



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:57 AM UTC

PDB ID : 6VMF / pdb_00006vmf
Title : Crystal structure of the Y766F mutant of GoxA soaked with glycine
Authors : Yukl, E.T.
Deposited on : 2020-01-27
Resolution : 2.24 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

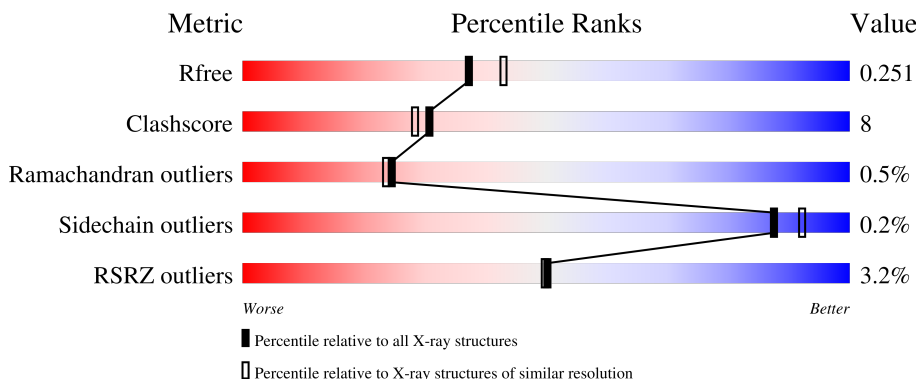
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	 2% 77% 15% 8%
1	B	816	 4% 75% 19% 5%
1	C	816	 3% 79% 15% • 6%
1	D	816	 3% 76% 19% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25629 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 Glycine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	754	Total	C	N	O	S	7	14	0
			6060	3832	1030	1178	20			
1	B	773	Total	C	N	O	S	0	11	0
			6202	3920	1054	1207	21			
1	C	770	Total	C	N	O	S	0	7	0
			6148	3889	1047	1192	20			
1	D	778	Total	C	N	O	S	0	4	0
			6194	3916	1054	1204	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	766	PHE	TYR	engineered mutation	UNP A0A161XU12
B	766	PHE	TYR	engineered mutation	UNP A0A161XU12
C	766	PHE	TYR	engineered mutation	UNP A0A161XU12
D	766	PHE	TYR	engineered mutation	UNP A0A161XU12

- Molecule 2 is MAGNESIUM ION (CCD ID: 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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

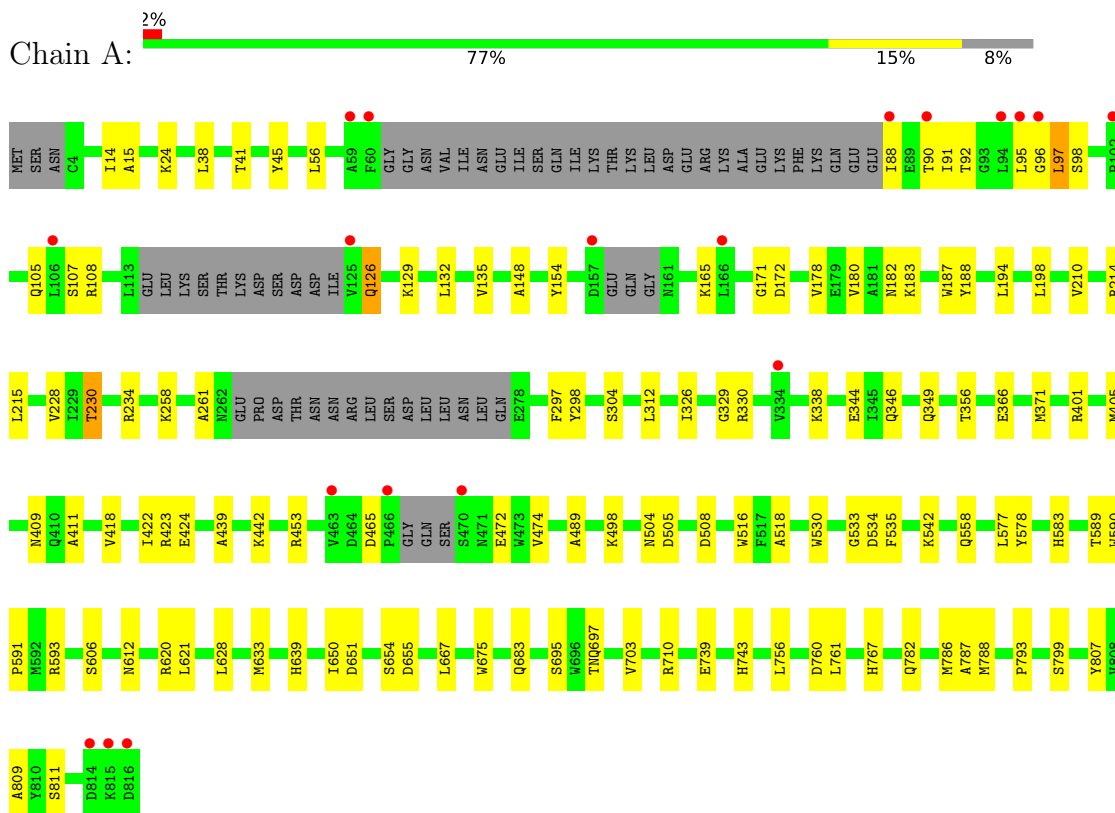
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	293	Total	O	0	0
			293	293		
4	B	208	Total	O	0	0
			208	208		
4	C	258	Total	O	0	0
			258	258		
4	D	247	Total	O	0	0
			247	247		

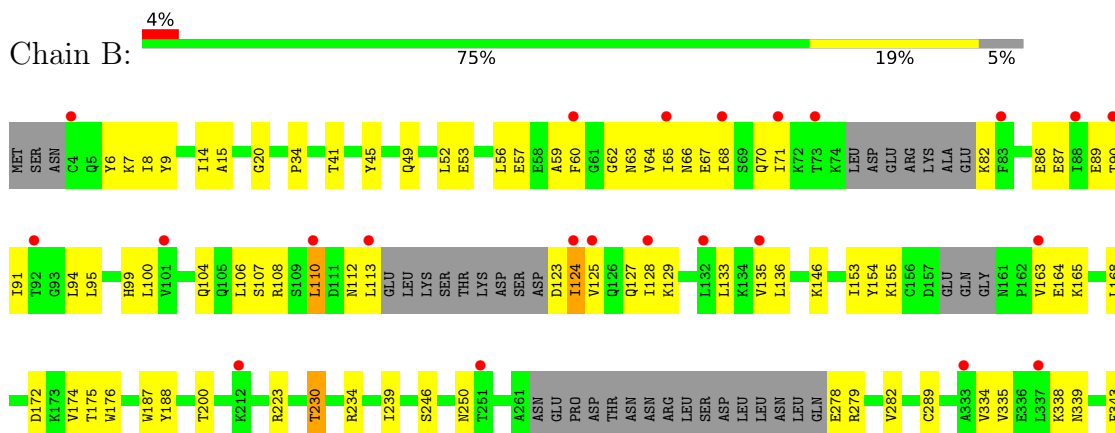
3 Residue-property plots

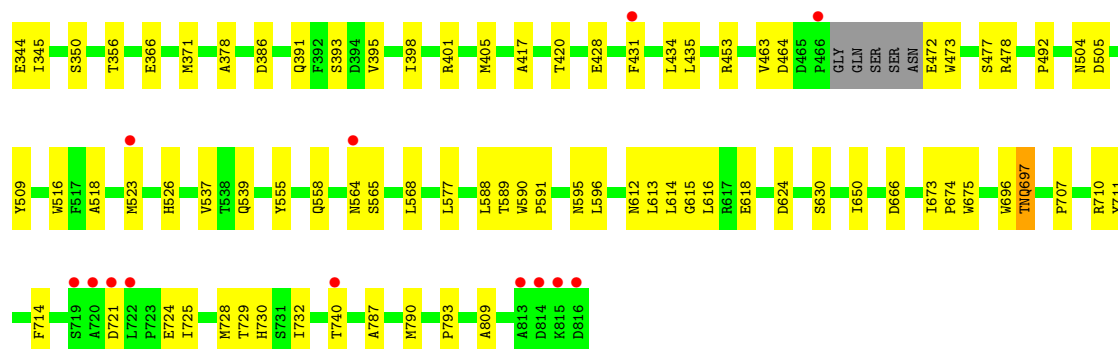
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycine oxidase

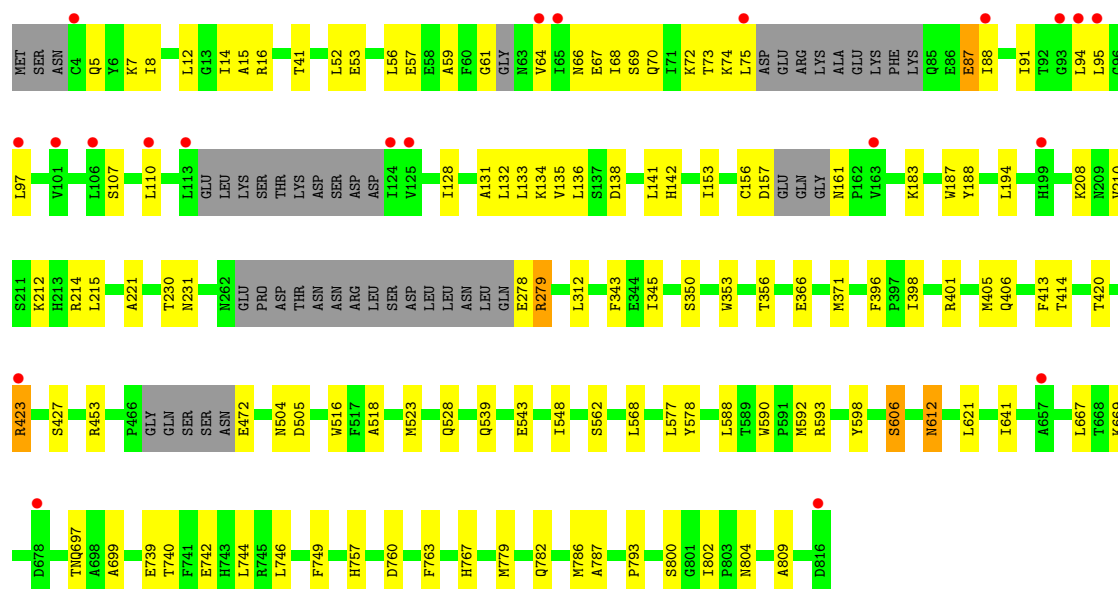
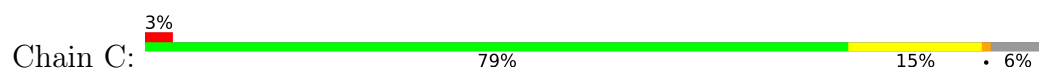


• Molecule 1: Glycine oxidase

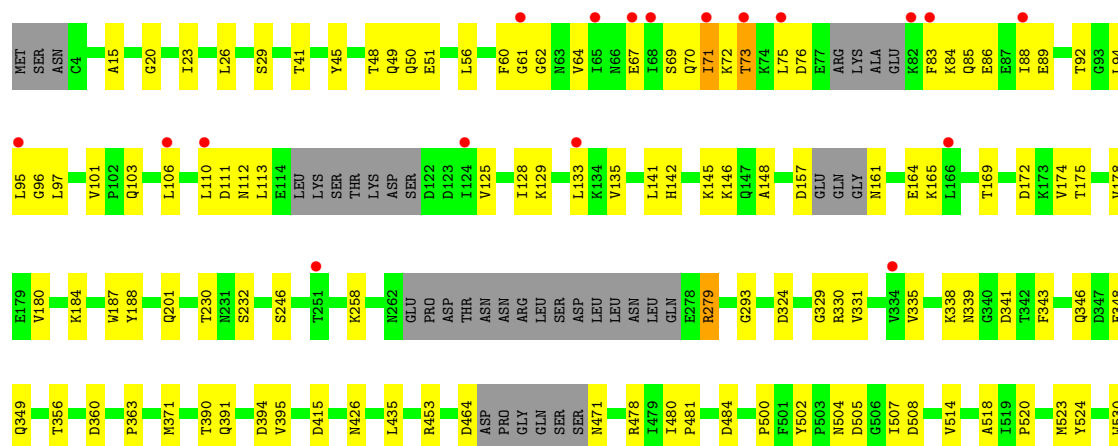
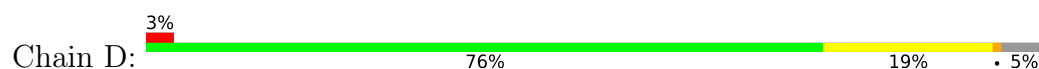


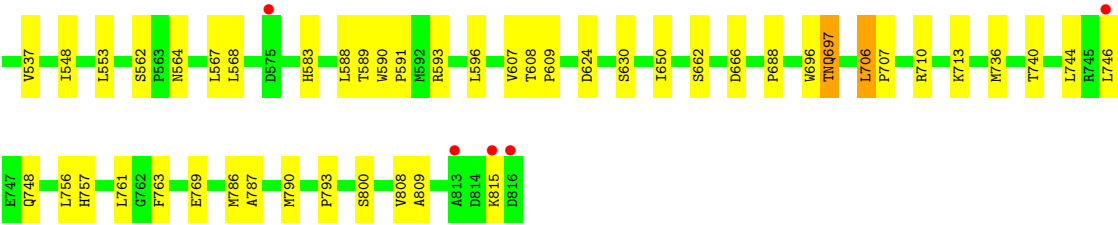


• Molecule 1: Glycine oxidase



• Molecule 1: Glycine oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.86Å 92.98Å 187.05Å 90.00° 95.06° 90.00°	Depositor
Resolution (Å)	48.42 – 2.24 48.42 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.42-2.24) 98.0 (48.42-2.24)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.202 , 0.250 0.203 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (1.13%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.757	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25629	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TNQ, SO4, MG

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	0.24	2/6185 (0.0%)	0.39	0/8425
1	B	0.18	0/6328	0.43	2/8609 (0.0%)
1	C	0.24	2/6272 (0.0%)	0.41	1/8536 (0.0%)
1	D	0.17	0/6319	0.40	0/8598
All	All	0.21	4/25104 (0.0%)	0.41	3/34168 (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	B	0	1
1	D	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	767	HIS	CD2-NE2	-7.28	1.29	1.37
1	A	767	HIS	CD2-NE2	-6.93	1.30	1.37
1	A	767	HIS	CG-ND1	-6.80	1.30	1.38
1	C	767	HIS	CG-ND1	-6.12	1.31	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	LEU	CA-C-N	-5.81	112.56	122.56
1	B	110	LEU	C-N-CA	-5.81	112.56	122.56
1	C	87	GLU	CA-CB-CG	5.69	125.48	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	123	ASP	Peptide
1	D	71	ILE	Peptide
1	D	73	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6060	0	5805	88	0
1	B	6202	0	5948	128	0
1	C	6148	0	5909	89	0
1	D	6194	0	5949	103	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	C	10	0	0	0	0
3	D	5	0	0	0	0
4	A	293	0	0	11	0
4	B	208	0	0	11	0
4	C	258	0	0	5	0
4	D	247	0	0	11	0
All	All	25629	0	23611	400	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 8.

All (400) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLN:HA	1:B:107:SER:HB3	1.43	1.01
1:D:394:ASP:OD2	4:D:1001:HOH:O	1.92	0.87
1:A:95:LEU:HD13	1:A:97:LEU:HG	1.54	0.87
1:B:568:LEU:HD22	1:B:616:LEU:HD11	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ILE:HA	1:C:94:LEU:HD12	1.61	0.83
1:C:562:SER:HB3	1:C:568:LEU:HD11	1.62	0.82
1:B:59:ALA:HB1	1:B:95:LEU:HB3	1.64	0.78
1:A:214:ARG:NH1	1:A:472:GLU:OE2	2.17	0.77
1:C:69:SER:HA	1:C:72:LYS:HB3	1.69	0.74
1:A:96:GLY:O	1:A:98:SER:N	2.19	0.74
1:C:606[A]:SER:HB3	1:C:612[A]:ASN:HA	1.69	0.73
1:D:562:SER:HB3	1:D:568:LEU:HD11	1.72	0.72
1:C:110:LEU:HD21	1:C:132:LEU:HD21	1.72	0.71
1:C:57:GLU:O	1:C:61:GLY:N	2.24	0.71
1:D:391:GLN:N	4:D:1001:HOH:O	2.15	0.71
1:B:154:TYR:CZ	1:B:165:LYS:HG2	2.27	0.70
1:B:34:PRO:HD2	1:B:568:LEU:HD12	1.73	0.69
1:B:435:LEU:HD23	1:B:537:VAL:HG21	1.74	0.69
1:A:304:SER:OG	4:A:1001:HOH:O	2.11	0.69
1:D:426:ASN:HD21	1:D:548:ILE:HG22	1.56	0.68
1:A:95:LEU:CD1	1:A:97:LEU:HG	2.23	0.67
1:C:53:GLU:O	1:C:56:LEU:HB2	1.94	0.67
1:C:87:GLU:O	1:C:91:ILE:HG12	1.94	0.67
1:B:14:ILE:HG21	1:B:577:LEU:HD11	1.77	0.66
1:B:86:GLU:HA	1:B:89:GLU:HB3	1.77	0.66
1:B:334:VAL:HG12	1:B:344:GLU:HG3	1.78	0.66
1:B:106:LEU:HD23	1:B:135:VAL:HG11	1.78	0.66
1:B:618:GLU:O	4:B:1001:HOH:O	2.14	0.66
1:A:799:SER:OG	4:A:1003:HOH:O	2.15	0.65
1:C:88:ILE:HG23	1:C:110:LEU:HD12	1.79	0.64
1:B:87:GLU:O	1:B:91:ILE:HG12	1.98	0.64
1:C:366:GLU:HB3	1:C:401:ARG:HG2	1.78	0.64
1:D:67:GLU:O	1:D:71:ILE:N	2.31	0.64
1:B:64:VAL:O	1:B:68:ILE:HG23	1.98	0.63
1:C:787:ALA:HB1	1:C:809:ALA:HB1	1.80	0.63
1:B:239:ILE:HD13	1:B:282:VAL:HG21	1.79	0.63
1:B:6:TYR:O	1:B:350[A]:SER:OG	2.16	0.63
1:B:335:VAL:HB	1:B:343:PHE:HB2	1.81	0.63
1:A:182:ASN:ND2	1:A:326:ILE:O	2.27	0.62
1:C:156:CYS:HG	1:C:161:ASN:N	1.97	0.62
1:A:228[B]:VAL:HG22	1:A:234:ARG:HG2	1.81	0.62
1:B:335:VAL:HG23	1:B:345:ILE:HD11	1.82	0.62
1:C:69:SER:HA	1:C:72:LYS:CB	2.30	0.62
1:C:210:VAL:HA	1:C:215:LEU:HD22	1.82	0.62
1:C:804:ASN:ND2	4:C:1020:HOH:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:SER:HA	1:D:72:LYS:HD3	1.82	0.61
1:B:278:GLU:N	4:B:1022:HOH:O	2.34	0.60
1:B:168:LEU:HD22	1:B:172:ASP:HB3	1.82	0.60
1:C:64:VAL:HG13	1:C:94:LEU:HD13	1.84	0.60
1:A:542:LYS:NZ	4:A:1029:HOH:O	2.34	0.60
1:B:163:VAL:HG23	1:B:164:GLU:H	1.65	0.60
1:B:729:THR:HG23	1:B:732:ILE:H	1.66	0.60
1:D:67:GLU:HA	1:D:70:GLN:HG3	1.84	0.60
1:C:420:THR:OG1	4:C:1001:HOH:O	2.17	0.59
1:A:442:LYS:N	4:A:1004:HOH:O	2.35	0.59
1:B:168:LEU:HD22	1:B:172:ASP:CB	2.33	0.59
1:C:59:ALA:HB1	1:C:95:LEU:HB2	1.85	0.59
1:C:73:THR:C	1:C:75:LEU:H	2.09	0.58
1:D:390:THR:HA	4:D:1001:HOH:O	2.03	0.58
1:A:439:ALA:O	4:A:1004:HOH:O	2.17	0.58
1:C:453:ARG:HG2	1:C:518:ALA:HB2	1.84	0.58
1:D:83:PHE:HE2	1:D:113:LEU:HD12	1.67	0.58
1:B:110:LEU:HD11	1:B:128:ILE:HA	1.86	0.58
1:B:64:VAL:HG23	1:B:94:LEU:HD22	1.86	0.57
1:A:15:ALA:O	1:A:356:THR:HA	2.05	0.57
1:D:88:ILE:HG23	1:D:110:LEU:HD12	1.86	0.57
1:A:95:LEU:HD13	1:A:97:LEU:CG	2.30	0.56
1:B:107:SER:OG	1:B:108:ARG:N	2.38	0.56
1:B:104:GLN:HA	1:B:107:SER:CB	2.27	0.56
1:D:89:GLU:O	1:D:92:THR:OG1	2.22	0.56
1:C:67:GLU:HG3	1:C:94:LEU:HD21	1.87	0.56
1:D:258:LYS:HG2	1:D:279:ARG:HD3	1.86	0.56
1:B:172:ASP:OD1	1:B:338:LYS:N	2.37	0.56
1:C:14:ILE:HG21	1:C:577:LEU:HD11	1.87	0.56
1:C:406:GLN:NE2	4:C:1003:HOH:O	2.21	0.56
1:A:366:GLU:OE1	1:A:401:ARG:NE	2.34	0.56
1:D:339:ASN:OD1	1:D:341:ASP:HB2	2.06	0.56
1:B:564[B]:ASN:OD1	1:B:564[B]:ASN:N	2.31	0.55
1:B:787:ALA:HB1	1:B:809:ALA:HB1	1.88	0.55
1:D:184:LYS:NZ	1:D:324:ASP:OD2	2.36	0.55
1:A:606:SER:HB2	1:A:612[A]:ASN:HA	1.89	0.55
1:C:95:LEU:HD13	1:C:97:LEU:HG	1.88	0.55
1:A:787:ALA:HB1	1:A:809:ALA:HB1	1.88	0.55
1:D:371:MET:HE3	1:D:588:LEU:HB2	1.89	0.55
1:C:7:LYS:HG2	1:C:350:SER:HA	1.88	0.55
1:B:65:ILE:HG12	1:B:65:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LEU:HD11	1:B:174:VAL:HG23	1.89	0.54
1:D:524:TYR:OH	4:D:1002:HOH:O	2.16	0.54
1:C:41:THR:HB	1:C:793:PRO:HD3	1.90	0.54
1:A:24:LYS:NZ	4:A:1041:HOH:O	2.41	0.54
1:B:523[A]:MET:HE1	1:B:614:LEU:HD21	1.90	0.54
1:D:73:THR:HG22	1:D:76:ASP:HB2	1.90	0.54
1:D:88:ILE:O	1:D:92:THR:HG23	2.07	0.54
1:D:49:GLN:HE21	1:D:133:LEU:HD21	1.74	0.53
1:D:84:LYS:HE3	1:D:85:GLN:HB3	1.89	0.53
1:D:15:ALA:O	1:D:356:THR:HA	2.08	0.53
1:A:88:ILE:HA	1:A:90:THR:HG22	1.89	0.53
1:C:760:ASP:O	1:C:782:GLN:HG3	2.09	0.53
1:D:435:LEU:HD23	1:D:537:VAL:HG21	1.91	0.53
1:B:589:THR:OG1	1:B:590:TRP:N	2.39	0.53
1:D:69:SER:O	1:D:72:LYS:HG2	2.09	0.53
1:A:187:TRP:CG	1:A:188:TYR:H	2.26	0.53
1:B:589:THR:HG23	1:B:591:PRO:HD2	1.91	0.53
1:A:41:THR:HB	1:A:793:PRO:HD3	1.92	0.52
1:B:65:ILE:HA	1:B:68:ILE:HG12	1.91	0.52
1:B:67:GLU:O	1:B:71:ILE:HD12	2.09	0.52
1:B:721:ASP:OD2	1:B:730:HIS:HE1	1.92	0.52
1:D:564[A]:ASN:ND2	1:D:567:LEU:HD22	2.25	0.52
1:A:695:SER:HB2	1:A:703:VAL:HG21	1.91	0.52
1:C:64:VAL:O	1:C:68:ILE:HG12	2.10	0.52
1:D:20:GLY:O	1:D:146:LYS:HE2	2.10	0.52
1:D:95:LEU:O	1:D:97:LEU:N	2.42	0.52
1:D:706[A]:LEU:HD23	1:D:808:VAL:HG22	1.92	0.52
1:C:16:ARG:O	4:C:1002:HOH:O	2.19	0.52
1:C:187:TRP:CG	1:C:188:TYR:H	2.28	0.51
1:B:154:TYR:HH	1:B:565:SER:HG	1.57	0.51
1:D:64:VAL:HG22	1:D:94:LEU:HB3	1.91	0.51
1:C:214:ARG:NH1	1:C:472:GLU:OE1	2.40	0.51
1:A:105:GLN:OE1	1:A:108:ARG:HD2	2.11	0.51
1:A:126:GLN:O	1:A:129:LYS:N	2.42	0.51
1:A:424:GLU:HB2	1:D:736:MET:HE2	1.92	0.51
1:A:178:VAL:HG11	1:A:297:PHE:HE2	1.76	0.51
1:D:787:ALA:HB1	1:D:809:ALA:HB1	1.92	0.51
1:B:492:PRO:O	4:B:1002:HOH:O	2.18	0.51
1:B:7:LYS:NZ	1:B:9:TYR:OH	2.44	0.50
1:B:64:VAL:HA	1:B:67:GLU:HB2	1.92	0.50
1:C:128:ILE:O	1:C:132:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:THR:OG1	1:D:50:GLN:HG3	2.12	0.50
1:C:15:ALA:O	1:C:356:THR:HA	2.11	0.50
1:D:103:GLN:HG3	1:D:106:LEU:HD11	1.93	0.50
1:A:504:ASN:CG	1:A:505:ASP:H	2.19	0.50
1:C:371:MET:HE3	1:C:588:LEU:HB2	1.94	0.50
1:B:463:VAL:HG22	1:B:473:TRP:CD1	2.46	0.50
1:D:51:GLU:OE2	1:D:145:LYS:NZ	2.35	0.50
1:A:172:ASP:OD2	1:A:338:LYS:HG3	2.12	0.50
1:B:99:HIS:CE1	1:B:100:LEU:HD13	2.47	0.50
1:B:125:VAL:O	1:B:128:ILE:HB	2.12	0.50
1:C:746:LEU:HA	1:C:802:ILE:HD11	1.94	0.50
1:B:82:LYS:HG2	1:B:113:LEU:C	2.36	0.49
1:B:175:THR:HG22	1:B:246:SER:HB2	1.94	0.49
1:B:666:ASP:OD2	4:B:1003:HOH:O	2.20	0.49
1:A:683:GLN:HG3	1:A:756:LEU:HD11	1.93	0.49
1:D:707:PRO:HG2	1:D:710:ARG:HG2	1.94	0.49
1:D:111:ASP:C	1:D:112:ASN:HD22	2.21	0.49
1:A:92:THR:HG21	1:A:107:SER:OG	2.13	0.49
1:B:108:ARG:O	1:B:112:ASN:ND2	2.46	0.49
1:B:339:ASN:ND2	4:B:1044:HOH:O	2.45	0.49
1:D:508:ASP:OD1	1:D:583:HIS:NE2	2.46	0.49
1:A:183:LYS:HE3	1:A:633:MET:HE2	1.95	0.48
1:B:187:TRP:CG	1:B:188:TYR:H	2.31	0.48
1:C:396:PHE:CE1	1:C:548:ILE:HG13	2.49	0.48
1:A:258:LYS:HG2	1:A:261:ALA:HA	1.94	0.48
1:A:312:LEU:HD11	1:C:312:LEU:HD11	1.96	0.48
1:B:8:ILE:HD13	1:B:176:TRP:HZ3	1.79	0.48
1:C:56:LEU:HD11	1:C:133:LEU:HB2	1.94	0.48
1:C:398[B]:ILE:HD11	1:C:523:MET:HE2	1.96	0.48
1:D:69:SER:HA	1:D:72:LYS:CD	2.43	0.48
1:A:90:THR:HG23	1:A:91:ILE:HG13	1.96	0.48
1:C:423[A]:ARG:HH11	1:C:423[A]:ARG:HB3	1.78	0.48
1:A:589:THR:HG23	1:A:591:PRO:HD2	1.96	0.48
1:B:371:MET:HE3	1:B:588:LEU:HB2	1.95	0.48
1:B:401:ARG:O	1:B:405:MET:HG2	2.14	0.48
1:A:24:LYS:NZ	4:A:1036:HOH:O	2.37	0.48
1:A:530:TRP:HA	1:A:535:PHE:CD1	2.48	0.48
1:C:606[B]:SER:HB2	1:C:612[B]:ASN:HA	1.96	0.48
1:D:26:LEU:HD11	1:D:51:GLU:HB3	1.96	0.48
1:D:596:LEU:HD21	1:D:650:ILE:HA	1.96	0.48
1:B:335:VAL:HG23	1:B:345:ILE:CD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:PRO:HG2	1:B:710:ARG:HG2	1.95	0.47
1:A:88:ILE:HG13	1:A:91:ILE:HD12	1.97	0.47
1:B:250:ASN:HA	1:B:289:CYS:O	2.15	0.47
1:D:64:VAL:HA	1:D:94:LEU:HD13	1.96	0.47
1:B:125:VAL:O	1:B:129:LYS:HG3	2.14	0.47
1:B:696:TRP:HB3	1:B:697:TNQ:CE3	2.45	0.47
1:D:187:TRP:CG	1:D:188:TYR:H	2.32	0.47
1:D:330:ARG:NH2	1:D:346:GLN:HG2	2.30	0.47
1:D:484:ASP:OD2	4:D:1003:HOH:O	2.21	0.47
1:D:590:TRP:O	1:D:593:ARG:HG2	2.14	0.47
1:B:386:ASP:N	1:B:386:ASP:OD1	2.47	0.47
1:A:418:VAL:O	1:A:422:ILE:HG12	2.15	0.47
1:B:154:TYR:OH	1:B:565:SER:OG	2.25	0.47
1:A:105:GLN:HG3	1:A:135:VAL:CG2	2.45	0.47
1:A:606:SER:HB2	1:A:612[B]:ASN:HA	1.97	0.47
1:B:740:THR:HG21	1:C:427:SER:HB3	1.97	0.47
1:A:453:ARG:HG2	1:A:518:ALA:HB2	1.97	0.47
1:C:73:THR:O	1:C:75:LEU:N	2.48	0.47
1:D:180:VAL:HA	1:D:329:GLY:HA3	1.95	0.47
1:D:815:LYS:HB3	1:D:815:LYS:HE3	1.52	0.47
1:D:175:THR:HG22	1:D:246:SER:HB3	1.96	0.46
1:B:155:LYS:HE3	1:B:164:GLU:HG2	1.97	0.46
1:A:198:LEU:HD11	1:A:650:ILE:HD11	1.96	0.46
1:A:401:ARG:O	1:A:405:MET:HG2	2.16	0.46
1:B:15:ALA:O	1:B:356:THR:HA	2.15	0.46
1:C:396:PHE:HE1	1:C:548:ILE:HG13	1.80	0.46
1:C:742:GLU:OE1	1:C:800:SER:HB3	2.15	0.46
1:D:481:PRO:HG3	1:D:688:PRO:HD3	1.98	0.46
1:D:761:LEU:HD21	1:D:786:MET:SD	2.55	0.46
1:A:675:TRP:NE1	4:A:1001:HOH:O	2.46	0.46
1:C:401:ARG:O	1:C:405:MET:HG2	2.15	0.46
1:D:415:ASP:O	4:D:1004:HOH:O	2.21	0.46
1:A:210:VAL:HA	1:A:215:LEU:HD12	1.98	0.46
1:A:423:ARG:CD	1:D:744:LEU:HD21	2.46	0.46
1:B:477:SER:OG	1:B:478:ARG:N	2.49	0.46
1:C:132:LEU:HA	1:C:135:VAL:HG23	1.98	0.46
1:C:157:ASP:OD1	1:C:161:ASN:HB3	2.15	0.46
1:A:194:LEU:HB2	1:A:590:TRP:CZ2	2.50	0.46
1:B:391:GLN:OE1	1:B:612:ASN:N	2.39	0.46
1:C:131:ALA:O	1:C:135:VAL:HG23	2.15	0.46
1:B:393:SER:HB2	1:B:613:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:GLU:HG3	1:D:349:GLN:NE2	2.31	0.46
1:A:45:TYR:HB2	1:A:788:MET:HG2	1.98	0.46
1:D:60:PHE:HZ	1:D:128:ILE:HG22	1.81	0.46
1:A:171:GLY:HA3	1:A:338:LYS:HG2	1.99	0.45
1:A:533:GLY:O	1:A:535:PHE:N	2.48	0.45
1:B:624:ASP:OD2	1:B:630:SER:OG	2.34	0.45
1:C:757:HIS:HA	1:C:763:PHE:CZ	2.51	0.45
1:D:41:THR:HB	1:D:793:PRO:HD3	1.97	0.45
1:B:8:ILE:HD13	1:B:176:TRP:CZ3	2.51	0.45
1:B:711:TYR:HA	1:B:714:PHE:CE2	2.51	0.45
1:A:230:THR:HA	1:B:464:ASP:OD2	2.17	0.45
1:B:175:THR:HA	1:B:246:SER:HA	1.98	0.45
1:B:345:ILE:HG23	1:B:350[B]:SER:HB2	1.98	0.45
1:B:673:ILE:HD12	1:B:674:PRO:HA	1.98	0.45
1:A:105:GLN:HG3	1:A:135:VAL:HG21	1.99	0.45
1:C:56:LEU:HG	1:C:133:LEU:HD23	1.98	0.45
1:D:69:SER:HA	1:D:72:LYS:HG2	1.98	0.45
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.66	0.45
1:D:83:PHE:CE2	1:D:113:LEU:HD12	2.48	0.45
1:A:180:VAL:HA	1:A:329:GLY:HA3	1.99	0.45
1:C:52:LEU:HD22	1:C:136:LEU:HB3	1.99	0.45
1:A:95:LEU:O	1:A:95:LEU:HD12	2.17	0.45
1:A:739:GLU:HG2	1:A:743:HIS:CE1	2.52	0.45
1:B:62:GLY:HA2	1:B:63:ASN:HA	1.62	0.45
1:B:428:GLU:OE1	1:B:428:GLU:HA	2.16	0.45
1:C:66:ASN:O	1:C:70:GLN:HG3	2.17	0.45
1:D:61:GLY:HA2	1:D:62:GLY:HA2	1.64	0.45
1:D:453:ARG:HG2	1:D:518:ALA:HB2	1.99	0.45
1:B:45:TYR:CD2	1:B:790:MET:HG2	2.52	0.45
1:C:592:MET:O	1:C:598:TYR:OH	2.34	0.45
1:D:101:VAL:HG11	1:D:135:VAL:HG12	1.98	0.45
1:B:49:GLN:NE2	1:B:133:LEU:HD21	2.32	0.45
1:B:67:GLU:O	1:B:68:ILE:C	2.59	0.45
1:C:64:VAL:O	1:C:68:ILE:N	2.47	0.45
1:C:504:ASN:CG	1:C:505:ASP:H	2.25	0.45
1:D:84:LYS:HD2	1:D:84:LYS:HA	1.74	0.45
1:A:787:ALA:HA	1:A:811:SER:HB3	1.99	0.44
1:B:113:LEU:HD11	1:B:127:GLN:HB3	1.98	0.44
1:C:231:ASN:N	1:D:464:ASP:OD2	2.44	0.44
1:A:96:GLY:C	1:A:98:SER:H	2.22	0.44
1:B:596:LEU:HD21	1:B:650:ILE:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ALA:O	4:A:1005:HOH:O	2.21	0.44
1:D:29:SER:HA	1:D:148:ALA:O	2.18	0.44
1:A:38:LEU:O	1:A:807:TYR:OH	2.27	0.44
1:A:558:GLN:OE1	4:A:1007:HOH:O	2.21	0.44
1:B:52:LEU:HD13	1:B:136:LEU:HB3	1.99	0.44
1:B:539:GLN:NE2	4:B:1050:HOH:O	2.47	0.44
1:D:75:LEU:HD21	1:D:83:PHE:HD1	1.81	0.44
1:D:172:ASP:OD1	1:D:338:LYS:N	2.50	0.44
1:A:655:ASP:OD1	4:A:1006:HOH:O	2.21	0.44
1:B:53:GLU:O	1:B:57:GLU:HG3	2.18	0.44
1:B:110:LEU:HD23	1:B:110:LEU:HA	1.63	0.44
1:C:12:LEU:HD13	1:C:353:TRP:HB3	2.00	0.44
1:C:590:TRP:O	1:C:593:ARG:HG2	2.18	0.44
1:B:395:VAL:HG12	1:B:526:HIS:HB3	1.99	0.44
1:B:417:ALA:HA	1:B:420:THR:HG22	1.99	0.44
1:B:729:THR:HG21	4:B:1200:HOH:O	2.16	0.44
1:D:174:VAL:HG11	1:D:293:GLY:HA2	2.00	0.44
1:D:279:ARG:HH11	1:D:279:ARG:HB2	1.83	0.44
1:B:86:GLU:HA	1:B:89:GLU:CB	2.47	0.44
1:D:335:VAL:HB	1:D:343:PHE:HB2	1.99	0.44
1:B:20:GLY:O	1:B:146:LYS:HE2	2.18	0.43
1:B:729:THR:HG22	1:B:732:ILE:HD12	2.00	0.43
1:C:73:THR:C	1:C:75:LEU:N	2.75	0.43
1:D:23:ILE:HD11	1:D:26:LEU:HB2	2.00	0.43
1:D:141:LEU:HG	1:D:142:HIS:CD2	2.53	0.43
1:B:57:GLU:HG2	1:B:129:LYS:HZ3	1.83	0.43
1:B:223:ARG:HD3	1:B:234:ARG:CZ	2.49	0.43
1:C:141:LEU:HG	1:C:142:HIS:CE1	2.53	0.43
1:C:539:GLN:O	1:C:543:GLU:HG2	2.17	0.43
1:A:590:TRP:O	1:A:593:ARG:HG2	2.19	0.43
1:C:95:LEU:HD12	1:C:95:LEU:O	2.18	0.43
1:B:200:THR:O	4:B:1004:HOH:O	2.21	0.43
1:B:366:GLU:HB3	1:B:401:ARG:HG2	1.99	0.43
1:B:7:LYS:HA	1:B:350[A]:SER:OG	2.18	0.43
1:D:504:ASN:CG	1:D:505:ASP:H	2.26	0.43
1:D:624:ASP:OD2	1:D:630:SER:OG	2.34	0.43
1:C:345:ILE:HG23	1:C:350:SER:HB2	2.00	0.43
1:B:398:ILE:HD11	1:B:523[A]:MET:CE	2.48	0.43
1:A:14:ILE:HG21	1:A:577:LEU:HD11	2.00	0.43
1:D:589:THR:HG23	1:D:591:PRO:HD2	1.99	0.43
1:A:504:ASN:HB2	1:A:516:TRP:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:GLY:O	1:B:616:LEU:HD23	2.19	0.43
1:A:621:LEU:HD11	1:A:667:LEU:HD11	2.01	0.42
1:B:8:ILE:HG12	1:B:153:ILE:HD13	2.01	0.42
1:C:134:LYS:HD3	1:C:138:ASP:OD2	2.19	0.42
1:B:555:TYR:HA	1:B:558:GLN:HG2	2.00	0.42
1:C:800:SER:OG	1:C:802:ILE:HG12	2.19	0.42
1:D:103:GLN:NE2	4:D:1057:HOH:O	2.52	0.42
1:D:164:GLU:HG3	1:D:165:LYS:O	2.19	0.42
1:B:41:THR:HB	1:B:793:PRO:HD3	2.01	0.42
1:B:724:GLU:HA	1:B:728:MET:O	2.19	0.42
1:C:208:LYS:HB2	1:C:208:LYS:HE3	1.57	0.42
1:C:7:LYS:HD3	1:C:156:CYS:SG	2.59	0.42
1:D:86:GLU:HA	1:D:89:GLU:HG2	2.01	0.42
1:D:178:VAL:HA	1:D:330:ARG:O	2.19	0.42
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.78	0.42
1:B:504:ASN:HB2	1:B:516:TRP:C	2.45	0.42
1:D:756:LEU:O	1:D:761:LEU:HD23	2.19	0.42
1:B:453:ARG:HG2	1:B:518:ALA:HB2	2.00	0.42
1:B:740:THR:HG22	4:B:1192:HOH:O	2.20	0.42
1:D:696:TRP:HB3	1:D:697:TNQ:CE3	2.50	0.42
1:A:628:LEU:HA	1:A:633:MET:SD	2.59	0.42
1:B:155:LYS:HE3	1:B:164:GLU:CG	2.50	0.42
1:D:478:ARG:NH2	4:D:1019:HOH:O	2.30	0.42
1:A:508:ASP:OD2	1:A:583:HIS:NE2	2.47	0.42
1:C:740:THR:O	1:C:744:LEU:HG	2.20	0.42
1:B:7:LYS:HG2	1:B:350[A]:SER:OG	2.20	0.42
1:C:208:LYS:HE2	1:C:212:LYS:HD3	2.02	0.42
1:D:746:LEU:HG	1:D:800:SER:O	2.19	0.42
1:A:371:MET:HE2	1:A:578:TYR:O	2.20	0.42
1:A:710:ARG:HA	1:A:710:ARG:HD3	1.81	0.42
1:B:504:ASN:CG	1:B:505:ASP:H	2.27	0.42
1:D:471:ASN:HD22	1:D:471:ASN:HA	1.62	0.42
1:A:344:GLU:HB3	1:A:346:GLN:HG3	2.01	0.41
1:A:639:HIS:HB3	1:B:509:TYR:CD1	2.55	0.41
1:B:9:TYR:OH	1:B:618:GLU:OE1	2.27	0.41
1:C:66:ASN:OD1	1:C:67:GLU:N	2.53	0.41
1:C:739:GLU:H	1:C:739:GLU:HG3	1.69	0.41
1:D:169:THR:OG1	1:D:338:LYS:HD2	2.21	0.41
1:D:178:VAL:HG12	1:D:331:VAL:HG13	2.02	0.41
1:D:201:GLN:HB2	4:D:1235:HOH:O	2.20	0.41
1:D:757:HIS:HA	1:D:763:PHE:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLN:H	1:A:349:GLN:CD	2.27	0.41
1:A:409:ASN:HD21	1:A:411:ALA:HB3	1.85	0.41
1:A:453:ARG:NH2	1:A:498:LYS:O	2.53	0.41
1:A:756:LEU:O	1:A:761[A]:LEU:HD12	2.19	0.41
1:B:68:ILE:HB	1:B:124:ILE:HG21	2.02	0.41
1:C:88:ILE:HG21	1:C:107:SER:O	2.20	0.41
1:C:621:LEU:HD11	1:C:667:LEU:HD11	2.02	0.41
1:D:504:ASN:HB3	1:D:514:VAL:O	2.20	0.41
1:D:662:SER:HB3	1:D:666:ASP:HB2	2.02	0.41
1:A:56:LEU:HD21	1:A:132:LEU:HB2	2.02	0.41
1:A:474:VAL:HG11	1:B:230:THR:HG22	2.01	0.41
1:A:620:ARG:HA	1:A:620:ARG:HD3	1.89	0.41
1:A:760:ASP:O	1:A:782:GLN:HG3	2.19	0.41
1:B:110:LEU:HD22	1:B:113:LEU:HB2	2.01	0.41
1:B:431:PHE:CE1	1:B:434:LEU:HD12	2.55	0.41
1:C:8:ILE:HG12	1:C:153:ILE:HD13	2.01	0.41
1:D:562:SER:OG	1:D:607:VAL:O	2.34	0.41
1:B:66:ASN:O	1:B:70:GLN:HG3	2.19	0.41
1:D:713:LYS:HE2	1:D:748:GLN:CD	2.45	0.41
1:B:56:LEU:HD22	1:B:133:LEU:HB2	2.03	0.41
1:B:56:LEU:O	1:B:60:PHE:HD1	2.03	0.41
1:B:590:TRP:CG	1:B:591:PRO:HD3	2.55	0.41
1:D:360:ASP:OD2	1:D:363:PRO:HA	2.20	0.41
1:A:761[B]:LEU:HD11	1:A:786:MET:SD	2.60	0.41
1:B:725:ILE:HD12	1:B:730:HIS:HA	2.02	0.41
1:A:88:ILE:CA	1:A:90:THR:HG22	2.50	0.41
1:A:651:ASP:HB3	1:A:654:SER:HB3	2.03	0.41
1:C:194:LEU:HB2	1:C:590:TRP:CZ2	2.55	0.41
1:C:413:PHE:CD2	1:C:414:THR:HG23	2.56	0.41
1:C:749:PHE:CD1	1:C:802:ILE:HG23	2.55	0.41
1:D:553:LEU:HD23	1:D:553:LEU:HA	1.87	0.41
1:A:154:TYR:OH	1:A:165:LYS:HE3	2.20	0.41
1:B:90:THR:O	1:B:94:LEU:HG	2.21	0.41
1:C:371:MET:HE2	1:C:578:TYR:O	2.20	0.41
1:C:779:MET:HE1	1:C:786:MET:HE2	2.02	0.41
1:D:157:ASP:OD1	1:D:161:ASN:HB3	2.21	0.41
1:A:187:TRP:CD1	1:A:188:TYR:H	2.39	0.41
1:A:330:ARG:NH2	1:A:346:GLN:O	2.43	0.41
1:B:86:GLU:CA	1:B:89:GLU:HB3	2.49	0.41
1:C:75:LEU:HD23	1:C:75:LEU:HA	1.80	0.41
1:C:183:LYS:HB2	1:C:669:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:GLU:O	1:C:279:ARG:HB2	2.20	0.41
1:C:405:MET:SD	1:C:699:ALA:HB2	2.61	0.41
1:C:528:GLN:HG3	4:C:1012:HOH:O	2.21	0.41
1:D:125:VAL:HA	1:D:128:ILE:HB	2.03	0.41
1:D:395:VAL:HG11	1:D:530:TRP:HB2	2.03	0.41
1:D:608:THR:HG23	1:D:609:PRO:HD2	2.03	0.41
1:A:590:TRP:CD2	1:A:591:PRO:HD3	2.56	0.41
1:C:504:ASN:HB2	1:C:516:TRP:C	2.46	0.41
1:D:480:ILE:HG21	1:D:507:ILE:HD11	2.03	0.41
1:D:520:PRO:HG2	1:D:523:MET:HG3	2.03	0.40
1:A:148:ALA:HB2	1:A:298:TYR:CD1	2.56	0.40
1:B:155:LYS:H	1:B:155:LYS:HG2	1.62	0.40
1:B:165:LYS:HE2	1:B:165:LYS:HB2	1.91	0.40
1:C:69:SER:CA	1:C:72:LYS:HB3	2.47	0.40
1:D:56:LEU:HD23	1:D:129:LYS:HE2	2.03	0.40
1:D:500:PRO:HB2	1:D:502:TYR:CE2	2.56	0.40
1:B:68:ILE:HG21	1:B:125:VAL:CG1	2.51	0.40
1:C:5:GLN:HG3	1:C:343:PHE:CD2	2.56	0.40
1:C:221:ALA:HB3	1:C:641:ILE:HG22	2.03	0.40
1:D:769:GLU:OE2	4:D:1006:HOH:O	2.22	0.40
1:B:146:LYS:HB3	4:B:1057:HOH:O	2.20	0.40
1:B:378:ALA:O	1:B:595:ASN:HB2	2.21	0.40
1:B:675:TRP:NE1	4:B:1036:HOH:O	2.41	0.40
1:D:740:THR:O	1:D:744:LEU:HG	2.22	0.40
1:B:6:TYR:CD2	1:B:335:VAL:HG21	2.56	0.40
1:D:45:TYR:CD2	1:D:790:MET:HG2	2.56	0.40
1:D:232:SER:OG	4:D:1005:HOH:O	2.21	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	755/816 (92%)	724 (96%)	26 (3%)	5 (1%)	18	16
1	B	770/816 (94%)	733 (95%)	34 (4%)	3 (0%)	30	30
1	C	762/816 (93%)	733 (96%)	26 (3%)	3 (0%)	30	30
1	D	769/816 (94%)	736 (96%)	30 (4%)	3 (0%)	30	30
All	All	3056/3264 (94%)	2926 (96%)	116 (4%)	14 (0%)	24	23

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	LEU
1	A	126	GLN
1	B	124	ILE
1	D	96	GLY
1	A	230	THR
1	A	534	ASP
1	B	279	ARG
1	C	74	LYS
1	C	230	THR
1	D	279	ARG
1	B	230	THR
1	C	279	ARG
1	D	230	THR
1	A	465	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	668/711 (94%)	668 (100%)	0	100	100
1	B	682/711 (96%)	680 (100%)	2 (0%)	86	90
1	C	676/711 (95%)	670 (99%)	6 (1%)	70	78
1	D	680/711 (96%)	678 (100%)	2 (0%)	86	90
All	All	2706/2844 (95%)	2696 (100%)	10 (0%)	87	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	472[A]	GLU
1	B	472[B]	GLU
1	C	423[A]	ARG
1	C	423[B]	ARG
1	C	606[A]	SER
1	C	606[B]	SER
1	C	612[A]	ASN
1	C	612[B]	ASN
1	D	706[A]	LEU
1	D	706[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	HIS
1	A	199	HIS
1	A	231	ASN
1	A	249	ASN
1	A	284	GLN
1	A	410	GLN
1	A	451	GLN
1	A	525	GLN
1	A	561	ASN
1	A	632	ASN
1	A	751	GLN
1	A	782	GLN
1	A	785	ASN
1	B	5	GLN
1	B	37	HIS
1	B	49	GLN
1	B	63	ASN
1	B	85	GLN
1	B	433	GLN
1	B	612	ASN
1	B	730	HIS
1	B	734	GLN
1	B	782	GLN
1	B	785	ASN
1	B	812	GLN
1	C	37	HIS
1	C	70	GLN

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Mol	Chain	Res	Type
1	C	112	ASN
1	C	242	GLN
1	C	525	GLN
1	C	767	HIS
1	C	778	GLN
1	C	785	ASN
1	C	812	GLN
1	D	37	HIS
1	D	49	GLN
1	D	105	GLN
1	D	112	ASN
1	D	142	HIS
1	D	383	GLN
1	D	410	GLN
1	D	426	ASN
1	D	471	ASN
1	D	525	GLN
1	D	528	GLN
1	D	600	GLN
1	D	751	GLN
1	D	785	ASN

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	C	697	1	20,21,22	3.49	6 (30%)	21,29,31	3.00	6 (28%)
1	TNQ	A	697	1	20,21,22	3.48	6 (30%)	21,29,31	3.06	7 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TNQ	B	697	1	20,21,22	3.44	6 (30%)	21,29,31	2.64	7 (33%)
1	TNQ	D	697	1	20,21,22	3.46	6 (30%)	21,29,31	2.76	9 (42%)

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	C	697	1	-	4/10/11/13	0/2/2/2
1	TNQ	A	697	1	-	4/10/11/13	0/2/2/2
1	TNQ	B	697	1	-	4/10/11/13	0/2/2/2
1	TNQ	D	697	1	-	4/10/11/13	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	697	TNQ	C2-N1	-12.12	1.26	1.45
1	C	697	TNQ	C2-N1	-12.01	1.26	1.45
1	A	697	TNQ	C2-N1	-11.96	1.26	1.45
1	B	697	TNQ	C2-N1	-11.94	1.26	1.45
1	B	697	TNQ	CH2-CZ2	6.46	1.49	1.40
1	C	697	TNQ	CH2-CZ2	6.19	1.49	1.40
1	A	697	TNQ	CH2-CZ2	6.10	1.49	1.40
1	D	697	TNQ	CH2-CZ2	5.55	1.48	1.40
1	A	697	TNQ	CD2-CE2	4.94	1.48	1.41
1	C	697	TNQ	CD2-CE2	4.80	1.47	1.41
1	D	697	TNQ	CD2-CE2	4.79	1.47	1.41
1	B	697	TNQ	CD2-CE2	4.48	1.47	1.41
1	C	697	TNQ	CD2-CG	3.31	1.49	1.44
1	A	697	TNQ	CD2-CG	3.15	1.49	1.44
1	D	697	TNQ	CE2-CZ2	3.06	1.49	1.40
1	D	697	TNQ	CD2-CG	3.00	1.48	1.44
1	A	697	TNQ	CE2-CZ2	2.92	1.49	1.40
1	B	697	TNQ	CE2-CZ2	2.90	1.49	1.40
1	C	697	TNQ	CE2-CZ2	2.82	1.48	1.40
1	B	697	TNQ	CD2-CG	2.53	1.48	1.44
1	D	697	TNQ	CD1-CG	2.50	1.40	1.36
1	B	697	TNQ	CD1-CG	2.22	1.40	1.36
1	C	697	TNQ	CD1-CG	2.16	1.40	1.36
1	A	697	TNQ	CE2-NE1	-2.02	1.34	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	697	TNQ	C1-C2-N1	8.89	127.07	110.77
1	C	697	TNQ	C1-C2-N1	8.57	126.48	110.77
1	A	697	TNQ	C2-N1-CH2	-8.25	111.74	123.94
1	C	697	TNQ	C2-N1-CH2	-8.13	111.91	123.94
1	D	697	TNQ	C1-C2-N1	7.40	124.34	110.77
1	B	697	TNQ	C1-C2-N1	7.08	123.75	110.77
1	D	697	TNQ	C2-N1-CH2	-6.76	113.93	123.94
1	B	697	TNQ	C2-N1-CH2	-6.22	114.73	123.94
1	D	697	TNQ	CZ2-CH2-N1	3.64	121.95	119.52
1	C	697	TNQ	CZ2-CH2-N1	3.47	121.84	119.52
1	B	697	TNQ	CD2-CE2-CZ2	-3.47	116.69	121.41
1	A	697	TNQ	CZ2-CH2-N1	3.43	121.81	119.52
1	B	697	TNQ	CZ2-CH2-N1	3.36	121.76	119.52
1	A	697	TNQ	CE2-NE1-CD1	3.11	111.61	108.93
1	D	697	TNQ	CD2-CE2-CZ2	-3.05	117.26	121.41
1	B	697	TNQ	CE3-CD2-CE2	2.86	122.36	119.14
1	D	697	TNQ	CE2-NE1-CD1	2.79	111.33	108.93
1	C	697	TNQ	CE2-NE1-CD1	2.60	111.17	108.93
1	C	697	TNQ	CD2-CE2-CZ2	-2.52	117.98	121.41
1	B	697	TNQ	CE2-NE1-CD1	2.37	110.97	108.93
1	A	697	TNQ	CD2-CE2-CZ2	-2.27	118.33	121.41
1	D	697	TNQ	CE3-CD2-CE2	2.26	121.68	119.14
1	B	697	TNQ	CZ3-CH2-N1	-2.24	118.05	121.75
1	A	697	TNQ	CE3-CZ3-CH2	2.16	123.74	119.57
1	D	697	TNQ	CD2-CG-CD1	-2.15	103.96	106.16
1	C	697	TNQ	CE3-CD2-CE2	2.09	121.50	119.14
1	A	697	TNQ	CE3-CD2-CE2	2.04	121.43	119.14
1	D	697	TNQ	CE3-CZ3-CH2	2.02	123.47	119.57
1	D	697	TNQ	CZ3-CH2-N1	-2.01	118.43	121.75

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	SO4	C	902	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	D	902	-	4,4,4	0.22	0	6,6,6	0.06	0
3	SO4	C	903	-	4,4,4	0.25	0	6,6,6	0.05	0

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, 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	752/816 (92%)	0.10	19 (2%) 58 59	13, 37, 89, 143	13 (1%)
1	B	772/816 (94%)	0.49	36 (4%) 36 35	19, 53, 123, 169	11 (1%)
1	C	769/816 (94%)	0.18	21 (2%) 56 57	17, 43, 112, 160	7 (0%)
1	D	777/816 (95%)	0.25	23 (2%) 52 52	16, 44, 112, 164	4 (0%)
All	All	3070/3264 (94%)	0.26	99 (3%) 50 50	13, 44, 112, 169	35 (1%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334[A]	VAL	6.4
1	D	816	ASP	5.4
1	B	124	ILE	4.3
1	B	466	PRO	4.1
1	B	71	ILE	4.1
1	C	124	ILE	4.1
1	B	212[A]	LYS	3.7
1	D	83	PHE	3.5
1	A	94	LEU	3.5
1	A	466	PRO	3.5
1	B	816	ASP	3.5
1	A	102	PRO	3.3
1	A	816	ASP	3.2
1	A	88	ILE	3.2
1	B	813	ALA	3.1
1	D	813	ALA	3.1
1	B	65	ILE	3.1
1	D	124	ILE	3.1
1	C	75	LEU	3.0
1	A	106	LEU	2.9
1	B	721	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	93	GLY	2.8
1	B	125	VAL	2.8
1	B	132	LEU	2.8
1	B	73	THR	2.8
1	B	128	ILE	2.7
1	C	65	ILE	2.7
1	D	61	GLY	2.7
1	D	133	LEU	2.7
1	B	720	ALA	2.7
1	B	113	LEU	2.7
1	A	125	VAL	2.7
1	B	814	ASP	2.7
1	B	88	ILE	2.7
1	C	110	LEU	2.7
1	C	64	VAL	2.6
1	B	4	CYS	2.6
1	C	97	LEU	2.6
1	A	96	GLY	2.5
1	D	71	ILE	2.5
1	D	73	THR	2.4
1	D	65	ILE	2.4
1	D	746	LEU	2.4
1	C	423[A]	ARG	2.4
1	C	657	ALA	2.4
1	A	470	SER	2.4
1	B	60	PHE	2.4
1	B	68	ILE	2.4
1	A	815	LYS	2.4
1	A	59	ALA	2.4
1	A	60	PHE	2.4
1	B	163	VAL	2.4
1	B	722	LEU	2.4
1	C	4	CYS	2.3
1	D	75	LEU	2.3
1	B	564[A]	ASN	2.3
1	D	575	ASP	2.3
1	B	333	ALA	2.3
1	B	90	THR	2.3
1	B	92	THR	2.3
1	C	199	HIS	2.3
1	D	68	ILE	2.3
1	D	82	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	523[A]	MET	2.3
1	A	90	THR	2.3
1	B	740	THR	2.3
1	C	88	ILE	2.3
1	C	101	VAL	2.3
1	C	125	VAL	2.3
1	D	334	VAL	2.3
1	B	337	LEU	2.3
1	A	157	ASP	2.3
1	B	83	PHE	2.2
1	C	95	LEU	2.2
1	D	106	LEU	2.2
1	D	815	LYS	2.2
1	A	463	VAL	2.2
1	B	101	VAL	2.2
1	B	135	VAL	2.2
1	B	251	THR	2.2
1	B	719	SER	2.2
1	D	166	LEU	2.2
1	C	163	VAL	2.2
1	A	814	ASP	2.2
1	C	816	ASP	2.2
1	B	815	LYS	2.2
1	C	678	ASP	2.2
1	C	94	LEU	2.1
1	D	251	THR	2.1
1	C	106	LEU	2.1
1	C	113	LEU	2.1
1	D	110	LEU	2.1
1	A	166	LEU	2.1
1	B	431	PHE	2.1
1	D	67	GLU	2.0
1	B	110	LEU	2.0
1	D	95	LEU	2.0
1	A	95	LEU	2.0
1	D	88	ILE	2.0

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

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($\text{\AA}^2$)	Q<0.9
1	TNQ	A	697	20/21	0.92	0.09	21,39,48,50	0
1	TNQ	C	697	20/21	0.92	0.09	23,35,48,60	0
1	TNQ	B	697	20/21	0.93	0.08	21,39,57,60	0
1	TNQ	D	697	20/21	0.95	0.08	18,37,48,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	SO4	C	902	5/5	0.84	0.10	93,95,96,97	0
3	SO4	D	902	5/5	0.87	0.08	74,76,82,97	0
3	SO4	C	903	5/5	0.91	0.07	97,101,106,110	0
2	MG	C	901	1/1	0.92	0.05	40,40,40,40	0
2	MG	B	901	1/1	0.94	0.05	49,49,49,49	0
2	MG	A	901	1/1	0.95	0.05	38,38,38,38	0
2	MG	D	901	1/1	0.96	0.06	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.