Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 03:58 PM EDT

PDB ID	:	6VMF
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 (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:

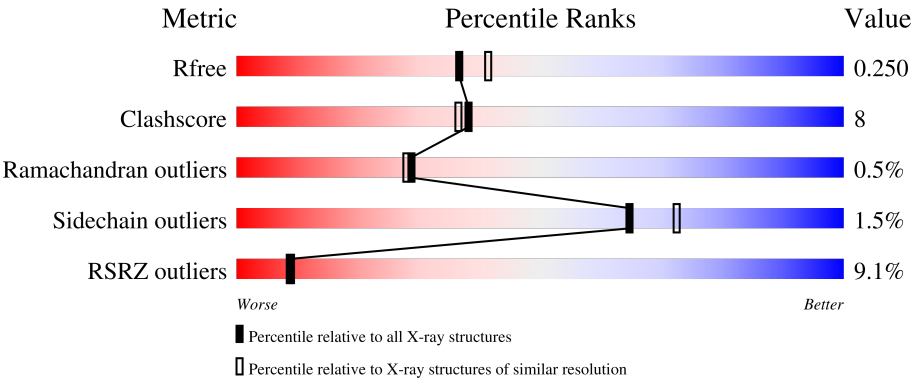
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.24 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}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (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 <=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	6% 78% 14% • 8%
1	B	816	12% 76% 18% • 5%
1	C	816	8% 79% 14% • 6%
1	D	816	8% 76% 19% • 5%

2 Entry composition (i)

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			

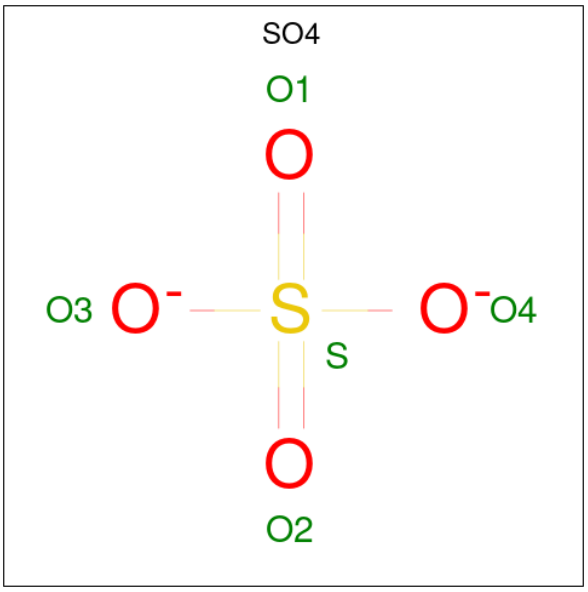
There are 4 discrepancies between the modelled and reference sequences:

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 (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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

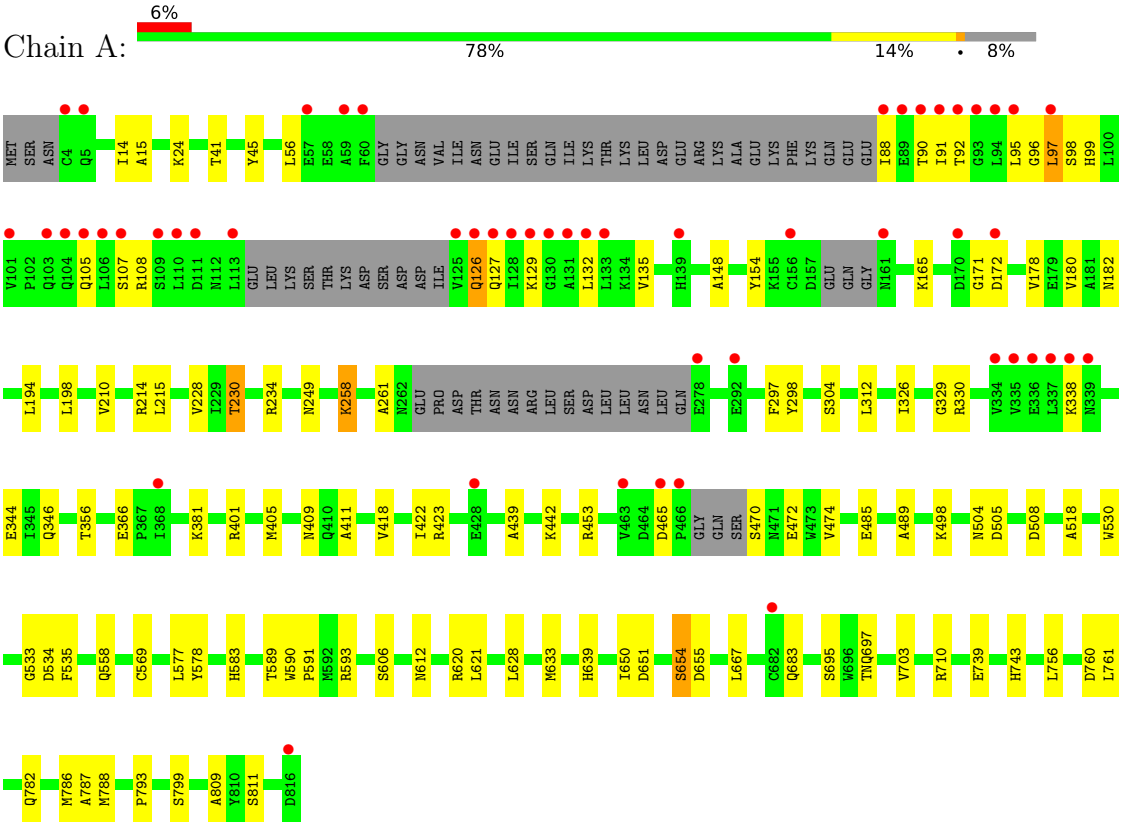
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	293	Total O 293 293	0	0
4	B	208	Total O 208 208	0	0
4	C	258	Total O 258 258	0	0
4	D	247	Total O 247 247	0	0

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.

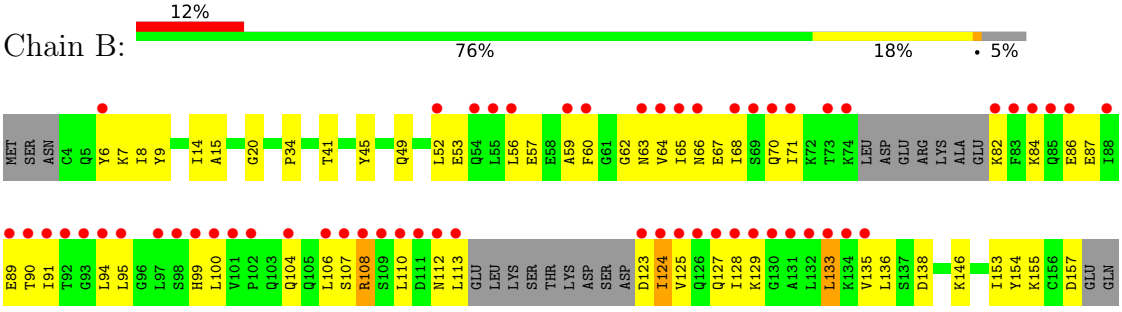
• Molecule 1: Glycine oxidase

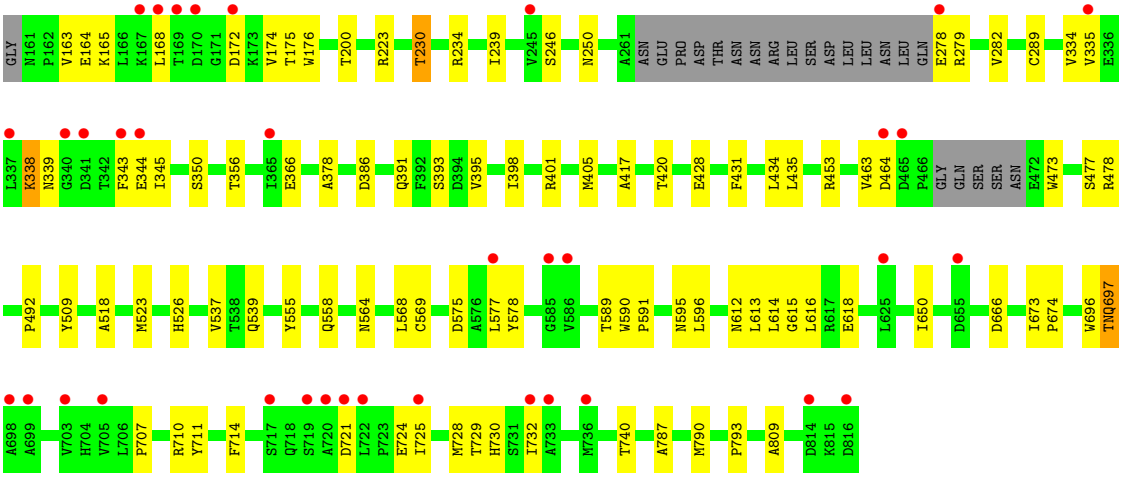
Chain A:



• Molecule 1: Glycine oxidase

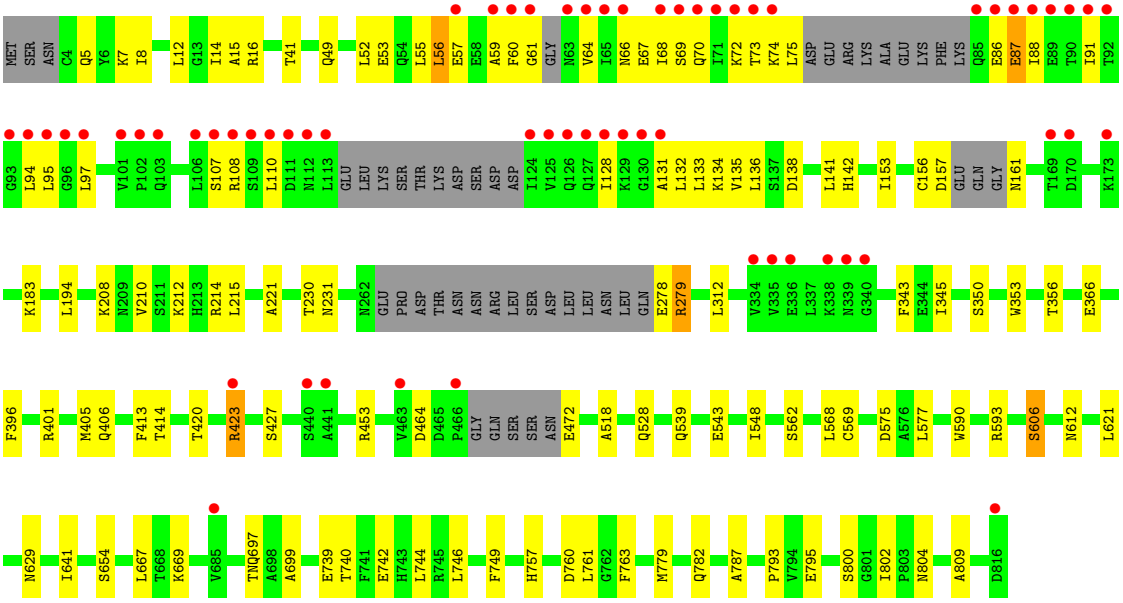
Chain B:





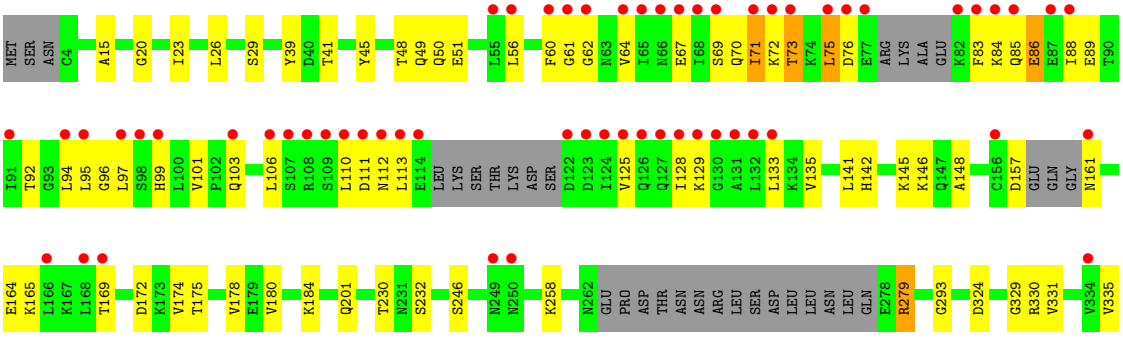
• Molecule 1: Glycine oxidase

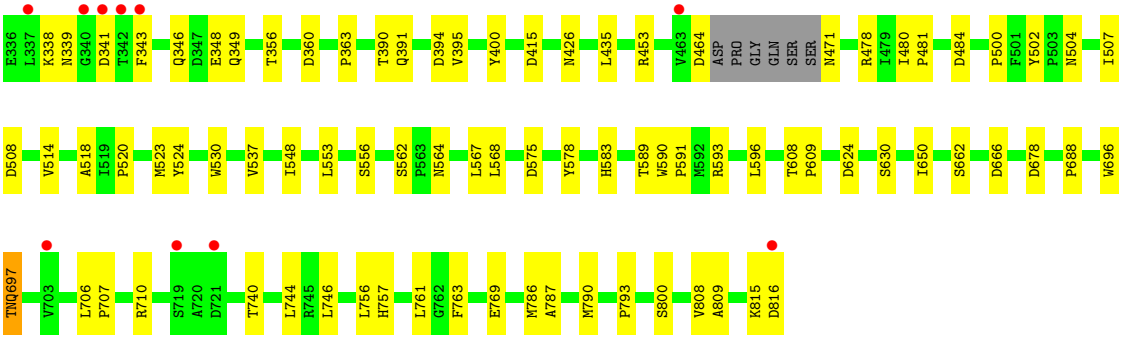
Chain C:



• Molecule 1: Glycine oxidase

Chain D:




E336 L337 K338 N339 G340 D341 T342 F343 Q346 D347 E348 Q349 T356 D360 P363 T390 Q391 D394 V395 Y400 D415 N426 L435 R453 V463 D464 ASP PRO GLY GLN SER SER N471 R478 I479 I480 P481 D484 P500 F501 Y502 P503 N504 I507
D508 V514 A518 I519 P520 M523 Y524 W530 V537 I548 L553 S556 S562 P563 N564 L567 L568 D575 Y578 H583 T589 W590 P591 M592 R593 L596 T608 P609 D624 S630 I650 S662 D666 D678 P688 W696
TNQ697 V703 L706 P707 R710 S719 A720 D721 T740 L744 R745 L746 L756 H757 L761 G762 F763 E769 M786 A787 M790 P793 S800 V808 A809 K815 D816

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.10 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.202 , 0.250 0.202 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (1.15%)	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)	0.31 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	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.*

[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: SO4, TNQ, 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	0.29	0/6185	0.47	0/8425
1	B	0.29	0/6328	0.49	0/8609
1	C	0.29	0/6272	0.49	2/8536 (0.0%)
1	D	0.27	0/6319	0.48	1/8598 (0.0%)
All	All	0.28	0/25104	0.48	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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	75	LEU	CA-CB-CG	7.45	132.44	115.30
1	C	56	LEU	CA-CB-CG	5.99	129.08	115.30
1	C	87	GLU	CA-CB-CG	5.49	125.48	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	123	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	D	71	ILE	Peptide
1	D	73	THR	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	6060	0	5805	76	0
1	B	6202	0	5948	119	0
1	C	6148	0	5909	81	0
1	D	6194	0	5949	98	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	8	0
4	B	208	0	0	10	0
4	C	258	0	0	5	0
4	D	247	0	0	11	0
All	All	25629	0	23611	367	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 (367) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:156:CYS:HG	1:C:161:ASN:N	1.93	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: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
1:D:524:TYR:OH	4:D:1002:HOH:O	2.16	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:B:589:THR:OG1	1:B:590:TRP:N	2.39	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
1:B:168:LEU:HD11	1:B:174:VAL:HG23	1.89	0.54
1:C:41:THR:HB	1:C:793:PRO:HD3	1.90	0.54
1:C:73:THR:C	1:C:75:LEU:H	2.09	0.54
1:A:24:LYS:NZ	4:A:1041:HOH:O	2.41	0.54
1:D:73:THR:HG22	1:D:76:ASP:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:ILE:O	1:D:92:THR:HG23	2.07	0.54
1:D:184:LYS:NZ	1:D:324:ASP:OD2	2.36	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:51:GLU:OE2	1:D:145:LYS:NZ	2.35	0.53
1:D:435:LEU:HD23	1:D:537:VAL:HG21	1.91	0.53
1:D:69:SER:O	1:D:72:LYS:HG2	2.09	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:523[A]:MET:HE1	1:B:614:LEU:HD21	1.92	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: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: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
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:B:463:VAL:HG22	1:B:473:TRP:CD1	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:401:ARG:O	1:B:405:MET:HG2	2.14	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:504:ASN:CG	1:A:505:ASP:H	2.19	0.45
1:A:533:GLY:O	1:A:535:PHE:N	2.48	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:B:82:LYS:HG2	1:B:113:LEU:C	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:64:VAL:O	1:C:68:ILE:N	2.47	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:B:596:LEU:HD21	1:B:650:ILE:HA	1.99	0.44
1:D:111:ASP:C	1:D:112:ASN:HD22	2.21	0.44
1:A:489:ALA:O	4:A:1005:HOH:O	2.21	0.44
1:D:624:ASP:OD2	1:D:630:SER:OG	2.34	0.44
1:D:29:SER:HA	1:D:148:ALA:O	2.18	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:D:23:ILE:HD11	1:D:26:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:LEU:HG	1:D:142:HIS:CD2	2.53	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: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: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: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:710:ARG:HA	1:A:710:ARG:HD3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:TYR:HH	1:D:400:TYR:HH	1.60	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
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:C:761[B]:LEU:HD21	1:C:779:MET:HE1	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:B:66:ASN:O	1:B:70:GLN:HG3	2.19	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:B:56:LEU:HD23	1:B:129:LYS:HZ2	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:157:ASP:OD1	1:D:161:ASN:HB3	2.21	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
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: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: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%)	22	20
1	B	770/816 (94%)	733 (95%)	34 (4%)	3 (0%)	34	35
1	C	762/816 (93%)	733 (96%)	26 (3%)	3 (0%)	34	35
1	D	769/816 (94%)	736 (96%)	30 (4%)	3 (0%)	34	35
All	All	3056/3264 (94%)	2926 (96%)	116 (4%)	14 (0%)	29	28

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 (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	668/711 (94%)	658 (98%)	10 (2%)	65	72
1	B	682/711 (96%)	673 (99%)	9 (1%)	69	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	676/711 (95%)	661 (98%)	15 (2%)	52 59
1	D	680/711 (96%)	673 (99%)	7 (1%)	76 82
All	All	2706/2844 (95%)	2665 (98%)	41 (2%)	65 72

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

Mol	Chain	Res	Type
1	A	99	HIS
1	A	127	GLN
1	A	249	ASN
1	A	258	LYS
1	A	381	LYS
1	A	470	SER
1	A	485	GLU
1	A	569	CYS
1	A	578	TYR
1	A	654	SER
1	B	84	LYS
1	B	108	ARG
1	B	133	LEU
1	B	138	ASP
1	B	157	ASP
1	B	338	LYS
1	B	569	CYS
1	B	575	ASP
1	B	578	TYR
1	C	49	GLN
1	C	55	LEU
1	C	60	PHE
1	C	86	GLU
1	C	108	ARG
1	C	423[A]	ARG
1	C	423[B]	ARG
1	C	464	ASP
1	C	569	CYS
1	C	575	ASP
1	C	606[A]	SER
1	C	606[B]	SER
1	C	629	ASN
1	C	654	SER
1	C	795	GLU

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Mol	Chain	Res	Type
1	D	86	GLU
1	D	99	HIS
1	D	556	SER
1	D	575	ASP
1	D	578	TYR
1	D	678	ASP
1	D	816	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	ASN
1	A	451	GLN
1	A	812	GLN
1	B	63	ASN
1	B	85	GLN
1	B	612	ASN
1	B	730	HIS
1	B	734	GLN
1	C	70	GLN
1	C	767	HIS
1	D	49	GLN
1	D	112	ASN
1	D	426	ASN
1	D	471	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	B	697	1	18,21,22	3.14	3 (16%)	16,29,31	2.71	4 (25%)
1	TNQ	A	697	1	18,21,22	3.15	3 (16%)	16,29,31	3.29	3 (18%)
1	TNQ	D	697	1	18,21,22	3.18	3 (16%)	16,29,31	2.85	3 (18%)
1	TNQ	C	697	1	18,21,22	3.15	3 (16%)	16,29,31	3.24	3 (18%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	697	TNQ	C2-N1	-11.96	1.26	1.45
1	C	697	TNQ	C2-N1	-11.86	1.26	1.45
1	A	697	TNQ	C2-N1	-11.81	1.26	1.45
1	B	697	TNQ	C2-N1	-11.79	1.26	1.45
1	D	697	TNQ	CZ2-CE2	3.87	1.49	1.42
1	A	697	TNQ	CZ2-CE2	3.64	1.49	1.42
1	B	697	TNQ	CZ2-CE2	3.59	1.49	1.42
1	C	697	TNQ	CZ2-CE2	3.46	1.48	1.42
1	B	697	TNQ	CH2-CZ2	3.16	1.49	1.40
1	C	697	TNQ	CH2-CZ2	3.02	1.49	1.40
1	A	697	TNQ	CH2-CZ2	2.98	1.49	1.40
1	D	697	TNQ	CH2-CZ2	2.70	1.48	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	697	TNQ	C1-C2-N1	8.78	127.07	110.96
1	A	697	TNQ	C2-N1-CH2	-8.54	111.74	123.98
1	C	697	TNQ	C1-C2-N1	8.46	126.48	110.96
1	C	697	TNQ	C2-N1-CH2	-8.42	111.91	123.98
1	D	697	TNQ	C1-C2-N1	7.29	124.34	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	697	TNQ	C2-N1-CH2	-7.01	113.93	123.98
1	B	697	TNQ	C1-C2-N1	6.97	123.75	110.96
1	B	697	TNQ	C2-N1-CH2	-6.45	114.73	123.98
1	B	697	TNQ	CG-CB-CA	-3.16	109.64	114.53
1	D	697	TNQ	CG-CB-CA	-2.60	110.51	114.53
1	C	697	TNQ	CG-CB-CA	-2.39	110.83	114.53
1	B	697	TNQ	CZ3-CH2-N1	-2.20	118.05	121.80
1	A	697	TNQ	CE3-CZ3-CH2	2.06	123.74	120.08

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	B	697	TNQ	O3-C1-C2-N1
1	C	697	TNQ	CZ2-CH2-N1-C2
1	C	697	TNQ	O2-C1-C2-N1
1	C	697	TNQ	O3-C1-C2-N1
1	D	697	TNQ	CZ2-CH2-N1-C2
1	A	697	TNQ	CZ3-CH2-N1-C2
1	B	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	B	697	TNQ	O2-C1-C2-N1
1	D	697	TNQ	O2-C1-C2-N1
1	A	697	TNQ	O2-C1-C2-N1
1	D	697	TNQ	O3-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 monosaccharides 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	903	-	4,4,4	0.15	0	6,6,6	0.04	0
3	SO4	C	902	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	D	902	-	4,4,4	0.13	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 (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	753/816 (92%)	0.26	53 (7%) 16 15	20, 37, 89, 143	0
1	B	772/816 (94%)	0.64	94 (12%) 4 3	26, 54, 123, 169	0
1	C	769/816 (94%)	0.38	63 (8%) 11 11	22, 43, 112, 160	0
1	D	777/816 (95%)	0.42	69 (8%) 9 9	21, 44, 112, 164	0
All	All	3071/3264 (94%)	0.43	279 (9%) 9 9	20, 44, 112, 169	0

All (279) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	61	GLY	8.7
1	C	110	LEU	8.4
1	B	128	ILE	8.4
1	C	65	ILE	8.2
1	A	106	LEU	8.2
1	D	73	THR	8.0
1	C	91	ILE	7.6
1	C	94	LEU	7.3
1	A	94	LEU	7.1
1	C	95	LEU	7.0
1	C	113	LEU	6.9
1	B	83	PHE	6.9
1	C	73	THR	6.7
1	B	88	ILE	6.7
1	D	71	ILE	6.6
1	C	109	SER	6.4
1	C	97	LEU	6.3
1	B	124	ILE	6.2
1	C	124	ILE	6.2
1	B	125	VAL	6.2
1	A	88	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	71	ILE	6.1
1	D	66	ASN	6.0
1	B	111	ASP	6.0
1	D	69	SER	6.0
1	C	60	PHE	5.9
1	B	132	LEU	5.9
1	B	106	LEU	5.8
1	C	64	VAL	5.7
1	A	92	THR	5.7
1	B	108	ARG	5.6
1	B	86	GLU	5.6
1	A	90	THR	5.5
1	D	123	ASP	5.5
1	C	68	ILE	5.5
1	D	113	LEU	5.4
1	D	124	ILE	5.3
1	A	59	ALA	5.3
1	D	721	ASP	5.2
1	D	83	PHE	5.1
1	A	110	LEU	5.1
1	A	60	PHE	5.1
1	B	112	ASN	5.1
1	B	168	LEU	5.1
1	B	721	ASP	5.0
1	D	122	ASP	5.0
1	D	64	VAL	4.9
1	C	111	ASP	4.9
1	B	68	ILE	4.9
1	D	94	LEU	4.8
1	A	128	ILE	4.8
1	A	127	GLN	4.8
1	B	95	LEU	4.8
1	D	91	ILE	4.7
1	C	112	ASN	4.7
1	B	169	THR	4.7
1	B	101	VAL	4.7
1	C	61	GLY	4.7
1	C	126	GLN	4.7
1	B	110	LEU	4.6
1	D	60	PHE	4.6
1	C	125	VAL	4.6
1	B	719	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	106	LEU	4.6
1	D	95	LEU	4.5
1	C	128	ILE	4.5
1	C	85	GLN	4.4
1	D	110	LEU	4.4
1	C	131	ALA	4.4
1	D	62	GLY	4.4
1	C	88	ILE	4.4
1	B	73	THR	4.4
1	C	96	GLY	4.3
1	B	133	LEU	4.3
1	B	65	ILE	4.3
1	D	87	GLU	4.3
1	B	94	LEU	4.2
1	C	66	ASN	4.2
1	D	75	LEU	4.1
1	C	71	ILE	4.1
1	A	466	PRO	4.1
1	B	60	PHE	4.1
1	A	125	VAL	4.0
1	D	125	VAL	4.0
1	B	127	GLN	4.0
1	D	107	SER	4.0
1	A	103	GLN	4.0
1	B	63	ASN	4.0
1	D	98	SER	4.0
1	D	65	ILE	4.0
1	B	126	GLN	4.0
1	C	127	GLN	4.0
1	B	56	LEU	3.9
1	B	89	GLU	3.9
1	B	91	ILE	3.9
1	A	109	SER	3.9
1	B	131	ALA	3.9
1	A	91	ILE	3.8
1	B	66	ASN	3.8
1	D	76	ASP	3.8
1	B	337	LEU	3.8
1	B	90	THR	3.7
1	C	63	ASN	3.7
1	A	4	CYS	3.7
1	C	108	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	88	ILE	3.7
1	D	106	LEU	3.7
1	D	99	HIS	3.7
1	B	64	VAL	3.6
1	B	74	LYS	3.6
1	A	463	VAL	3.6
1	A	105	GLN	3.6
1	A	89	GLU	3.6
1	A	107	SER	3.6
1	A	95	LEU	3.5
1	B	129	LYS	3.5
1	B	720	ALA	3.5
1	A	101	VAL	3.5
1	B	104	GLN	3.5
1	D	343	PHE	3.5
1	D	68	ILE	3.5
1	C	466	PRO	3.4
1	B	92	THR	3.4
1	B	341	ASP	3.4
1	B	135	VAL	3.4
1	B	85	GLN	3.4
1	C	103	GLN	3.4
1	B	113	LEU	3.4
1	D	816	ASP	3.3
1	C	107	SER	3.3
1	D	161	ASN	3.3
1	C	93	GLY	3.3
1	A	126	GLN	3.3
1	C	129	LYS	3.3
1	B	59	ALA	3.2
1	B	170	ASP	3.2
1	D	129	LYS	3.2
1	A	111	ASP	3.2
1	D	111	ASP	3.2
1	D	131	ALA	3.2
1	D	128	ILE	3.2
1	C	816	ASP	3.2
1	B	134	LYS	3.2
1	D	334	VAL	3.2
1	A	278	GLU	3.2
1	B	100	LEU	3.2
1	B	84	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	132	LEU	3.1
1	C	89	GLU	3.1
1	B	107	SER	3.0
1	C	340	GLY	3.0
1	D	97	LEU	3.0
1	B	245	VAL	3.0
1	D	168	LEU	3.0
1	B	816	ASP	3.0
1	D	127	GLN	3.0
1	A	129	LYS	3.0
1	B	343	PHE	3.0
1	B	344	GLU	3.0
1	B	335	VAL	3.0
1	D	463	VAL	3.0
1	C	101	VAL	2.9
1	B	814	ASP	2.9
1	C	441	ALA	2.9
1	A	93	GLY	2.9
1	D	85	GLN	2.9
1	D	56	LEU	2.9
1	B	733	ALA	2.9
1	B	82	LYS	2.9
1	D	84	LYS	2.9
1	A	130	GLY	2.9
1	C	69	SER	2.8
1	C	86	GLU	2.8
1	A	113	LEU	2.8
1	C	59	ALA	2.8
1	D	133	LEU	2.8
1	A	161	ASN	2.7
1	A	57	GLU	2.7
1	C	72	LYS	2.7
1	A	339	ASN	2.7
1	B	340	GLY	2.7
1	C	70	GLN	2.7
1	B	55	LEU	2.7
1	B	736	MET	2.7
1	B	278	GLU	2.7
1	D	67	GLU	2.7
1	A	334[A]	VAL	2.7
1	C	169	THR	2.7
1	D	114	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	725	ILE	2.7
1	A	816	ASP	2.7
1	B	465	ASP	2.7
1	D	169	THR	2.7
1	B	172	ASP	2.6
1	C	92	THR	2.6
1	B	98	SER	2.6
1	B	464	ASP	2.6
1	D	108	ARG	2.6
1	B	6	TYR	2.6
1	C	170	ASP	2.6
1	C	440	SER	2.5
1	A	133	LEU	2.5
1	B	705	VAL	2.5
1	A	172	ASP	2.5
1	A	465	ASP	2.5
1	D	77	GLU	2.5
1	D	166	LEU	2.5
1	C	335	VAL	2.5
1	D	112	ASN	2.5
1	A	131	ALA	2.5
1	B	585	GLY	2.5
1	A	336	GLU	2.5
1	D	82	LYS	2.5
1	B	717[A]	SER	2.5
1	D	130	GLY	2.4
1	B	97	LEU	2.4
1	D	337	LEU	2.4
1	B	655	ASP	2.4
1	A	338	LYS	2.4
1	A	428	GLU	2.4
1	A	139	HIS	2.4
1	C	57	GLU	2.4
1	B	699	ALA	2.3
1	C	685	VAL	2.3
1	D	703	VAL	2.3
1	A	170	ASP	2.3
1	B	586	VAL	2.3
1	C	130	GLY	2.3
1	C	102	PRO	2.3
1	B	698	ALA	2.3
1	A	337	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	340	GLY	2.3
1	B	625	LEU	2.3
1	C	339	ASN	2.3
1	C	336	GLU	2.2
1	C	74	LYS	2.2
1	C	463	VAL	2.2
1	A	292	GLU	2.2
1	D	719	SER	2.2
1	B	732	ILE	2.2
1	A	156	CYS	2.2
1	D	109	SER	2.2
1	D	156	CYS	2.2
1	A	368	ILE	2.2
1	B	52	LEU	2.2
1	B	93	GLY	2.2
1	B	123	ASP	2.2
1	A	5	GLN	2.2
1	B	70	GLN	2.2
1	D	103	GLN	2.2
1	C	423[A]	ARG	2.2
1	A	97	LEU	2.2
1	C	87	GLU	2.2
1	B	167	LYS	2.1
1	D	72	LYS	2.1
1	A	335	VAL	2.1
1	D	342	THR	2.1
1	B	577	LEU	2.1
1	A	104	GLN	2.1
1	B	54	GLN	2.1
1	B	365	ILE	2.1
1	D	341	ASP	2.1
1	B	130	GLY	2.1
1	B	69	SER	2.1
1	A	132	LEU	2.1
1	C	90	THR	2.1
1	C	334	VAL	2.1
1	B	102	PRO	2.1
1	C	173	LYS	2.0
1	C	338	LYS	2.0
1	D	249	ASN	2.0
1	D	250	ASN	2.0
1	D	126	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	722	LEU	2.0
1	B	109	SER	2.0
1	B	99	HIS	2.0
1	B	703	VAL	2.0
1	A	682	CYS	2.0
1	D	55	LEU	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	0.93	0.18	21,39,48,50	0
1	TNQ	C	697	20/21	0.95	0.15	23,35,48,60	0
1	TNQ	B	697	20/21	0.96	0.16	21,39,57,60	0
1	TNQ	D	697	20/21	0.96	0.17	18,37,48,48	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
2	MG	B	901	1/1	0.80	0.15	49,49,49,49	0
2	MG	C	901	1/1	0.85	0.19	40,40,40,40	0
3	SO4	C	903	5/5	0.93	0.25	97,101,106,110	0
3	SO4	C	902	5/5	0.95	0.20	93,95,96,97	0
3	SO4	D	902	5/5	0.95	0.21	74,76,82,97	0
2	MG	D	901	1/1	0.97	0.10	45,45,45,45	0
2	MG	A	901	1/1	0.98	0.18	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.