



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 04:14 PM EDT

PDB ID : 6UBZ
Title : Crystal structure of D678A GoxA bound to glycine at pH 5.5
Authors : Yukl, E.T.
Deposited on : 2019-09-13
Resolution : 1.83 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

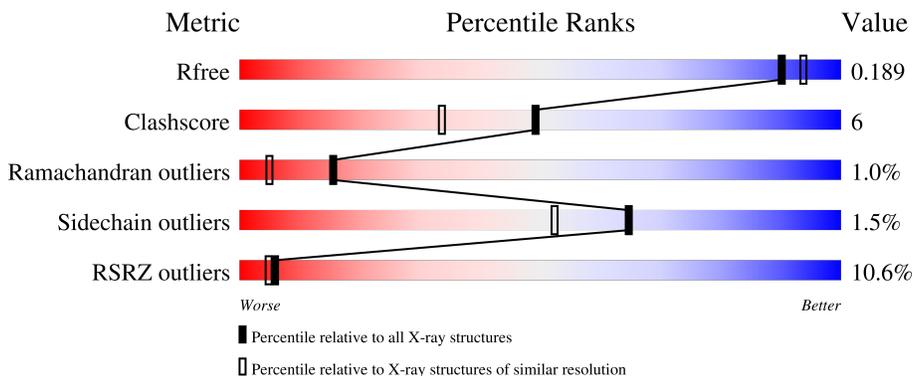
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	816	 12% 85% 10% ...
1	B	816	 9% 85% 9% ...
1	C	816	 9% 86% 9% ...
1	D	816	 11% 82% 13% ...

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27437 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 Uncharacterized protein GoxA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	783	6243	3946	1061	1215	21	0	7	0
1	A	791	6258	3954	1065	1219	20	0	1	0
1	C	785	6264	3958	1067	1218	21	0	7	0
1	D	780	6193	3916	1057	1199	21	0	4	0

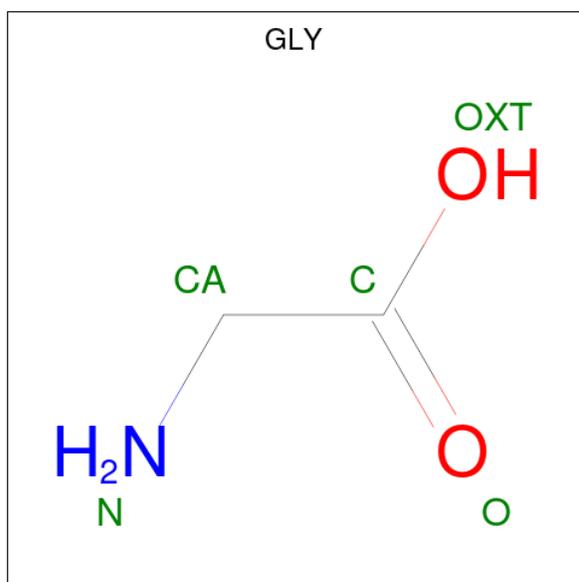
There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	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 GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			5	2	1	2		
3	A	1	Total	C	N	O	0	0
			5	2	1	2		
3	C	1	Total	C	N	O	0	0
			5	2	1	2		
3	D	1	Total	C	N	O	0	0
			5	2	1	2		

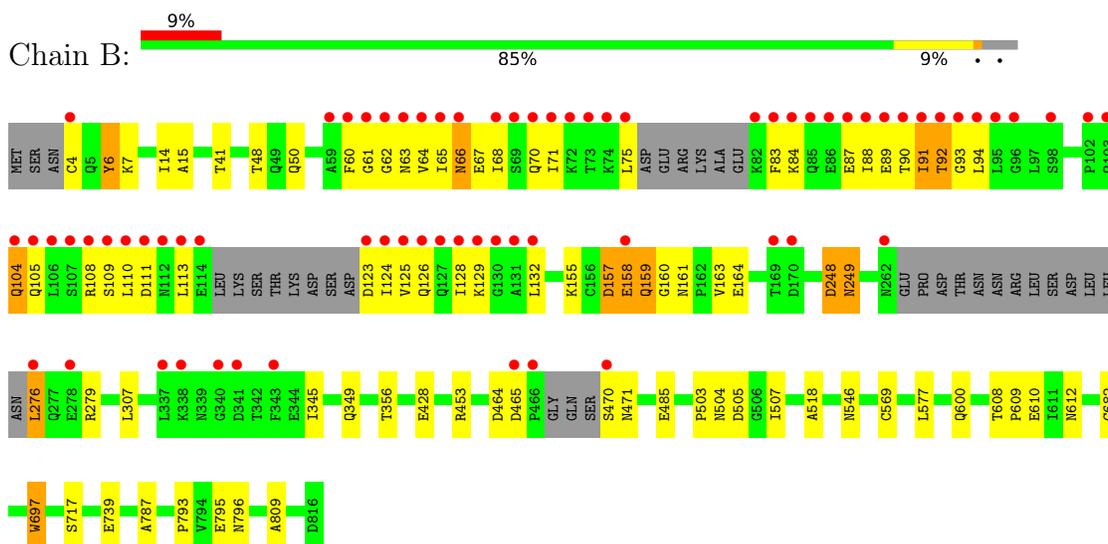
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	672	Total	O	0	1
			673	673		
4	A	554	Total	O	0	0
			554	554		
4	C	650	Total	O	0	0
			650	650		
4	D	578	Total	O	0	0
			578	578		

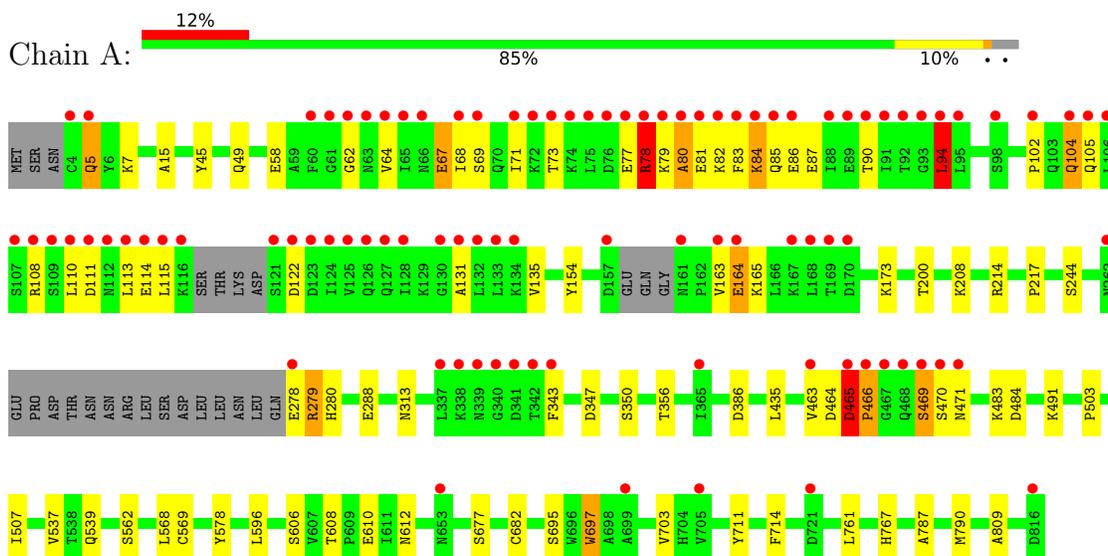
3 Residue-property plots [i](#)

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.

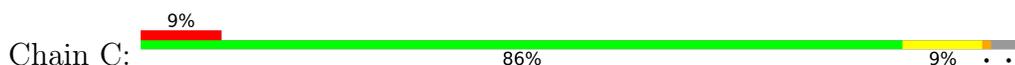
- Molecule 1: Uncharacterized protein GoxA

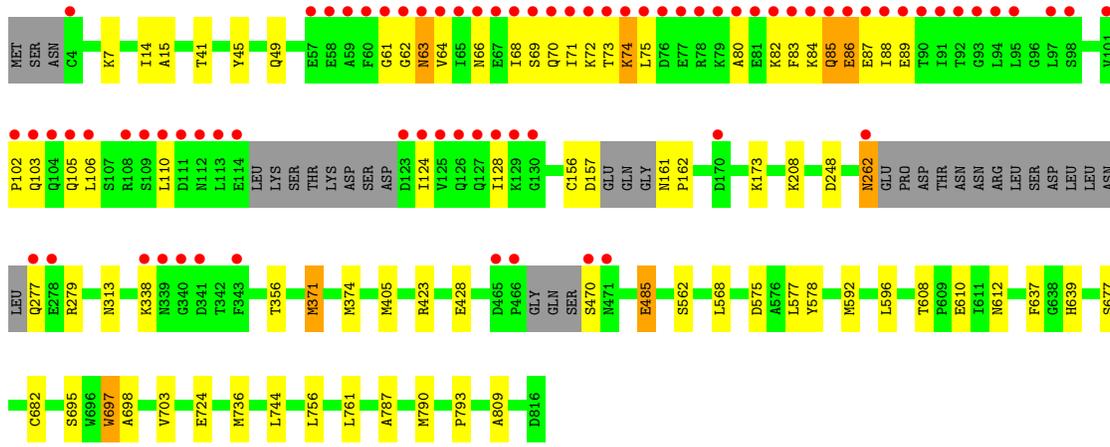


- Molecule 1: Uncharacterized protein GoxA

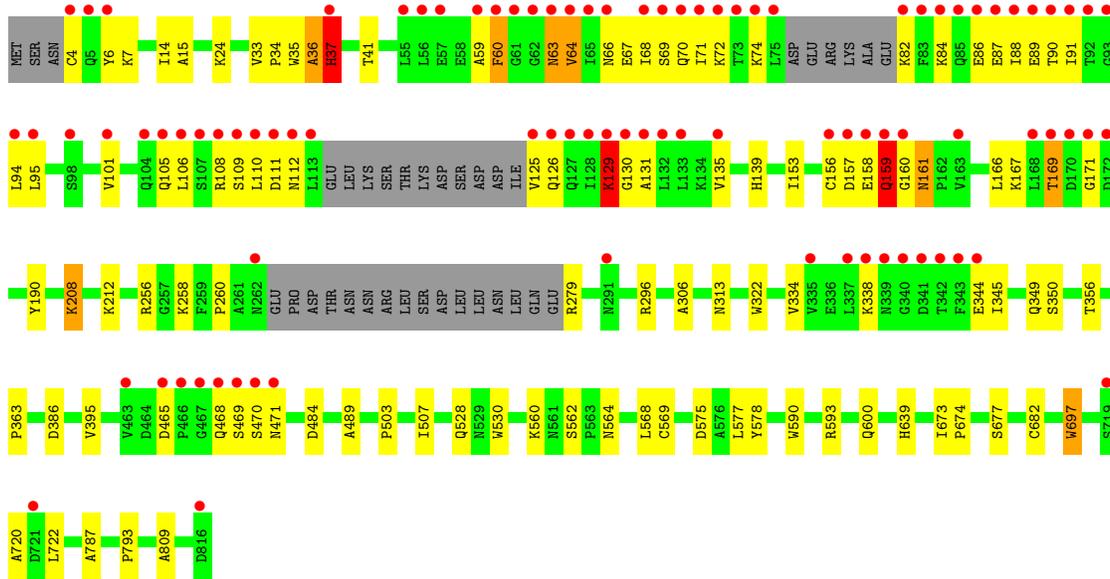
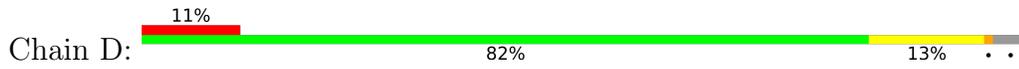


- Molecule 1: Uncharacterized protein GoxA





• Molecule 1: Uncharacterized protein GoxA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.33Å 93.40Å 187.99Å 90.00° 95.20° 90.00°	Depositor
Resolution (Å)	47.35 – 1.83 47.35 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.35-1.83) 99.2 (47.35-1.83)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.83Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.162 , 0.189 0.163 , 0.189	Depositor DCC
R_{free} test set	16599 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtrriage
Anisotropy	0.590	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	27437	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.39	2/6390 (0.0%)	0.58	3/8695 (0.0%)
1	B	1.08	6/6374 (0.1%)	1.03	13/8675 (0.1%)
1	C	0.40	0/6395	0.59	2/8702 (0.0%)
1	D	0.37	0/6326	0.58	1/8610 (0.0%)
All	All	0.63	8/25485 (0.0%)	0.72	19/34682 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
1	D	0	3
All	All	0	8

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	TYR	CD1-CE1	49.48	2.13	1.39
1	B	6	TYR	CD2-CE2	49.36	2.13	1.39
1	B	6	TYR	CE1-CZ	-20.20	1.12	1.38
1	B	6	TYR	CE2-CZ	-20.04	1.12	1.38
1	B	6	TYR	CG-CD2	-17.77	1.16	1.39
1	B	6	TYR	CG-CD1	-17.64	1.16	1.39
1	A	78	ARG	CB-CG	-6.01	1.36	1.52
1	A	78	ARG	NE-CZ	5.69	1.40	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	TYR	CE1-CZ-CE2	-35.52	62.96	119.80
1	B	6	TYR	CG-CD2-CE2	-30.20	97.14	121.30
1	B	6	TYR	CG-CD1-CE1	-30.12	97.21	121.30
1	B	6	TYR	CD1-CG-CD2	-29.50	85.45	117.90
1	B	6	TYR	CB-CG-CD2	26.18	136.71	121.00
1	B	6	TYR	CB-CG-CD1	26.17	136.70	121.00
1	B	6	TYR	CD1-CE1-CZ	-12.67	108.40	119.80
1	B	6	TYR	CZ-CE2-CD2	-12.40	108.64	119.80
1	B	6	TYR	CE1-CZ-OH	10.59	148.68	120.10
1	B	6	TYR	OH-CZ-CE2	10.44	148.29	120.10
1	A	78	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	78	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	C	371	MET	CG-SD-CE	7.12	111.59	100.20
1	A	78	ARG	NH1-CZ-NH2	6.79	126.87	119.40
1	B	248	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	C	592	MET	CG-SD-CE	5.50	109.00	100.20
1	D	159	GLN	N-CA-C	-5.35	96.56	111.00
1	B	276	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	158	GLU	CA-CB-CG	5.08	124.58	113.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	465	ASP	Peptide
1	A	469	SER	Peptide
1	A	80	ALA	Peptide
1	A	94	LEU	Peptide
1	B	91	ILE	Peptide
1	D	169	THR	Peptide
1	D	36	ALA	Peptide
1	D	37[B]	HIS	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	6258	0	6028	64	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6243	0	6005	80	1
1	C	6264	0	6032	59	0
1	D	6193	0	5966	86	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	5	0	2	2	0
3	B	5	0	2	3	0
3	C	5	0	2	1	0
3	D	5	0	2	1	0
4	A	554	0	0	9	0
4	B	673	0	0	12	1
4	C	650	0	0	6	0
4	D	578	0	0	9	0
All	All	27437	0	24039	291	2

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 (291) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:LYS:NZ	1:C:83:PHE:O	1.61	1.31
1:C:86:GLU:HB3	1:C:89:GLU:HB2	1.41	1.01
1:D:157:ASP:OD2	1:D:160:GLY:N	1.93	1.01
1:D:86:GLU:HA	1:D:89:GLU:HG2	1.47	0.94
1:D:36:ALA:HA	1:D:560:LYS:HZ1	1.33	0.93
1:B:158:GLU:HB2	1:B:161:ASN:HB2	1.50	0.92
1:B:92:THR:O	1:B:94:LEU:N	2.05	0.88
1:C:371:MET:CE	1:C:374:MET:HB2	2.09	0.82
1:B:158:GLU:O	1:B:161:ASN:N	2.15	0.78
1:A:471:ASN:ND2	4:A:1002:HOH:O	2.16	0.78
1:B:50:GLN:OE1	4:B:1001:HOH:O	2.01	0.78
1:B:61:GLY:HA2	1:B:64:VAL:H	1.49	0.77
1:D:313:ASN:ND2	1:D:677:SER:OG	2.18	0.75
1:B:697:TRQ:O6	3:B:902:GLY:N	2.19	0.75
1:B:163:VAL:HG23	1:B:164:GLU:HG2	1.69	0.74
1:A:79:LYS:NZ	4:A:1004:HOH:O	2.19	0.74
1:D:36:ALA:HA	1:D:560:LYS:NZ	2.02	0.73
1:D:562:SER:HB3	1:D:568:LEU:HD11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428[B]:GLU:OE1	4:B:1002:HOH:O	2.07	0.71
1:D:71:ILE:HA	1:D:74:LYS:HZ3	1.55	0.71
1:B:110:LEU:HA	1:B:113:LEU:HD13	1.72	0.70
1:B:157:ASP:HA	1:B:158:GLU:C	2.11	0.70
1:C:639:HIS:N	4:C:1002:HOH:O	2.23	0.70
1:B:63:ASN:OD1	1:B:66:ASN:ND2	2.24	0.70
1:D:159:GLN:HA	1:D:159:GLN:OE1	1.91	0.70
1:B:83:PHE:HB3	1:B:87:GLU:HG3	1.74	0.69
1:B:123:ASP:N	4:B:1004:HOH:O	2.24	0.69
1:C:371:MET:HE3	1:C:374:MET:HB2	1.75	0.69
1:B:88:ILE:HA	1:B:91:ILE:HG22	1.76	0.68
1:A:214:ARG:NH2	1:C:637:PHE:O	2.26	0.68
1:D:484:ASP:OD1	4:D:1001:HOH:O	2.10	0.68
1:C:82:LYS:CE	1:C:83:PHE:O	2.40	0.68
1:D:256:ARG:HG2	1:D:258:LYS:HZ3	1.59	0.67
1:A:313:ASN:ND2	1:A:677:SER:OG	2.21	0.67
1:D:720:ALA:HB1	1:D:722:LEU:HD12	1.77	0.67
1:D:70:GLN:OE1	4:D:1002:HOH:O	2.12	0.66
1:D:157:ASP:OD2	1:D:160:GLY:CA	2.43	0.66
1:C:313:ASN:ND2	1:C:677:SER:OG	2.23	0.65
1:B:84:LYS:O	1:B:87:GLU:HB3	1.97	0.65
1:D:66:ASN:O	1:D:70:GLN:HG2	1.97	0.65
1:C:86:GLU:CB	1:C:89:GLU:HB2	2.22	0.65
1:A:466:PRO:O	1:A:471:ASN:HB3	1.98	0.64
1:C:262:ASN:HB2	1:C:279:ARG:HH21	1.63	0.64
1:A:288:GLU:OE1	4:A:1001:HOH:O	2.16	0.63
1:C:612[A]:ASN:ND2	4:C:1005:HOH:O	2.31	0.63
1:B:248:ASP:O	1:B:249:ASN:HB2	1.98	0.63
1:B:90:THR:O	1:B:94:LEU:HD13	1.99	0.62
1:B:349:GLN:HE22	1:B:600:GLN:HB2	1.64	0.62
1:B:4:CYS:SG	1:B:7:LYS:HE3	2.40	0.62
1:D:349:GLN:HE22	1:D:600:GLN:HB2	1.65	0.62
1:D:468:GLN:HB3	1:D:470:SER:HB2	1.83	0.61
1:C:82:LYS:HZ2	1:C:83:PHE:C	1.86	0.61
1:D:208:LYS:HE2	1:D:212:LYS:HD2	1.83	0.61
1:C:682:CYS:SG	1:C:697:TRQ:HB3	2.41	0.60
1:A:87:GLU:HA	1:A:90:THR:HG22	1.83	0.60
3:C:902:GLY:N	4:C:1008:HOH:O	2.34	0.60
1:C:64:VAL:O	1:C:68:ILE:HG12	2.02	0.60
1:B:104:GLN:NE2	1:B:108:ARG:HH21	2.00	0.60
1:D:34:PRO:O	4:D:1003:HOH:O	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:SER:OG	1:B:796[A]:ASN:HB2	2.01	0.59
1:B:157:ASP:OD2	1:B:159:GLN:OE1	2.20	0.59
1:A:503:PRO:HB3	1:A:507:ILE:HD13	1.85	0.59
1:D:159:GLN:OE1	1:D:160:GLY:O	2.19	0.59
1:D:256:ARG:HG2	1:D:258:LYS:NZ	2.18	0.58
1:B:124:ILE:HD12	1:B:125:VAL:HG23	1.85	0.58
1:D:160:GLY:H	1:D:161:ASN:HB2	1.68	0.58
1:B:61:GLY:HA3	1:B:65:ILE:HD12	1.85	0.57
1:B:68:ILE:HD13	1:B:125:VAL:HG22	1.85	0.57
1:D:468:GLN:HB3	1:D:470:SER:H	1.69	0.57
1:B:84:LYS:HD2	1:B:84:LYS:N	2.19	0.57
1:C:110:LEU:HD21	1:C:128:ILE:HG23	1.86	0.57
1:D:37[B]:HIS:NE2	1:D:363:PRO:O	2.37	0.57
1:B:503:PRO:HB3	1:B:507:ILE:HD13	1.87	0.56
1:C:86:GLU:HA	1:C:88:ILE:N	2.19	0.56
1:B:66:ASN:O	1:B:70:GLN:HG3	2.04	0.56
1:A:80:ALA:HB1	1:A:82:LYS:N	2.20	0.56
1:D:471:ASN:ND2	4:D:1013:HOH:O	2.39	0.56
1:B:67:GLU:HG2	1:B:94:LEU:HD21	1.88	0.56
1:B:71:ILE:HG21	1:B:87:GLU:OE1	2.05	0.55
1:C:82:LYS:HD3	1:C:83:PHE:O	2.06	0.55
1:D:787:ALA:HB1	1:D:809:ALA:HB1	1.88	0.55
1:C:82:LYS:CD	1:C:83:PHE:O	2.54	0.55
1:C:371:MET:HE2	1:C:374:MET:HB2	1.87	0.55
1:B:124:ILE:HD12	1:B:125:VAL:N	2.22	0.55
1:C:608:THR:HG22	1:C:610:GLU:H	1.71	0.55
3:B:902:GLY:OXT	1:A:767:HIS:NE2	2.36	0.54
1:C:61:GLY:O	1:C:63:ASN:HB3	2.07	0.54
1:A:110:LEU:HA	1:A:113:LEU:HD12	1.89	0.54
1:B:307:LEU:HA	4:B:1003:HOH:O	2.08	0.54
1:C:7:LYS:HD3	1:C:156:CYS:SG	2.48	0.54
1:C:371:MET:HE3	1:C:371:MET:HA	1.88	0.54
1:D:503:PRO:HB3	1:D:507:ILE:HD13	1.90	0.54
1:A:110:LEU:HA	1:A:113:LEU:CD1	2.38	0.54
1:B:608:THR:HG23	4:B:1006:HOH:O	2.06	0.53
1:A:15:ALA:O	1:A:356:THR:HA	2.08	0.53
1:B:787:ALA:HB1	1:B:809:ALA:HB1	1.89	0.53
1:D:260:PRO:O	1:D:279:ARG:HD3	2.08	0.53
1:D:190:TYR:O	4:D:1004:HOH:O	2.19	0.53
1:B:682:CYS:SG	1:B:697:TRQ:HB3	2.48	0.53
1:D:15:ALA:O	1:D:356:THR:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:VAL:HG13	1:D:126:GLN:NE2	2.23	0.53
1:A:200:THR:O	1:A:208:LYS:HG3	2.09	0.52
1:C:173:LYS:NZ	1:C:248:ASP:OD2	2.35	0.52
1:D:564[B]:ASN:ND2	1:D:564[B]:ASN:H	2.07	0.52
1:B:104:GLN:HE21	1:B:108:ARG:HH21	1.55	0.52
1:B:157:ASP:HA	1:B:158:GLU:O	2.09	0.52
1:A:562:SER:HB3	1:A:568:LEU:HD11	1.91	0.52
1:A:83:PHE:O	1:A:84:LYS:HB2	2.10	0.52
1:A:682:CYS:SG	1:A:697:TRQ:HB3	2.50	0.52
1:A:386:ASP:OD1	1:A:386:ASP:N	2.43	0.52
1:B:609:PRO:HD2	4:B:1006:HOH:O	2.10	0.51
1:C:102:PRO:HB2	1:C:105:GLN:HG3	1.91	0.51
1:C:103:GLN:HA	1:C:106:LEU:HD12	1.92	0.51
1:B:75:LEU:HD11	1:B:84:LYS:NZ	2.26	0.51
1:D:465:ASP:O	1:D:471:ASN:HB3	2.11	0.51
1:A:787:ALA:HB1	1:A:809:ALA:HB1	1.93	0.51
1:A:539:GLN:OE1	4:A:1003:HOH:O	2.19	0.51
1:C:428:GLU:HA	1:C:428:GLU:OE1	2.11	0.50
1:D:68:ILE:O	1:D:71:ILE:N	2.30	0.50
1:B:105:GLN:O	1:B:109:SER:OG	2.20	0.50
3:A:902:GLY:N	4:A:1023:HOH:O	2.44	0.50
1:D:169:THR:O	1:D:171:GLY:N	2.44	0.50
1:A:69:SER:O	1:A:73:THR:HG23	2.11	0.50
1:C:73:THR:C	1:C:75:LEU:H	2.13	0.50
1:D:87:GLU:O	1:D:91:ILE:HG13	2.12	0.50
1:B:61:GLY:HA2	1:B:64:VAL:N	2.23	0.50
1:C:562:SER:HB3	1:C:568:LEU:HD11	1.93	0.50
1:B:125:VAL:HA	1:B:128:ILE:CG2	2.42	0.49
1:B:276:LEU:HD13	1:B:276:LEU:O	2.12	0.49
1:A:80:ALA:HB1	1:A:82:LYS:H	1.76	0.49
1:B:612[B]:ASN:ND2	4:B:1020:HOH:O	2.45	0.49
1:A:105:GLN:HA	1:A:108:ARG:HB2	1.93	0.49
1:A:278:GLU:HG2	1:A:279:ARG:N	2.28	0.49
1:B:125:VAL:HA	1:B:128:ILE:HG22	1.94	0.49
1:A:77:GLU:O	1:A:78:ARG:HB2	2.13	0.49
1:C:75:LEU:HG	1:C:80:ALA:HB3	1.93	0.49
1:D:66:ASN:HA	1:D:69:SER:OG	2.12	0.49
1:D:131:ALA:O	1:D:135:VAL:HG23	2.13	0.49
1:B:610:GLU:N	1:B:610:GLU:OE1	2.46	0.49
1:C:485:GLU:CD	1:C:485:GLU:H	2.17	0.48
1:C:371:MET:CE	1:C:374:MET:CB	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:LEU:C	1:D:112:ASN:H	2.17	0.48
1:D:157:ASP:OD2	1:D:160:GLY:HA2	2.13	0.48
1:D:59:ALA:O	1:D:95:LEU:HD23	2.13	0.48
1:B:75:LEU:HD21	1:B:84:LYS:NZ	2.28	0.48
1:D:60:PHE:HA	1:D:64:VAL:HG11	1.96	0.48
1:B:349:GLN:HG2	4:B:1394:HOH:O	2.14	0.48
1:B:717:SER:OG	1:B:796[B]:ASN:HB3	2.13	0.48
1:A:78:ARG:HA	1:A:78:ARG:HD2	1.37	0.47
1:D:63:ASN:HB3	1:D:67:GLU:CG	2.44	0.47
1:D:86:GLU:O	1:D:90:THR:HG23	2.14	0.47
1:D:71:ILE:HA	1:D:74:LYS:NZ	2.28	0.47
1:C:262:ASN:HB2	1:C:279:ARG:NH2	2.27	0.47
1:C:682:CYS:HB2	1:C:697:TRQ:HZ3	1.64	0.47
1:B:279:ARG:HG3	1:B:279:ARG:HH11	1.79	0.47
1:D:171:GLY:HA3	1:D:338:LYS:HB2	1.96	0.47
1:D:101:VAL:HG21	1:D:106:LEU:HD21	1.95	0.47
1:B:15:ALA:O	1:B:356:THR:HA	2.14	0.47
1:C:84:LYS:CD	1:C:85:GLN:H	2.27	0.47
1:D:153:ILE:HD12	1:D:345:ILE:HD12	1.96	0.47
1:D:682:CYS:HB2	1:D:697:TRQ:HZ3	1.69	0.47
1:A:217:PRO:HB3	4:A:1410:HOH:O	2.14	0.47
1:B:128:ILE:O	1:B:132:LEU:HG	2.15	0.47
1:B:349:GLN:NE2	1:B:600:GLN:OE1	2.48	0.47
1:A:682:CYS:HB2	1:A:697:TRQ:HZ3	1.72	0.47
1:A:695[A]:SER:HB2	1:A:703:VAL:HG21	1.97	0.47
1:C:71:ILE:O	1:C:75:LEU:HB2	2.14	0.47
1:D:468:GLN:CB	1:D:470:SER:HB2	2.45	0.47
1:A:491:LYS:NZ	4:A:1031:HOH:O	2.47	0.46
1:C:695[A]:SER:HB2	1:C:703:VAL:HG21	1.97	0.46
1:A:435:LEU:HD23	1:A:537:VAL:HG21	1.98	0.46
1:B:68:ILE:CG2	1:B:124:ILE:HD13	2.46	0.46
1:C:15:ALA:O	1:C:356:THR:HA	2.15	0.46
1:B:158:GLU:O	1:B:160:GLY:N	2.48	0.46
1:A:608:THR:HG22	1:A:610:GLU:H	1.80	0.46
1:D:64:VAL:O	1:D:68:ILE:HG13	2.15	0.46
1:D:105:GLN:OE1	1:D:139:HIS:HE1	1.98	0.46
1:D:7:LYS:HD2	1:D:350:SER:HA	1.98	0.46
1:D:682:CYS:SG	1:D:697:TRQ:HB3	2.55	0.46
1:A:82:LYS:HE3	1:A:111:ASP:O	2.16	0.46
1:D:94:LEU:HD23	1:D:94:LEU:HA	1.81	0.45
1:B:60:PHE:CZ	1:B:129:LYS:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PRO:HG2	1:A:105:GLN:HE22	1.80	0.45
1:D:386:ASP:OD1	1:D:386:ASP:N	2.45	0.45
1:D:35:TRP:HB2	4:D:1003:HOH:O	2.16	0.45
1:A:465:ASP:OD1	1:A:465:ASP:N	2.49	0.45
1:A:214:ARG:CZ	1:A:214:ARG:HB3	2.47	0.45
1:A:483:LYS:HG3	1:A:484:ASP:N	2.30	0.45
1:C:677:SER:HB2	4:C:1089:HOH:O	2.16	0.45
1:D:84:LYS:HB2	1:D:84:LYS:HE2	1.87	0.45
1:B:71:ILE:HG21	1:B:87:GLU:CD	2.37	0.45
1:D:6:TYR:CE1	1:D:166:LEU:HD13	2.52	0.45
1:D:334:VAL:HG22	1:D:344:GLU:OE1	2.17	0.45
1:A:67:GLU:O	1:A:71:ILE:HG13	2.17	0.45
1:A:606:SER:HA	1:A:612:ASN:HD22	1.82	0.45
1:D:24[B]:LYS:HE3	1:D:296:ARG:CZ	2.47	0.45
1:D:590:TRP:O	1:D:593:ARG:HG2	2.17	0.45
1:B:41:THR:HB	1:B:793:PRO:HD3	1.98	0.44
1:B:91:ILE:HG12	1:B:91:ILE:O	2.17	0.44
1:D:349:GLN:NE2	1:D:600:GLN:HB2	2.31	0.44
1:A:280:HIS:HE1	4:A:1070:HOH:O	1.99	0.44
1:D:14:ILE:HG21	1:D:577:LEU:HD11	2.00	0.44
1:C:70:GLN:O	1:C:71:ILE:HD13	2.18	0.44
1:A:596:LEU:HD23	1:A:596:LEU:HA	1.85	0.44
1:B:158:GLU:HB2	1:B:161:ASN:CB	2.33	0.44
1:B:464:ASP:O	1:B:471:ASN:HA	2.17	0.44
1:D:70:GLN:O	1:D:74:LYS:NZ	2.50	0.44
1:A:114:GLU:O	1:A:115:LEU:HD23	2.18	0.44
1:B:682:CYS:HB2	1:B:697:TRQ:HZ3	1.56	0.44
1:A:131:ALA:O	1:A:135:VAL:HG23	2.18	0.44
1:A:697:TRQ:O6	3:A:902:GLY:HA2	2.18	0.44
1:C:84:LYS:HD2	1:C:85:GLN:H	1.83	0.44
1:C:405:MET:CE	1:C:698:ALA:HB3	2.47	0.44
1:B:504:ASN:CG	1:B:505:ASP:H	2.21	0.44
1:C:45:TYR:CD2	1:C:790:MET:HG2	2.53	0.44
1:D:88:ILE:HG23	1:D:110:LEU:HD12	1.99	0.44
1:D:129:LYS:HG3	1:D:129:LYS:O	2.18	0.44
1:B:61:GLY:N	1:B:64:VAL:HB	2.33	0.43
1:B:155:LYS:NZ	4:B:1033:HOH:O	2.50	0.43
1:B:739:GLU:H	1:B:739:GLU:CD	2.21	0.43
1:B:75:LEU:HD21	1:B:84:LYS:HZ2	1.82	0.43
1:D:489:ALA:O	4:D:1005:HOH:O	2.21	0.43
1:C:66:ASN:O	1:C:69:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLN:NE2	1:A:86:GLU:H	2.17	0.43
1:C:277:GLN:HB3	1:C:279:ARG:NH1	2.34	0.43
1:C:736:MET:SD	1:C:744:LEU:HD12	2.59	0.43
1:B:6:TYR:HB2	1:B:345:ILE:HD11	2.01	0.42
1:D:110:LEU:O	1:D:112:ASN:N	2.52	0.42
1:D:639:HIS:N	4:D:1033:HOH:O	2.52	0.42
1:B:453:ARG:HG2	1:B:518:ALA:HB2	2.00	0.42
3:B:902:GLY:N	4:B:1039:HOH:O	2.51	0.42
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.95	0.42
1:A:471:ASN:ND2	1:A:471:ASN:O	2.52	0.42
1:C:156:CYS:HB3	1:C:157:ASP:H	1.75	0.42
1:A:463:VAL:HG12	1:A:466:PRO:HA	2.01	0.42
1:D:157:ASP:O	1:D:160:GLY:HA3	2.19	0.42
1:D:36:ALA:N	1:D:37[B]:HIS:CB	2.82	0.42
1:D:528:GLN:HG3	4:D:1027:HOH:O	2.19	0.42
1:B:48:THR:HB	4:B:1001:HOH:O	2.20	0.42
1:D:306:ALA:HB2	1:D:322:TRP:CE2	2.54	0.42
1:B:108:ARG:HA	1:B:111:ASP:HB2	2.02	0.42
1:A:163:VAL:HG23	1:A:163:VAL:O	2.19	0.42
1:D:33:VAL:CG1	1:D:560:LYS:HE3	2.49	0.42
1:B:128:ILE:HG23	1:B:129:LYS:N	2.35	0.42
1:B:68:ILE:HG12	1:B:91:ILE:CD1	2.49	0.42
1:C:14:ILE:HG21	1:C:577:LEU:HD11	2.01	0.42
1:A:82:LYS:HD2	1:A:82:LYS:HA	1.84	0.42
1:A:154:TYR:CZ	1:A:165:LYS:HG2	2.55	0.42
1:D:63:ASN:HB3	1:D:67:GLU:HG3	2.01	0.42
1:D:68:ILE:O	1:D:71:ILE:HG12	2.20	0.42
1:B:428[B]:GLU:H	1:B:428[B]:GLU:HG3	1.77	0.41
1:A:45:TYR:CD2	1:A:790:MET:HG2	2.54	0.41
1:D:7:LYS:HG3	1:D:156:CYS:SG	2.59	0.41
1:D:125:VAL:HG13	1:D:126:GLN:HE21	1.83	0.41
1:B:6:TYR:HB2	1:B:345:ILE:CD1	2.49	0.41
1:B:155:LYS:O	1:B:163:VAL:HG22	2.20	0.41
1:C:83:PHE:CZ	1:C:124:ILE:HD11	2.55	0.41
1:C:262:ASN:CB	1:C:279:ARG:HH21	2.31	0.41
1:C:724:GLU:HG2	4:C:1270:HOH:O	2.20	0.41
1:D:67:GLU:HG3	1:D:94:LEU:HD11	2.03	0.41
1:C:596:LEU:HA	1:C:596:LEU:HD23	1.78	0.41
1:C:756:LEU:O	1:C:761[B]:LEU:HD12	2.20	0.41
1:B:14:ILE:HG21	1:B:577:LEU:HD11	2.02	0.41
1:D:673:ILE:HD12	1:D:674:PRO:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLU:CG	1:A:82:LYS:HG2	2.51	0.41
1:A:606:SER:HB2	1:A:612:ASN:HA	2.03	0.41
1:B:546:ASN:ND2	4:B:1010:HOH:O	2.53	0.41
1:C:41:THR:HB	1:C:793:PRO:HD3	2.02	0.41
1:C:161:ASN:HB3	1:C:162:PRO:HD3	2.03	0.41
1:C:787:ALA:HB1	1:C:809:ALA:HB1	2.02	0.41
1:A:49:GLN:HB3	4:A:1425:HOH:O	2.21	0.41
1:A:86:GLU:O	1:A:90:THR:HG22	2.21	0.41
1:A:104:GLN:NE2	1:A:105:GLN:HG3	2.35	0.41
1:A:64:VAL:O	1:A:68:ILE:HG13	2.21	0.40
1:D:41:THR:HB	1:D:793:PRO:HD3	2.03	0.40
1:B:795:GLU:HA	1:B:795:GLU:OE1	2.21	0.40
1:A:5:GLN:HE21	1:A:343:PHE:HD1	1.69	0.40
1:A:7:LYS:HG2	1:A:350:SER:HA	2.02	0.40
1:A:163:VAL:O	1:A:164:GLU:O	2.40	0.40
1:C:596:LEU:HD21	4:C:1389:HOH:O	2.20	0.40
1:D:87:GLU:HA	1:D:90:THR:OG1	2.21	0.40
1:D:171:GLY:CA	1:D:338:LYS:HB2	2.51	0.40
1:B:108:ARG:HA	1:B:111:ASP:OD2	2.21	0.40
1:A:711:TYR:HA	1:A:714:PHE:CE2	2.56	0.40
1:A:761:LEU:HD23	1:A:761:LEU:HA	1.96	0.40
1:C:423:ARG:HH11	1:C:423:ARG:HD3	1.77	0.40
1:D:344:GLU:OE1	1:D:344:GLU:HA	2.21	0.40
1:D:395:VAL:HG11	1:D:530:TRP:HB2	2.03	0.40
1:D:697:TRQ:O6	3:D:902:GLY:HA2	2.21	0.40
1:A:347:ASP:OD1	1:A:350:SER:HB2	2.21	0.40
1:C:84:LYS:O	1:C:88:ILE:HG13	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1006:HOH:O	4:B:1105:HOH:O[2_558]	2.02	0.18
1:B:62:GLY:N	1:A:67:GLU:OE2[1_455]	2.08	0.12

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	783/816 (96%)	747 (95%)	27 (3%)	9 (1%)	14	4
1	B	779/816 (96%)	744 (96%)	29 (4%)	6 (1%)	19	7
1	C	781/816 (96%)	757 (97%)	19 (2%)	5 (1%)	25	12
1	D	775/816 (95%)	736 (95%)	28 (4%)	11 (1%)	11	3
All	All	3118/3264 (96%)	2984 (96%)	103 (3%)	31 (1%)	15	5

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	157	ASP
1	B	249	ASN
1	A	78	ARG
1	A	94	LEU
1	C	62	GLY
1	D	63	ASN
1	D	64	VAL
1	D	129	LYS
1	B	93	GLY
1	B	126	GLN
1	A	84	LYS
1	A	164	GLU
1	A	466	PRO
1	A	470	SER
1	C	63	ASN
1	D	37[A]	HIS
1	D	37[B]	HIS
1	D	60	PHE
1	D	111	ASP
1	D	469	SER
1	B	92	THR
1	A	279	ARG

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Mol	Chain	Res	Type
1	A	469	SER
1	C	87	GLU
1	B	159	GLN
1	C	74	LYS
1	C	86	GLU
1	D	158	GLU
1	D	161	ASN
1	A	62	GLY
1	D	130	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	687/710 (97%)	676 (98%)	11 (2%)	62	49
1	B	686/710 (97%)	679 (99%)	7 (1%)	76	68
1	C	688/710 (97%)	677 (98%)	11 (2%)	62	49
1	D	679/710 (96%)	667 (98%)	12 (2%)	59	44
All	All	2740/2840 (96%)	2699 (98%)	41 (2%)	65	52

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	66	ASN
1	B	89	GLU
1	B	104	GLN
1	B	465	ASP
1	B	470	SER
1	B	485	GLU
1	B	569	CYS
1	A	5	GLN
1	A	58	GLU
1	A	67	GLU
1	A	104	GLN
1	A	122	ASP

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Mol	Chain	Res	Type
1	A	173	LYS
1	A	244	SER
1	A	464	ASP
1	A	465	ASP
1	A	569	CYS
1	A	578	TYR
1	C	49	GLN
1	C	72	LYS
1	C	74	LYS
1	C	85	GLN
1	C	208	LYS
1	C	262	ASN
1	C	338	LYS
1	C	470	SER
1	C	485	GLU
1	C	575	ASP
1	C	578	TYR
1	D	4	CYS
1	D	72	LYS
1	D	82	LYS
1	D	108	ARG
1	D	109	SER
1	D	129	LYS
1	D	159	GLN
1	D	167	LYS
1	D	208	LYS
1	D	569	CYS
1	D	575	ASP
1	D	578	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	5	GLN
1	B	54	GLN
1	B	63	ASN
1	B	66	ASN
1	B	70	GLN
1	B	103	GLN
1	B	104	GLN
1	B	105	GLN
1	B	112	ASN

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Mol	Chain	Res	Type
1	B	161	ASN
1	B	346	GLN
1	B	349	GLN
1	A	5	GLN
1	A	54	GLN
1	A	66	ASN
1	A	70	GLN
1	A	85	GLN
1	A	103	GLN
1	A	104	GLN
1	A	105	GLN
1	A	112	ASN
1	A	139	HIS
1	A	142	HIS
1	A	147	GLN
1	A	262	ASN
1	A	280	HIS
1	A	612	ASN
1	A	635	GLN
1	A	778	GLN
1	C	5	GLN
1	C	54	GLN
1	C	242	GLN
1	C	262	ASN
1	D	49	GLN
1	D	103	GLN
1	D	105	GLN
1	D	139	HIS
1	D	142	HIS
1	D	262	ASN
1	D	346	GLN
1	D	600	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	TRQ	A	697	1	13,17,18	1.90	3 (23%)	14,24,26	1.87	5 (35%)
1	TRQ	B	697	1	13,17,18	1.74	3 (23%)	14,24,26	1.79	3 (21%)
1	TRQ	D	697	1	13,17,18	1.79	2 (15%)	14,24,26	1.97	4 (28%)
1	TRQ	C	697	1	13,17,18	1.69	2 (15%)	14,24,26	1.76	3 (21%)

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	TRQ	A	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	B	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	D	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	C	697	1	-	0/4/19/21	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	TRQ	CE2-CZ2	-4.24	1.44	1.50
1	D	697	TRQ	CE2-CZ2	-4.18	1.44	1.50
1	B	697	TRQ	CE2-CZ2	-4.05	1.44	1.50
1	C	697	TRQ	CE2-CZ2	-3.96	1.44	1.50
1	A	697	TRQ	CB-CG	-3.03	1.47	1.51
1	A	697	TRQ	CH2-CZ2	-2.81	1.50	1.54
1	D	697	TRQ	CB-CG	-2.70	1.48	1.51
1	B	697	TRQ	CB-CG	-2.43	1.48	1.51
1	B	697	TRQ	CH2-CZ2	-2.30	1.51	1.54
1	C	697	TRQ	CB-CG	-2.12	1.48	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	697	TRQ	CZ2-CE2-NE1	4.41	126.98	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	697	TRQ	CZ2-CE2-NE1	4.39	126.96	119.94
1	D	697	TRQ	CZ2-CE2-NE1	4.01	126.35	119.94
1	D	697	TRQ	CB-CG-CD1	-3.75	123.34	127.97
1	A	697	TRQ	CZ2-CE2-NE1	3.45	125.45	119.94
1	A	697	TRQ	O6-CH2-CZ2	-3.32	116.25	118.51
1	D	697	TRQ	CE3-CZ3-CH2	3.09	123.42	121.08
1	C	697	TRQ	CB-CG-CD1	-2.96	124.31	127.97
1	B	697	TRQ	CB-CG-CD1	-2.85	124.44	127.97
1	D	697	TRQ	O7-CZ2-CH2	2.81	122.31	119.00
1	C	697	TRQ	O7-CZ2-CH2	2.63	122.09	119.00
1	A	697	TRQ	CB-CG-CD1	-2.55	124.82	127.97
1	A	697	TRQ	O7-CZ2-CH2	2.42	121.85	119.00
1	B	697	TRQ	O7-CZ2-CH2	2.29	121.70	119.00
1	A	697	TRQ	O7-CZ2-CE2	2.27	124.24	121.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	697	TRQ	3	0
1	B	697	TRQ	3	0
1	D	697	TRQ	3	0
1	C	697	TRQ	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLY	C	902	-	4,4,4	1.16	1 (25%)	3,4,4	1.47	0
3	GLY	A	902	-	4,4,4	1.16	1 (25%)	3,4,4	1.38	0
3	GLY	B	902	-	4,4,4	1.39	1 (25%)	3,4,4	1.17	0
3	GLY	D	902	-	4,4,4	1.19	1 (25%)	3,4,4	1.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLY	C	902	-	-	0/2/2/2	-
3	GLY	A	902	-	-	1/2/2/2	-
3	GLY	B	902	-	-	0/2/2/2	-
3	GLY	D	902	-	-	0/2/2/2	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	GLY	OXT-C	-2.44	1.22	1.30
3	D	902	GLY	OXT-C	-2.15	1.23	1.30
3	A	902	GLY	OXT-C	-2.09	1.23	1.30
3	C	902	GLY	OXT-C	-2.08	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	GLY	OXT-C-CA-N

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	902	GLY	1	0
3	A	902	GLY	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	GLY	3	0
3	D	902	GLY	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	790/816 (96%)	0.35	94 (11%) 4 3	15, 30, 86, 122	0
1	B	782/816 (95%)	0.21	70 (8%) 9 8	12, 22, 81, 117	0
1	C	784/816 (96%)	0.24	76 (9%) 7 6	12, 24, 79, 116	0
1	D	779/816 (95%)	0.34	92 (11%) 4 4	14, 28, 87, 123	0
All	All	3135/3264 (96%)	0.28	332 (10%) 6 5	12, 26, 83, 123	0

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	68	ILE	10.8
1	D	68	ILE	9.7
1	C	61	GLY	9.3
1	C	62	GLY	9.2
1	B	83	PHE	9.2
1	A	469	SER	9.1
1	D	467	GLY	8.6
1	D	75	LEU	8.4
1	A	115	LEU	8.3
1	A	116	LYS	8.2
1	C	75	LEU	8.1
1	B	71	ILE	8.1
1	D	468	GLN	7.8
1	A	121	SER	7.7
1	A	124	ILE	7.7
1	C	65	ILE	7.6
1	C	94	LEU	7.6
1	C	88	ILE	7.3
1	D	83	PHE	7.2
1	B	73	THR	7.2
1	B	125	VAL	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	128	ILE	7.1
1	C	114	GLU	7.1
1	D	158	GLU	7.1
1	D	86	GLU	7.0
1	A	466	PRO	7.0
1	C	83	PHE	6.9
1	C	76	ASP	6.8
1	C	66	ASN	6.7
1	A	68	ILE	6.7
1	A	83	PHE	6.7
1	D	61	GLY	6.6
1	C	68	ILE	6.6
1	C	80	ALA	6.6
1	D	469	SER	6.6
1	B	276	LEU	6.6
1	B	61	GLY	6.5
1	B	113	LEU	6.5
1	B	123	ASP	6.4
1	A	75	LEU	6.4
1	A	80	ALA	6.4
1	C	81	GLU	6.4
1	A	78	ARG	6.3
1	C	69	SER	6.3
1	B	110	LEU	6.2
1	A	128	ILE	6.1
1	A	81	GLU	6.1
1	B	124	ILE	6.1
1	C	124	ILE	6.0
1	A	468	GLN	6.0
1	D	73	THR	6.0
1	B	75	LEU	5.9
1	A	113	LEU	5.9
1	D	71	ILE	5.9
1	C	70	GLN	5.8
1	B	108	ARG	5.8
1	C	73	THR	5.7
1	B	90	THR	5.6
1	D	65	ILE	5.6
1	B	91	ILE	5.5
1	D	127	GLN	5.5
1	D	466	PRO	5.5
1	A	79	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	466	PRO	5.4
1	B	85	GLN	5.4
1	B	4	CYS	5.4
1	D	169	THR	5.4
1	D	95	LEU	5.4
1	D	72	LYS	5.4
1	B	114	GLU	5.3
1	A	125	VAL	5.3
1	B	466	PRO	5.3
1	A	61	GLY	5.2
1	B	64	VAL	5.2
1	D	94	LEU	5.2
1	C	60	PHE	5.2
1	A	108	ARG	5.2
1	C	91	ILE	5.2
1	B	112	ASN	5.2
1	C	79	LYS	5.1
1	C	113	LEU	5.1
1	C	123	ASP	5.1
1	B	86	GLU	5.1
1	A	467	GLY	5.0
1	A	343	PHE	5.0
1	A	465	ASP	5.0
1	D	87	GLU	4.9
1	D	85	GLN	4.9
1	B	127	GLN	4.8
1	C	112	ASN	4.8
1	D	128	ILE	4.8
1	B	111	ASP	4.8
1	D	126	GLN	4.8
1	A	85	GLN	4.7
1	B	84	LYS	4.7
1	C	95	LEU	4.7
1	B	89	GLU	4.7
1	C	108	ARG	4.6
1	A	111	ASP	4.6
1	A	122	ASP	4.6
1	D	113	LEU	4.6
1	D	64	VAL	4.6
1	C	63	ASN	4.6
1	C	84	LYS	4.6
1	D	82	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	160	GLY	4.5
1	A	4	CYS	4.5
1	D	84	LYS	4.5
1	B	72	LYS	4.5
1	C	87	GLU	4.4
1	C	90	THR	4.4
1	D	131	ALA	4.4
1	A	88	ILE	4.4
1	C	72	LYS	4.3
1	D	69	SER	4.3
1	A	340	GLY	4.3
1	A	86	GLU	4.3
1	A	114	GLU	4.2
1	A	127	GLN	4.2
1	C	85	GLN	4.2
1	C	64	VAL	4.2
1	C	77	GLU	4.2
1	D	62	GLY	4.1
1	D	341	ASP	4.1
1	D	108	ARG	4.1
1	A	63	ASN	4.1
1	D	129	LYS	4.1
1	C	128	ILE	4.1
1	D	56	LEU	4.1
1	D	91	ILE	4.1
1	A	163	VAL	4.1
1	D	112	ASN	4.0
1	B	82	LYS	4.0
1	B	465	ASP	4.0
1	D	110	LEU	4.0
1	B	88	ILE	4.0
1	D	470	SER	4.0
1	D	130	GLY	3.9
1	D	60	PHE	3.9
1	C	110	LEU	3.9
1	A	112	ASN	3.9
1	C	4	CYS	3.9
1	A	76	ASP	3.9
1	C	71	ILE	3.9
1	C	126	GLN	3.9
1	C	106	LEU	3.8
1	B	70	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	71	ILE	3.8
1	B	158	GLU	3.8
1	C	93	GLY	3.7
1	B	109	SER	3.7
1	B	74	LYS	3.7
1	D	159	GLN	3.7
1	D	111	ASP	3.7
1	D	66	ASN	3.7
1	D	63	ASN	3.6
1	C	89	GLU	3.6
1	C	125	VAL	3.6
1	D	88	ILE	3.6
1	D	90	THR	3.6
1	B	87	GLU	3.6
1	B	131	ALA	3.6
1	A	106	LEU	3.6
1	D	343	PHE	3.6
1	C	92	THR	3.6
1	C	127	GLN	3.6
1	B	94	LEU	3.6
1	C	59	ALA	3.6
1	B	92	THR	3.6
1	B	102	PRO	3.6
1	A	72	LYS	3.5
1	D	92	THR	3.5
1	D	133	LEU	3.5
1	A	107	SER	3.5
1	D	89	GLU	3.5
1	D	109	SER	3.5
1	A	73	THR	3.5
1	A	262	ASN	3.5
1	D	107	SER	3.5
1	A	66	ASN	3.4
1	D	262	ASN	3.4
1	A	60	PHE	3.4
1	A	110	LEU	3.4
1	D	74	LYS	3.4
1	C	105	GLN	3.4
1	C	262	ASN	3.4
1	D	338	LYS	3.4
1	C	277	GLN	3.4
1	B	93	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	337	LEU	3.4
1	B	107	SER	3.3
1	A	109	SER	3.3
1	A	82	LYS	3.3
1	D	171	GLY	3.3
1	A	74	LYS	3.3
1	C	102	PRO	3.3
1	A	130	GLY	3.2
1	B	60	PHE	3.2
1	B	65	ILE	3.2
1	B	470	SER	3.2
1	A	342	THR	3.2
1	D	163	VAL	3.2
1	A	463	VAL	3.1
1	A	62	GLY	3.1
1	A	169	THR	3.1
1	C	170	ASP	3.1
1	A	84	LYS	3.1
1	D	721	ASP	3.1
1	D	125	VAL	3.1
1	A	5	GLN	3.1
1	B	62	GLY	3.1
1	D	816	ASP	3.0
1	C	340	GLY	3.0
1	D	132	LEU	3.0
1	D	156	CYS	3.0
1	C	86	GLU	3.0
1	A	339	ASN	3.0
1	C	74	LYS	3.0
1	A	132	LEU	3.0
1	A	90	THR	3.0
1	B	104	GLN	3.0
1	A	104	GLN	3.0
1	C	111	ASP	3.0
1	A	341	ASP	2.9
1	A	102	PRO	2.9
1	C	82	LYS	2.9
1	A	77	GLU	2.9
1	A	470	SER	2.9
1	D	106	LEU	2.9
1	C	78	ARG	2.8
1	B	126	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	4	CYS	2.8
1	B	106	LEU	2.8
1	A	471	ASN	2.8
1	B	69	SER	2.8
1	C	98	SER	2.8
1	B	95	LEU	2.7
1	C	109	SER	2.7
1	A	92	THR	2.7
1	D	104	GLN	2.7
1	D	93	GLY	2.7
1	A	131	ALA	2.7
1	D	339	ASN	2.7
1	B	278	GLU	2.7
1	D	59	ALA	2.7
1	C	470	SER	2.7
1	A	816	ASP	2.7
1	D	70	GLN	2.7
1	A	170	ASP	2.6
1	D	340	GLY	2.6
1	C	278	GLU	2.6
1	C	103	GLN	2.6
1	D	170	ASP	2.6
1	D	5	GLN	2.6
1	A	65	ILE	2.6
1	A	91	ILE	2.6
1	C	339	ASN	2.6
1	A	123	ASP	2.6
1	B	130	GLY	2.6
1	D	57	GLU	2.5
1	B	132	LEU	2.5
1	A	95	LEU	2.5
1	C	343	PHE	2.5
1	A	161	ASN	2.5
1	C	58	GLU	2.5
1	A	64	VAL	2.5
1	D	465	ASP	2.5
1	A	168	LEU	2.5
1	A	93	GLY	2.4
1	D	172	ASP	2.4
1	A	133	LEU	2.4
1	B	338	LYS	2.4
1	B	96	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	699	ALA	2.4
1	B	103	GLN	2.4
1	C	130	GLY	2.4
1	A	278	GLU	2.4
1	C	129	LYS	2.4
1	B	341	ASP	2.4
1	B	105	GLN	2.4
1	D	101	VAL	2.4
1	C	338	LYS	2.3
1	A	89	GLU	2.3
1	B	340	GLY	2.3
1	D	135	VAL	2.3
1	A	164	GLU	2.3
1	D	37[A]	HIS	2.3
1	D	55	LEU	2.3
1	B	66	ASN	2.3
1	D	335	VAL	2.3
1	D	342	THR	2.3
1	C	341	ASP	2.3
1	C	67	GLU	2.2
1	B	59	ALA	2.2
1	D	98	SER	2.2
1	B	170	ASP	2.2
1	A	105	GLN	2.2
1	A	126	GLN	2.2
1	B	129	LYS	2.2
1	B	63	ASN	2.2
1	A	653	ASN	2.2
1	B	169	THR	2.2
1	A	98	SER	2.2
1	D	471	ASN	2.2
1	C	97	LEU	2.2
1	C	465	ASP	2.2
1	A	167	LYS	2.2
1	C	104	GLN	2.2
1	D	105	GLN	2.2
1	A	134	LYS	2.2
1	A	338	LYS	2.1
1	A	94	LEU	2.1
1	D	168	LEU	2.1
1	C	101	VAL	2.1
1	D	344	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	471	ASN	2.1
1	D	6	TYR	2.1
1	A	157	ASP	2.1
1	D	157	ASP	2.1
1	A	721	ASP	2.0
1	D	291	ASN	2.0
1	B	337	LEU	2.0
1	A	705	VAL	2.0
1	D	463	VAL	2.0
1	B	343	PHE	2.0
1	C	57	GLU	2.0
1	B	262	ASN	2.0
1	A	337	LEU	2.0
1	A	365	ILE	2.0
1	B	98	SER	2.0
1	A	69	SER	2.0
1	D	719	SER	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, 95th 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	TRQ	B	697	16/17	0.96	0.12	13,15,27,30	0
1	TRQ	A	697	16/17	0.97	0.14	16,18,29,29	0
1	TRQ	C	697	16/17	0.97	0.12	10,15,24,25	0
1	TRQ	D	697	16/17	0.97	0.11	15,18,28,29	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, 95th 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(\AA^2)	Q<0.9
3	GLY	B	902	5/5	0.85	0.19	29,31,34,35	0
3	GLY	D	902	5/5	0.93	0.14	34,36,41,44	0
3	GLY	C	902	5/5	0.94	0.12	29,34,36,39	0
3	GLY	A	902	5/5	0.96	0.14	35,39,43,46	0
2	MG	A	901	1/1	0.99	0.09	22,22,22,22	0
2	MG	D	901	1/1	0.99	0.06	22,22,22,22	0
2	MG	C	901	1/1	1.00	0.07	16,16,16,16	0
2	MG	B	901	1/1	1.00	0.07	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.