C:183:LYS:HE3	1:C:664:PRO:O	2.15	0.47
1:D:86:GLU:HA	1:D:89:GLU:CB	2.40	0.47
1:C:258:LYS:HD3	1:C:279:ARG:HD3	1.96	0.47
1:C:632:ASN:HA	1:C:635:GLN:HG2	1.95	0.47
1:D:121:SER:HB3	1:D:122:ASP:H	1.50	0.47
1:B:544:SER:HA	1:B:550:GLU:OE1	2.15	0.47
1:A:72:LYS:O	1:A:75:LEU:HB3	2.15	0.47
1:B:57:GLU:OE2	1:B:129:LYS:NZ	2.48	0.47
1:D:260:PRO:O	1:D:279:ARG:HD3	2.16	0.46
1:B:76:ASP:O	1:B:79:LYS:HD3	2.15	0.46
1:D:66:ASN:HA	1:D:69:SER:HB3	1.96	0.46
1:C:110:LEU:HD21	1:C:128:ILE:HG23	1.98	0.46
1:B:91:ILE:HA	1:B:94:LEU:HD22	1.98	0.46
1:A:619:PHE:O	1:A:620:ARG:HG2	2.16	0.46
1:B:121:SER:C	1:B:123:ASP:H	2.18	0.46
1:C:590:TRP:O	1:C:593:ARG:HG2	2.16	0.46
1:D:63:ASN:OD1	1:D:63:ASN:N	2.49	0.46
1:D:69:SER:HA	1:D:72:LYS:HD2	1.98	0.46
1:D:757:HIS:HA	1:D:763:PHE:CZ	2.50	0.46
1:D:335:VAL:HB	1:D:343:PHE:HB2	1.98	0.46
1:D:78:ARG:O	1:D:78:ARG:HD3	2.17	0.45
1:B:61:GLY:HA2	1:B:62:GLY:HA2	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:THR:HG22	1:C:94:LEU:HD13	1.99	0.45
1:D:504:ASN:HB3	1:D:514:VAL:O	2.16	0.45
1:A:606:SER:HB2	1:A:612:ASN:HA	1.99	0.45
1:D:69:SER:O	1:D:72:LYS:HG2	2.16	0.45
1:A:99:HIS:CE1	1:A:100:LEU:HG	2.51	0.45
1:A:123:ASP:N	1:A:123:ASP:OD1	2.47	0.45
1:D:126:GLN:OE1	1:D:129:LYS:HD3	2.17	0.45
1:D:57:GLU:OE1	1:D:129:LYS:HD2	2.16	0.45
1:D:155:LYS:H	1:D:155:LYS:HG2	1.61	0.45
1:A:85:GLN:O	1:A:89:GLU:HG3	2.17	0.45
1:B:757:HIS:HA	1:B:763:PHE:CZ	2.52	0.45
1:C:20:GLY:O	1:C:146:LYS:HE2	2.17	0.45
1:D:306:ALA:HB2	1:D:322:TRP:CE2	2.53	0.44
1:A:45:TYR:CD2	1:A:790:MET:HG2	2.52	0.44
1:A:596:LEU:HD23	1:A:660:TRP:CZ2	2.52	0.44
1:C:683:GLN:HG3	1:C:756:LEU:CD1	2.48	0.44
1:D:695:SER:HB2	1:D:703:VAL:HG21	1.99	0.44
1:A:590:TRP:O	1:A:593:ARG:HG2	2.17	0.44
1:B:80:ALA:CA	1:B:81:GLU:HB2	2.45	0.44
1:B:787:ALA:HB1	1:B:809:ALA:HB1	1.99	0.44
1:B:213:HIS:HB2	1:B:215:LEU:CD1	2.48	0.44
1:B:590:TRP:O	1:B:593:ARG:HG2	2.17	0.44
1:D:26:LEU:HD11	1:D:51:GLU:HB3	2.00	0.44
1:A:82:LYS:CA	1:A:115:LEU:HD23	2.48	0.44
1:B:7:LYS:HG2	1:B:350:SER:HA	2.00	0.44
1:B:288:GLU:O	1:B:295:LEU:HD12	2.18	0.44
1:A:153:ILE:HD12	1:A:174:VAL:HG21	1.99	0.43
1:C:757:HIS:HA	1:C:763:PHE:CZ	2.52	0.43
1:A:71:ILE:O	1:A:75:LEU:N	2.50	0.43
1:A:367:PRO:O	1:A:401:ARG:HD3	2.18	0.43
1:A:757:HIS:HA	1:A:763:PHE:CZ	2.53	0.43
1:A:92:THR:HA	1:A:95:LEU:HD12	2.01	0.43
1:B:56:LEU:HD22	1:B:60:PHE:HE2	1.83	0.43
1:B:89:GLU:HA	1:B:92:THR:OG1	2.19	0.43
1:D:635:GLN:HB3	1:D:658:TRP:CZ2	2.54	0.43
1:D:61:GLY:HA2	1:D:62:GLY:HA2	1.69	0.43
1:B:252:GLN:HG3	1:B:288:GLU:HG3	2.00	0.43
1:B:80:ALA:HB1	1:B:82:LYS:H	1.84	0.43
1:C:7:LYS:HG3	1:C:156:CYS:SG	2.58	0.43
1:D:562:SER:HB3	1:D:568:LEU:HD11	1.99	0.43
1:C:696:TRP:HB3	1:C:697:TNQ:CE3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HB3	1:A:97:LEU:HG	2.00	0.43
1:A:562:SER:HB3	1:A:568:LEU:HD11	2.00	0.43
1:D:78:ARG:O	1:D:79:LYS:HB2	2.19	0.43
1:B:618:GLU:OE2	1:B:620:ARG:NH1	2.52	0.42
1:D:97:LEU:HD23	1:D:100:LEU:HD12	2.01	0.42
1:D:426:ASN:HD21	1:D:548:ILE:HG22	1.84	0.42
1:C:64:VAL:HG13	1:C:94:LEU:CD2	2.49	0.42
1:D:101:VAL:HG11	1:D:135:VAL:CG1	2.49	0.42
1:D:253:VAL:HB	1:D:287:ILE:HG13	2.01	0.42
1:C:61:GLY:HA2	1:C:62:GLY:HA2	1.64	0.42
1:B:27:SER:OG	1:B:296:ARG:NH2	2.44	0.42
1:C:673:ILE:HD12	1:C:674:PRO:HA	2.01	0.42
1:D:91:ILE:HD13	1:D:91:ILE:HG21	1.75	0.42
1:A:83:PHE:O	1:A:84:LYS:HG2	2.20	0.42
1:A:105:GLN:OE1	1:A:139:HIS:NE2	2.48	0.42
1:D:258:LYS:HD2	1:D:262:ASN:ND2	2.34	0.42
1:D:74:LYS:HA	1:D:77:GLU:OE2	2.20	0.42
1:A:7:LYS:HG3	1:A:156:CYS:SG	2.59	0.42
1:A:8:ILE:O	1:A:620:ARG:NH2	2.52	0.42
1:B:711:TYR:HA	1:B:714:PHE:CE2	2.55	0.42
1:D:110:LEU:HD21	1:D:132:LEU:HD21	2.02	0.42
1:D:313:ASN:ND2	1:D:677:SER:OG	2.35	0.42
1:C:696:TRP:HB3	1:C:697:TNQ:CD2	2.50	0.42
1:D:45:TYR:HB2	1:D:788:MET:HG2	2.02	0.42
1:A:84:LYS:O	1:A:85:GLN:C	2.58	0.42
1:A:246:SER:C	1:A:248:ASP:N	2.72	0.42
1:A:677:SER:HB2	4:A:1100:HOH:O	2.20	0.42
1:B:75:LEU:O	1:B:79:LYS:HA	2.20	0.41
1:C:503:PRO:HB3	1:C:507:ILE:HD12	2.02	0.41
1:A:683:GLN:HG3	1:A:756:LEU:HD11	2.01	0.41
1:B:68:ILE:HA	1:B:71:ILE:CG2	2.46	0.41
1:B:85:GLN:HA	1:B:88:ILE:CG1	2.49	0.41
1:B:372:TYR:HB3	1:B:575:ASP:OD1	2.20	0.41
1:C:358:PRO:HB3	1:C:675:TRP:CE3	2.56	0.41
1:D:64:VAL:HG22	1:D:94:LEU:HG	2.02	0.41
1:D:84:LYS:HG3	1:D:85:GLN:N	2.27	0.41
1:D:86:GLU:O	1:D:90:THR:HG23	2.20	0.41
1:D:441:ALA:O	1:D:445:ARG:HG3	2.21	0.41
1:B:81:GLU:HG3	1:B:115:LEU:O	2.20	0.41
1:B:504:ASN:HB3	1:B:514:VAL:O	2.20	0.41
1:B:695:SER:HB2	1:B:703:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ASN:OD1	1:B:251:THR:HG23	2.20	0.41
1:A:116:LYS:HA	1:A:116:LYS:HD3	1.87	0.41
1:B:80:ALA:CB	1:B:82:LYS:H	2.33	0.41
1:C:504:ASN:HB2	1:C:516:TRP:C	2.41	0.41
1:A:64:VAL:O	1:A:68:ILE:HG13	2.20	0.41
1:C:787:ALA:HA	1:C:810:TYR:O	2.21	0.41
1:D:74:LYS:O	1:D:77:GLU:HB3	2.20	0.41
1:A:82:LYS:N	1:A:115:LEU:HD23	2.35	0.41
1:A:639:HIS:HB3	1:D:509:TYR:CD1	2.56	0.41
1:D:235:LYS:HG2	1:D:634:TYR:CD1	2.56	0.41
1:D:435:LEU:HD23	1:D:537:VAL:HG21	2.03	0.41
1:D:471[A]:ASN:ND2	4:D:1029:HOH:O	2.51	0.41
1:B:619:PHE:O	1:B:620:ARG:HG2	2.20	0.41
1:D:741:PHE:CE1	1:D:745:ARG:HD2	2.56	0.41
1:A:115:LEU:H	1:A:115:LEU:HD22	1.85	0.40
1:D:582:PHE:CD1	1:D:589:THR:HA	2.56	0.40
1:A:696:TRP:HB3	1:A:697:TNQ:CD2	2.51	0.40
1:B:115:LEU:O	1:B:116:LYS:HB2	2.22	0.40
1:A:153:ILE:HG13	1:A:176:TRP:CZ2	2.57	0.40
1:A:246:SER:C	1:A:248:ASP:H	2.23	0.40
1:A:787:ALA:HA	1:A:810:TYR:O	2.22	0.40
1:C:92:THR:CG2	1:C:103:GLN:HE22	2.21	0.40
1:D:67:GLU:O	1:D:71:ILE:HG12	2.20	0.40
1:D:80:ALA:HA	1:D:81:GLU:CB	2.51	0.40
1:A:71:ILE:HG12	1:A:74:LYS:HE2	2.04	0.40
1:A:337:LEU:HD12	1:A:341:ASP:HB2	2.03	0.40
1:B:4:CYS:O	1:B:156:CYS:HB2	2.22	0.40
1:B:85:GLN:CD	1:B:88:ILE:HD11	2.42	0.40
1:C:235:LYS:HG2	1:C:634:TYR:CD1	2.56	0.40
1:D:696:TRP:HB3	1:D:697:TNQ:CD2	2.51	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	774/816 (95%)	742 (96%)	28 (4%)	4 (0%)	29	22
1	B	783/816 (96%)	752 (96%)	25 (3%)	6 (1%)	19	12
1	C	761/816 (93%)	722 (95%)	31 (4%)	8 (1%)	14	8
1	D	779/816 (96%)	741 (95%)	28 (4%)	10 (1%)	12	6
All	All	3097/3264 (95%)	2957 (96%)	112 (4%)	28 (1%)	17	11

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	B	94	LEU
1	B	279	ARG
1	C	63	ASN
1	C	96	GLY
1	D	81	GLU
1	D	94	LEU
1	D	279	ARG
1	C	93	GLY
1	C	94	LEU
1	C	109	SER
1	D	122	ASP
1	A	279	ARG
1	B	111	ASP
1	C	92	THR
1	C	279	ARG
1	D	82	LYS
1	D	85	GLN
1	D	164	GLU
1	A	230	THR
1	B	84	LYS
1	C	164	GLU
1	D	78	ARG
1	D	83	PHE
1	A	164	GLU
1	D	93	GLY
1	B	93	GLY
1	B	164	GLU

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	682/711 (96%)	676 (99%)	6 (1%)	78	83
1	B	688/711 (97%)	681 (99%)	7 (1%)	76	81
1	C	669/711 (94%)	662 (99%)	7 (1%)	76	81
1	D	684/711 (96%)	674 (98%)	10 (2%)	65	69
All	All	2723/2844 (96%)	2693 (99%)	30 (1%)	73	78

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	ARG
1	A	578	TYR
1	A	622	LYS
1	A	654	SER
1	A	731	SER
1	A	746	LEU
1	B	78	ARG
1	B	122	ASP
1	B	157	ASP
1	B	170	ASP
1	B	560	LYS
1	B	575	ASP
1	B	578	TYR
1	C	4	CYS
1	C	107	SER
1	C	246	SER
1	C	575	ASP
1	C	578	TYR
1	C	731	SER
1	C	796	ASN
1	D	4	CYS
1	D	54	GLN
1	D	66	ASN
1	D	121	SER

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Mol	Chain	Res	Type
1	D	279	ARG
1	D	339	ASN
1	D	471[A]	ASN
1	D	471[B]	ASN
1	D	575	ASP
1	D	578	TYR

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

Mol	Chain	Res	Type
1	C	70	GLN
1	C	103	GLN
1	C	142	HIS
1	C	796	ASN
1	D	339	ASN
1	D	349	GLN
1	D	433	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TNQ	A	697	1	18,21,22	3.10	3 (16%)	16,29,31	3.00	3 (18%)
1	TNQ	C	697	1	18,21,22	3.04	4 (22%)	16,29,31	2.84	4 (25%)
1	TNQ	D	697	1	18,21,22	3.09	3 (16%)	16,29,31	2.90	3 (18%)
1	TNQ	B	697	1	18,21,22	3.00	4 (22%)	16,29,31	2.73	4 (25%)

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
1	TNQ	A	697	1	-	4/9/11/13	0/2/2/2
1	TNQ	C	697	1	-	4/9/11/13	0/2/2/2
1	TNQ	D	697	1	-	4/9/11/13	0/2/2/2
1	TNQ	B	697	1	-	4/9/11/13	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	TNQ	C2-N1	-11.35	1.27	1.45
1	D	697	TNQ	C2-N1	-11.31	1.27	1.45
1	C	697	TNQ	C2-N1	-11.27	1.27	1.45
1	B	697	TNQ	C2-N1	-10.94	1.28	1.45
1	A	697	TNQ	CZ2-CE2	4.15	1.49	1.42
1	D	697	TNQ	CZ2-CE2	4.05	1.49	1.42
1	B	697	TNQ	CZ2-CE2	3.97	1.49	1.42
1	C	697	TNQ	CZ2-CE2	3.50	1.48	1.42
1	D	697	TNQ	CH2-CZ2	3.18	1.49	1.40
1	C	697	TNQ	CH2-CZ2	3.05	1.49	1.40
1	A	697	TNQ	CH2-CZ2	3.04	1.49	1.40
1	B	697	TNQ	CH2-CZ2	3.02	1.49	1.40
1	B	697	TNQ	CE3-CZ3	2.18	1.41	1.36
1	C	697	TNQ	CE3-CZ3	2.06	1.40	1.36

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	697	TNQ	C1-C2-N1	8.49	126.54	110.96
1	D	697	TNQ	C1-C2-N1	8.29	126.18	110.96
1	C	697	TNQ	C1-C2-N1	8.26	126.12	110.96
1	B	697	TNQ	C1-C2-N1	8.15	125.92	110.96
1	A	697	TNQ	C2-N1-CH2	-6.81	114.21	123.98
1	D	697	TNQ	C2-N1-CH2	-6.50	114.67	123.98
1	C	697	TNQ	C2-N1-CH2	-5.86	115.57	123.98
1	B	697	TNQ	C2-N1-CH2	-4.97	116.86	123.98
1	B	697	TNQ	O3-C1-C2	2.60	121.76	112.74
1	A	697	TNQ	CB-CG-CD2	2.55	130.22	126.25
1	D	697	TNQ	CB-CG-CD2	2.34	129.88	126.25
1	C	697	TNQ	O3-C1-C2	2.21	120.43	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	697	TNQ	CE3-CZ3-CH2	2.17	123.94	120.08
1	C	697	TNQ	CG-CB-CA	-2.07	111.33	114.53

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	697	TNQ	O2-C1-C2-N1
1	C	697	TNQ	O3-C1-C2-N1
1	C	697	TNQ	CZ3-CH2-N1-C2
1	D	697	TNQ	CZ3-CH2-N1-C2
1	A	697	TNQ	CZ3-CH2-N1-C2
1	A	697	TNQ	CZ2-CH2-N1-C2
1	B	697	TNQ	CZ2-CH2-N1-C2
1	C	697	TNQ	CZ2-CH2-N1-C2
1	D	697	TNQ	CZ2-CH2-N1-C2
1	B	697	TNQ	CZ3-CH2-N1-C2
1	A	697	TNQ	O2-C1-C2-N1
1	A	697	TNQ	O3-C1-C2-N1
1	B	697	TNQ	O2-C1-C2-N1
1	B	697	TNQ	O3-C1-C2-N1
1	D	697	TNQ	O2-C1-C2-N1
1	D	697	TNQ	O3-C1-C2-N1

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	697	TNQ	2	0
1	C	697	TNQ	2	0
1	D	697	TNQ	2	0
1	B	697	TNQ	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	783/816 (95%)	-0.16	32 (4%)	37	46	16, 29, 77, 117	0
1	B	790/816 (96%)	0.01	53 (6%)	17	24	17, 32, 89, 174	0
1	C	770/816 (94%)	-0.10	41 (5%)	26	35	16, 31, 83, 135	0
1	D	786/816 (96%)	0.11	64 (8%)	12	16	21, 37, 99, 157	0
All	All	3129/3264 (95%)	-0.03	190 (6%)	21	28	16, 32, 88, 174	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	GLY	12.0
1	D	61	GLY	9.5
1	B	75	LEU	8.0
1	D	81	GLU	8.0
1	B	83	PHE	7.8
1	D	83	PHE	7.3
1	D	91	ILE	7.1
1	B	80	ALA	6.9
1	D	80	ALA	6.8
1	C	62	GLY	6.7
1	D	113	LEU	6.5
1	B	115	LEU	6.3
1	B	121	SER	6.1
1	B	62	GLY	6.1
1	C	115	LEU	6.0
1	D	68	ILE	5.9
1	D	88	ILE	5.8
1	B	78	ARG	5.7
1	D	82	LYS	5.6
1	C	68	ILE	5.6
1	B	116	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	109	SER	5.4
1	B	110	LEU	5.4
1	C	70	GLN	5.3
1	B	74	LYS	5.3
1	B	81	GLU	5.2
1	B	61	GLY	5.2
1	A	113	LEU	5.1
1	A	75	LEU	5.1
1	D	79	LYS	5.1
1	C	111	ASP	5.1
1	B	68	ILE	5.0
1	C	60	PHE	5.0
1	C	102	PRO	5.0
1	A	115	LEU	4.8
1	D	71	ILE	4.7
1	B	86	GLU	4.6
1	C	65	ILE	4.5
1	B	114	GLU	4.5
1	D	73	THR	4.4
1	C	114	GLU	4.3
1	C	64	VAL	4.2
1	B	111	ASP	4.2
1	B	71	ILE	4.1
1	B	124	ILE	4.1
1	A	94	LEU	4.1
1	C	113	LEU	4.1
1	C	88	ILE	4.1
1	B	79	LYS	4.1
1	D	66	ASN	4.1
1	A	249	ASN	4.0
1	A	116	LYS	4.0
1	D	75	LEU	4.0
1	D	112	ASN	4.0
1	D	110	LEU	4.0
1	C	61	GLY	3.9
1	B	88	ILE	3.9
1	D	122	ASP	3.8
1	D	76	ASP	3.7
1	D	170	ASP	3.7
1	B	262	ASN	3.7
1	B	64	VAL	3.7
1	C	262	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	337	LEU	3.6
1	B	91	ILE	3.6
1	C	66	ASN	3.6
1	A	74	LYS	3.6
1	C	92	THR	3.5
1	C	124	ILE	3.5
1	D	65	ILE	3.5
1	A	114	GLU	3.5
1	B	65	ILE	3.5
1	C	112	ASN	3.5
1	B	95	LEU	3.4
1	D	92	THR	3.4
1	D	111	ASP	3.4
1	A	83	PHE	3.4
1	B	112	ASN	3.3
1	C	127	GLN	3.3
1	B	128	ILE	3.3
1	C	71	ILE	3.3
1	D	121	SER	3.3
1	B	82	LYS	3.2
1	B	60	PHE	3.2
1	B	125	VAL	3.2
1	D	77	GLU	3.2
1	B	107	SER	3.2
1	D	78	ARG	3.2
1	D	109	SER	3.2
1	D	70	GLN	3.2
1	A	124	ILE	3.2
1	D	262	ASN	3.2
1	C	91	ILE	3.2
1	A	61	GLY	3.2
1	B	77	GLU	3.2
1	D	126	GLN	3.2
1	D	169	THR	3.2
1	B	89	GLU	3.1
1	A	62	GLY	3.1
1	D	87	GLU	3.1
1	B	92	THR	3.1
1	B	122	ASP	3.1
1	C	99	HIS	3.1
1	A	262	ASN	3.1
1	D	60	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	130	GLY	3.1
1	D	108	ARG	3.1
1	D	343	PHE	3.1
1	B	4	CYS	3.0
1	A	248	ASP	3.0
1	A	110	LEU	3.0
1	D	95	LEU	3.0
1	B	85	GLN	3.0
1	C	63	ASN	2.9
1	B	113	LEU	2.9
1	D	128	ILE	2.9
1	D	64	VAL	2.8
1	C	97	LEU	2.8
1	D	338	LYS	2.8
1	B	721	ASP	2.8
1	D	94	LEU	2.8
1	D	72	LYS	2.7
1	D	129	LYS	2.7
1	C	108	ARG	2.7
1	B	163	VAL	2.7
1	D	123	ASP	2.7
1	D	163	VAL	2.7
1	D	127	GLN	2.6
1	C	90	THR	2.6
1	D	342	THR	2.6
1	B	109	SER	2.6
1	D	133	LEU	2.6
1	A	68	ILE	2.6
1	C	105	GLN	2.6
1	D	85	GLN	2.6
1	A	85	GLN	2.5
1	A	338	LYS	2.5
1	D	97	LEU	2.5
1	A	125	VAL	2.5
1	C	5	GLN	2.5
1	B	123	ASP	2.5
1	C	95	LEU	2.4
1	C	103	GLN	2.4
1	B	101	VAL	2.4
1	C	339	ASN	2.4
1	A	86	GLU	2.4
1	A	111	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	98	SER	2.4
1	B	340	GLY	2.4
1	D	106	LEU	2.4
1	D	63	ASN	2.4
1	C	59	ALA	2.3
1	D	172	ASP	2.3
1	B	66	ASN	2.3
1	D	69	SER	2.3
1	A	132	LEU	2.3
1	C	67	GLU	2.3
1	A	127	GLN	2.3
1	C	104	GLN	2.3
1	D	4	CYS	2.3
1	D	335	VAL	2.2
1	D	102	PRO	2.2
1	D	84	LYS	2.2
1	A	102	PRO	2.2
1	C	428	GLU	2.2
1	D	253	VAL	2.2
1	C	106	LEU	2.2
1	B	719	SER	2.2
1	B	97	LEU	2.2
1	D	86	GLU	2.2
1	D	89	GLU	2.2
1	A	65	ILE	2.1
1	A	337	LEU	2.1
1	D	74	LYS	2.1
1	B	127	GLN	2.1
1	A	170	ASP	2.1
1	B	108	ARG	2.1
1	B	70	GLN	2.1
1	B	278	GLU	2.1
1	B	73	THR	2.1
1	A	71	ILE	2.1
1	A	123	ASP	2.1
1	D	125	VAL	2.1
1	A	84	LYS	2.0
1	B	343	PHE	2.0
1	C	128	ILE	2.0
1	C	163	VAL	2.0
1	A	169	THR	2.0
1	C	94	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	135	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	TNQ	A	697	20/21	0.97	0.13	15,25,34,35	0
1	TNQ	B	697	20/21	0.97	0.13	16,23,35,37	0
1	TNQ	C	697	20/21	0.97	0.13	17,25,34,37	0
1	TNQ	D	697	20/21	0.97	0.14	20,26,34,34	0

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
3	NA	B	902	1/1	0.93	0.06	54,54,54,54	0
2	MG	C	901	1/1	0.97	0.10	27,27,27,27	0
2	MG	A	901	1/1	0.97	0.06	28,28,28,28	0
2	MG	D	901	1/1	0.98	0.07	39,39,39,39	0
2	MG	B	901	1/1	0.98	0.09	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.