



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:12 AM UTC

PDB ID : 6EER / pdb_00006eer
Title : Structure of glycine-bound GoxA from Pseudoalteromonas luteoviolacea
Authors : Yukl, E.T.; Avalos, D.
Deposited on : 2018-08-15
Resolution : 1.82 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

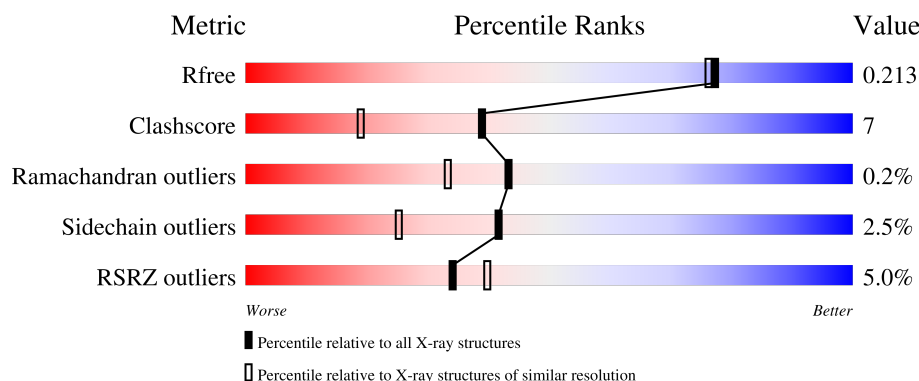
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	5% 82% 11% 6%
1	B	816	5% 82% 14% • •
1	C	816	5% 82% 12% • 5%
1	D	816	4% 82% 13% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	C	903	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 27935 atoms, of which 30 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 GoxA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	768	Total	C	N	O	S	0	14	0
			6161	3891	1049	1201	20			
1	B	786	Total	C	N	O	S	0	10	0
			6298	3976	1073	1228	21			
1	C	777	Total	C	N	O	S	0	7	0
			6202	3921	1057	1204	20			
1	D	784	Total	C	N	O	S	0	5	0
			6241	3941	1062	1218	20			

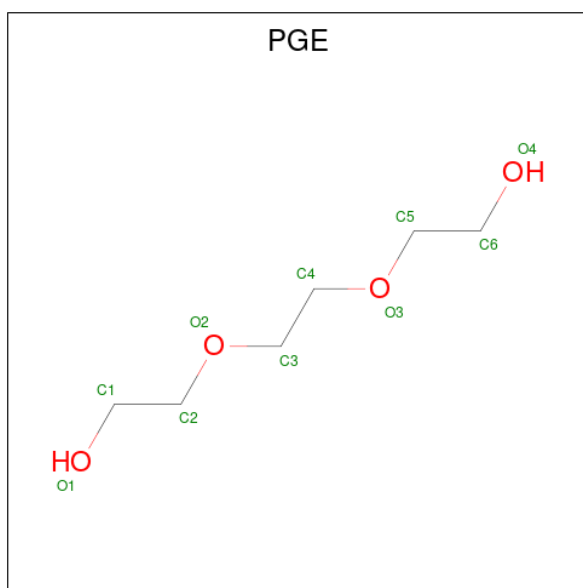
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 SODIUM ION (CCD ID: NA) (formula: Na).

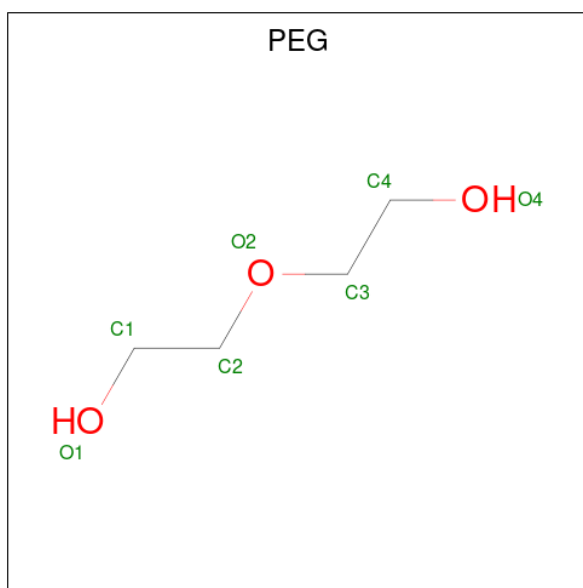
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	H	O	0	0
			10	2	6	2		

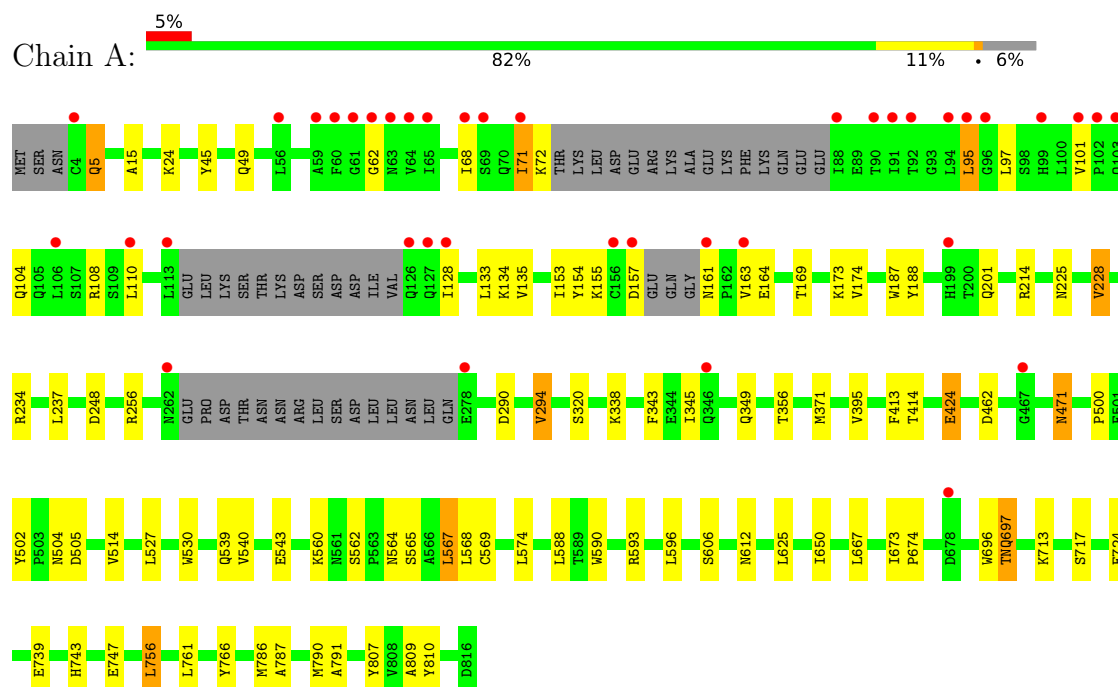
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	776	Total	O	0	5
			781	781		
7	B	699	Total	O	0	5
			704	704		
7	C	772	Total	O	0	3
			775	775		
7	D	705	Total	O	0	9
			714	714		

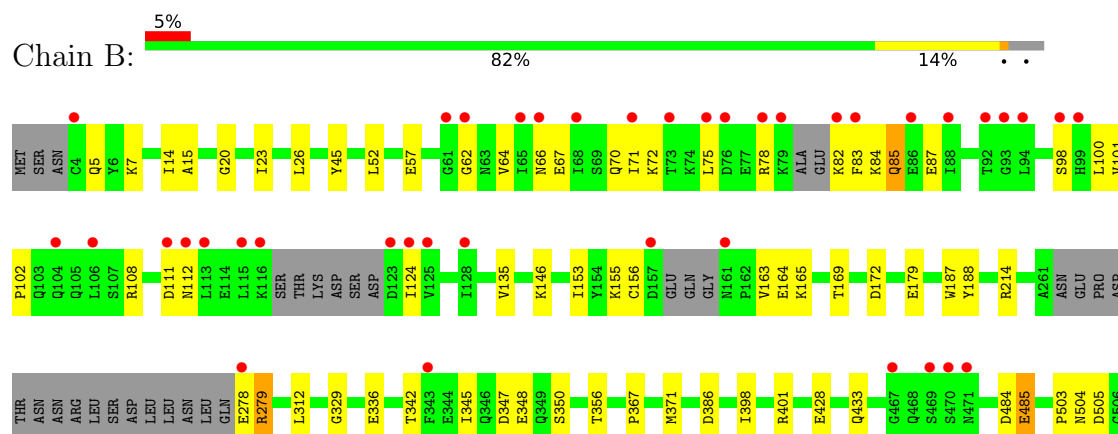
3 Residue-property plots [i](#)

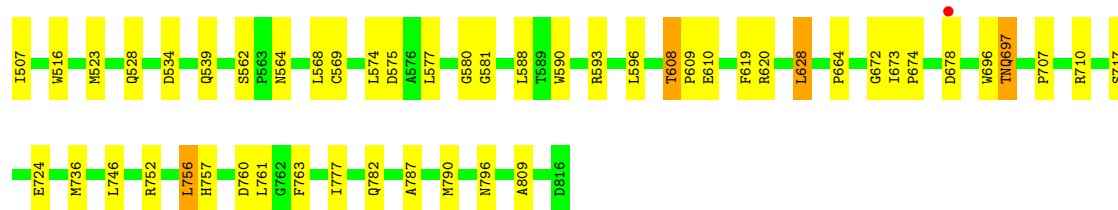
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

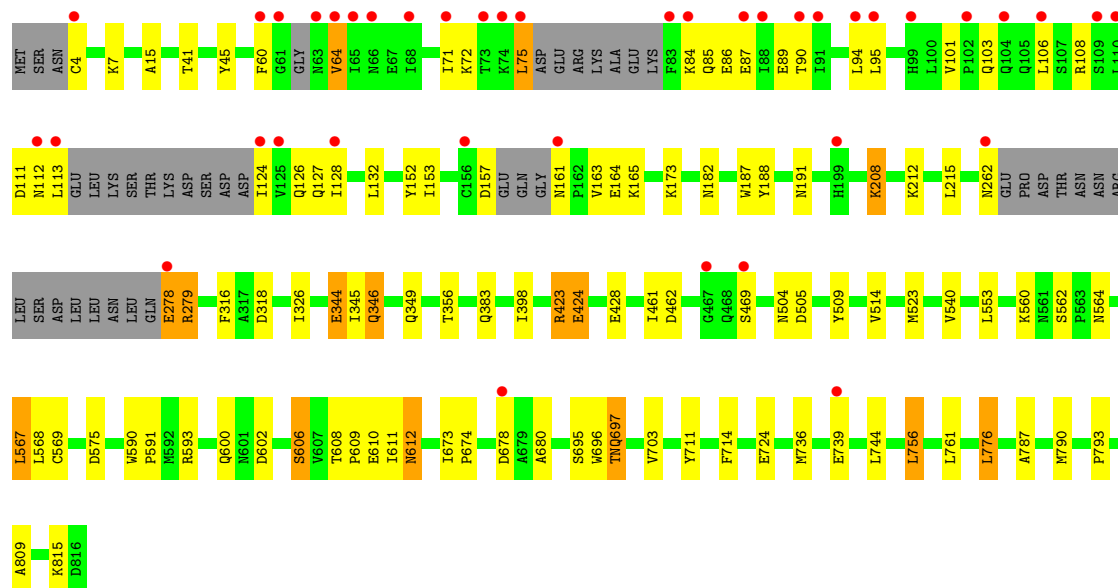
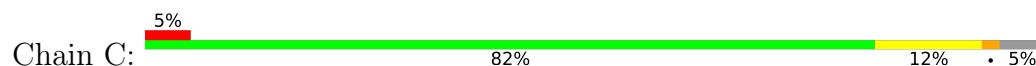


• Molecule 1: GoxA

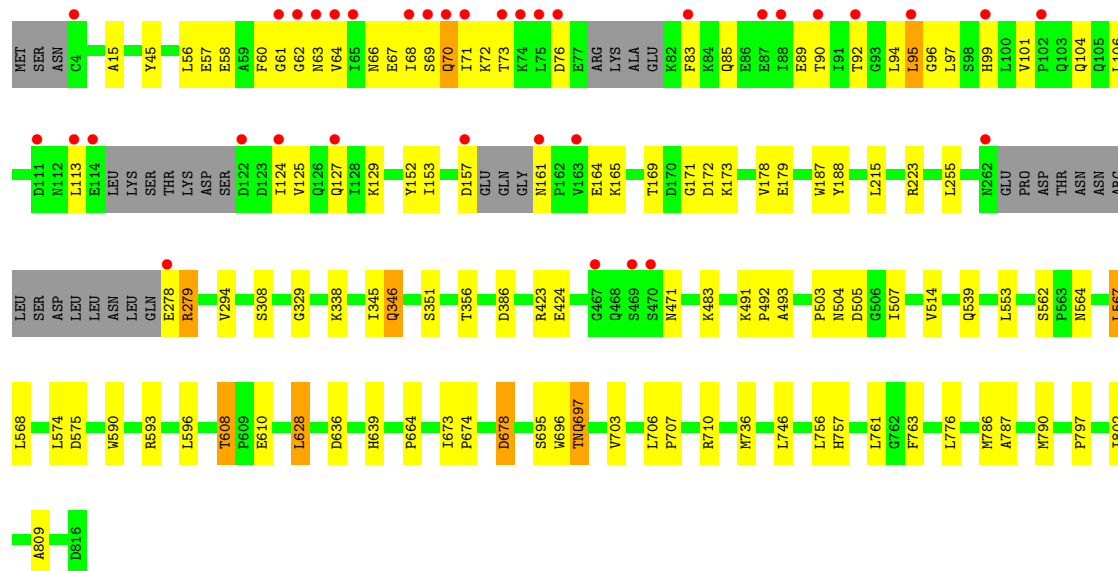
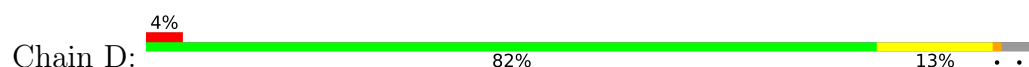




• Molecule 1: GoxA



• Molecule 1: GoxA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.24Å 93.46Å 187.90Å 90.00° 95.02° 90.00°	Depositor
Resolution (Å)	48.30 – 1.82 48.30 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.30-1.82) 99.4 (48.30-1.82)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.82Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.175 , 0.213 0.176 , 0.213	Depositor DCC
R_{free} test set	17055 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27935	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.37% 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: EDO, TNQ, PEG, NA, PGE, 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	0.30	0/6287	0.53	1/8563 (0.0%)
1	B	0.26	0/6425	0.50	0/8739
1	C	0.30	0/6328	0.53	0/8612
1	D	0.31	1/6368 (0.0%)	0.52	0/8667
All	All	0.29	1/25408 (0.0%)	0.52	1/34581 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	776	LEU	C-O	-6.91	1.16	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ILE	N-CA-C	-5.40	107.10	111.91

There are no chirality outliers.

There are no planarity outliers.

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	6161	0	5903	68	0
1	B	6298	0	6048	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6202	0	5957	87	0
1	D	6241	0	5984	88	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	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	10	14	14	0	0
5	C	7	10	10	8	0
6	D	4	6	6	3	0
7	A	781	0	0	13	0
7	B	704	0	0	12	0
7	C	775	0	0	13	0
7	D	714	0	0	9	0
All	All	27905	30	23922	331	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 7.

All (331) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:GLU:HG2	1:D:94:LEU:HD11	1.28	1.15
1:B:179:GLU:HB2	1:B:628:LEU:HD22	1.54	0.88
1:D:179:GLU:HB2	1:D:628:LEU:HD22	1.56	0.86
1:D:83:PHE:HZ	1:D:124:ILE:HD11	1.41	0.84
1:C:191:ASN:HA	5:C:903:PEG:H31	1.61	0.83
1:D:492:PRO:HA	6:D:903:EDO:H21	1.60	0.81
1:B:672:GLY:HA3	1:B:678:ASP:OD1	1.82	0.79
1:D:67:GLU:CG	1:D:94:LEU:HD11	2.13	0.78
1:C:423[A]:ARG:HH11	1:C:423[A]:ARG:HB3	1.47	0.78
1:C:383:GLN:HG2	7:C:1224:HOH:O	1.84	0.77
1:D:169:THR:OG1	1:D:338:LYS:HE3	1.85	0.76
1:B:528[B]:GLN:NE2	7:B:1001:HOH:O	2.17	0.76
1:D:608:THR:HG22	1:D:610:GLU:H	1.50	0.75
1:B:678:ASP:HB3	7:B:1140:HOH:O	1.87	0.74
1:B:398:ILE:HD11	1:B:523[A]:MET:HE2	1.69	0.74
1:B:345:ILE:HG23	1:B:350[A]:SER:OG	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:493:ALA:H	6:D:903:EDO:H11	1.52	0.73
1:A:5:GLN:HG3	1:A:343:PHE:CD2	2.24	0.72
1:C:103:GLN:HA	1:C:106:LEU:HD12	1.71	0.72
1:B:619:PHE:O	1:B:620:ARG:HD2	1.88	0.71
1:C:606[A]:SER:HB3	1:C:612[A]:ASN:HA	1.72	0.71
1:B:564[B]:ASN:OD1	1:B:564[B]:ASN:N	2.18	0.70
1:D:539:GLN:OE1	7:D:1001:HOH:O	2.08	0.70
1:D:706[A]:LEU:HD13	1:D:706[A]:LEU:C	2.17	0.69
1:A:225:ASN:O	1:A:228[A]:VAL:HG23	1.93	0.69
1:A:724:GLU:HG2	7:A:1346:HOH:O	1.92	0.69
1:A:95:LEU:O	1:A:95:LEU:HD12	1.93	0.68
1:D:67:GLU:OE1	1:D:71:ILE:HG23	1.93	0.68
1:A:228[B]:VAL:HG22	1:A:234:ARG:HG2	1.74	0.67
1:B:564[B]:ASN:ND2	7:B:1007:HOH:O	2.26	0.67
1:A:157:ASP:OD1	1:A:161:ASN:HB3	1.94	0.67
1:C:163:VAL:HG23	1:C:164:GLU:HG2	1.77	0.67
1:B:608:THR:HG22	1:B:610:GLU:H	1.58	0.66
1:B:155:LYS:HE3	1:B:156:CYS:O	1.95	0.65
1:D:338:LYS:HG3	7:D:1082:HOH:O	1.97	0.65
1:B:163:VAL:HG23	1:B:164:GLU:H	1.62	0.65
1:C:112:ASN:O	1:C:112:ASN:ND2	2.30	0.65
1:D:15:ALA:O	1:D:356:THR:HA	1.97	0.64
1:D:564[B]:ASN:OD1	7:D:1002:HOH:O	2.15	0.64
1:D:68:ILE:HD12	1:D:125:VAL:HG22	1.80	0.64
1:D:171:GLY:HA3	1:D:338:LYS:HB3	1.78	0.64
1:B:672:GLY:HA3	1:B:678:ASP:CG	2.23	0.64
1:B:398:ILE:HD11	1:B:523[A]:MET:CE	2.27	0.64
1:D:64:VAL:O	1:D:68:ILE:HG13	1.96	0.64
1:C:86:GLU:O	1:C:90:THR:HG23	1.98	0.63
1:B:15:ALA:O	1:B:356:THR:HA	1.99	0.63
1:C:608:THR:HG22	1:C:610:GLU:H	1.64	0.63
1:A:95:LEU:HD13	1:A:97:LEU:HD12	1.80	0.63
1:C:64:VAL:HG12	1:C:94:LEU:HD23	1.80	0.63
1:C:318:ASP:OD2	5:C:903:PEG:H42	1.98	0.62
1:C:612[B]:ASN:ND2	7:C:1006:HOH:O	2.31	0.62
1:C:152:TYR:CD1	1:C:165:LYS:HE2	2.34	0.62
1:D:101:VAL:HG21	1:D:106:LEU:HD21	1.81	0.62
1:C:84:LYS:HD3	1:C:85:GLN:N	2.15	0.62
1:A:713:LYS:NZ	7:A:1008:HOH:O	2.33	0.62
1:C:423[A]:ARG:HH11	1:C:423[A]:ARG:CB	2.11	0.62
1:D:673:ILE:HD12	1:D:674:PRO:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485[A]:GLU:CD	1:B:485[A]:GLU:H	2.07	0.61
1:D:101:VAL:CG2	1:D:106:LEU:HD21	2.29	0.61
1:A:564:ASN:ND2	1:A:567:LEU:HD22	2.16	0.61
1:C:64:VAL:HG12	1:C:94:LEU:HB3	1.82	0.61
1:B:82:LYS:HG2	1:B:83:PHE:H	1.66	0.60
1:C:60:PHE:HA	1:C:64:VAL:HG21	1.83	0.60
1:C:428:GLU:HA	1:C:428:GLU:OE1	2.02	0.60
1:A:596:LEU:HD11	1:A:650:ILE:HD12	1.84	0.59
1:A:471:ASN:ND2	7:A:1013:HOH:O	2.34	0.59
1:B:82:LYS:HG2	1:B:83:PHE:N	2.17	0.59
1:A:101:VAL:HG11	1:A:135:VAL:CG2	2.33	0.59
1:A:739:GLU:HG2	1:A:743:HIS:CE1	2.37	0.59
1:D:63:ASN:O	1:D:66:ASN:HB2	2.01	0.59
1:B:628:LEU:HD13	1:B:664:PRO:HG2	1.85	0.59
1:A:155:LYS:O	1:A:163:VAL:HG22	2.02	0.59
1:C:64:VAL:CG1	1:C:94:LEU:HB3	2.33	0.59
1:C:608:THR:HG23	1:C:609:PRO:HD2	1.85	0.59
1:B:72:LYS:HA	1:B:75:LEU:HB2	1.85	0.58
1:D:628:LEU:HD13	1:D:664:PRO:HG2	1.84	0.58
1:C:344:GLU:HG3	1:C:346:GLN:NE2	2.18	0.58
1:D:95:LEU:O	1:D:97:LEU:N	2.36	0.58
1:C:15:ALA:O	1:C:356:THR:HA	2.04	0.58
1:D:562:SER:OG	1:D:564[B]:ASN:ND2	2.37	0.58
1:C:316:PHE:CE1	5:C:903:PEG:H32	2.39	0.57
1:C:423[A]:ARG:HH11	1:C:423[A]:ARG:CG	2.17	0.57
1:C:724:GLU:HG2	7:C:1167:HOH:O	2.04	0.57
1:A:539:GLN:O	1:A:543:GLU:HG2	2.04	0.57
1:C:673:ILE:HD12	1:C:674:PRO:HA	1.86	0.57
1:C:398[B]:ILE:HD11	1:C:523:MET:HE2	1.87	0.56
1:D:608:THR:HG22	1:D:610:GLU:N	2.19	0.56
1:A:756:LEU:O	1:A:761[A]:LEU:HD12	2.05	0.56
1:B:155:LYS:O	1:B:163:VAL:HG22	2.05	0.56
1:B:312:LEU:HD13	1:B:777:ILE:HD13	1.88	0.56
1:C:157:ASP:OD1	1:C:161:ASN:HB3	2.05	0.56
1:D:99:HIS:H	1:D:99:HIS:CD2	2.22	0.56
1:C:208:LYS:HE2	1:C:212:LYS:HB2	1.88	0.56
1:C:349:GLN:H	1:C:349:GLN:CD	2.13	0.56
1:B:7:LYS:HG2	1:B:350[B]:SER:HA	1.88	0.56
1:B:72:LYS:HE2	1:B:124:ILE:HG21	1.88	0.56
1:B:724:GLU:HG2	7:B:1379:HOH:O	2.06	0.56
1:B:164:GLU:CD	1:B:165:LYS:H	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:GLU:HG2	1:D:94:LEU:CD1	2.19	0.55
1:D:113:LEU:HD13	1:D:127:GLN:HG3	1.86	0.55
1:A:72:LYS:O	1:A:72:LYS:HG3	2.05	0.55
1:B:717[B]:SER:OG	1:B:796[B]:ASN:HB2	2.07	0.55
1:D:85:GLN:O	1:D:89:GLU:HG2	2.06	0.55
1:A:68:ILE:O	1:A:72:LYS:HB2	2.06	0.55
1:C:564[A]:ASN:ND2	1:C:567:LEU:HD22	2.22	0.55
1:D:104:GLN:CD	1:D:104:GLN:H	2.13	0.55
1:A:49:GLN:NE2	1:A:133:LEU:HD21	2.22	0.55
1:D:69:SER:O	1:D:73:THR:HG23	2.07	0.55
1:D:85:GLN:NE2	1:D:89:GLU:OE2	2.40	0.55
1:B:7:LYS:HG2	1:B:350[A]:SER:HA	1.89	0.54
1:C:278:GLU:O	1:C:279:ARG:HB2	2.06	0.54
1:C:469:SER:HB3	1:D:636:ASP:O	2.07	0.54
1:C:514:VAL:HG12	1:C:514:VAL:O	2.07	0.54
1:D:56:LEU:CD2	1:D:129:LYS:HG3	2.38	0.54
1:D:164:GLU:HG3	1:D:165:LYS:H	1.72	0.54
1:A:187:TRP:CG	1:A:188:TYR:H	2.26	0.54
1:D:57:GLU:OE1	1:D:57:GLU:HA	2.06	0.54
1:B:485[A]:GLU:HG3	7:B:1090:HOH:O	2.09	0.53
1:A:5:GLN:HG3	1:A:343:PHE:HD2	1.74	0.53
1:C:85:GLN:O	1:C:89:GLU:HG2	2.08	0.53
1:C:124:ILE:O	1:C:128:ILE:HD12	2.09	0.53
1:C:173:LYS:NZ	7:C:1015:HOH:O	2.39	0.53
1:B:433:GLN:HB3	7:B:1003:HOH:O	2.08	0.53
1:A:612[A]:ASN:ND2	7:A:1020:HOH:O	2.40	0.53
1:C:756:LEU:HD12	1:C:761[B]:LEU:CD2	2.39	0.53
1:B:608:THR:HG23	1:B:609:PRO:HD2	1.90	0.53
1:C:4:CYS:SG	1:C:7:LYS:HE3	2.48	0.53
1:D:346:GLN:HA	1:D:351:SER:OG	2.10	0.52
1:A:15:ALA:O	1:A:356:THR:HA	2.09	0.52
1:A:787:ALA:HB1	1:A:809:ALA:HB1	1.92	0.52
1:C:187:TRP:CG	1:C:188:TYR:H	2.27	0.52
1:A:673:ILE:HD12	1:A:674:PRO:HA	1.92	0.52
1:B:707:PRO:HG2	1:B:710:ARG:HG2	1.91	0.52
1:D:187:TRP:CG	1:D:188:TYR:H	2.29	0.51
1:B:20:GLY:O	1:B:146:LYS:HE2	2.11	0.51
1:A:790:MET:HE3	1:A:810:TYR:CD1	2.46	0.51
1:D:223:ARG:NH1	7:D:1023:HOH:O	2.43	0.51
1:B:26:LEU:HD21	1:B:52:LEU:HD23	1.93	0.51
1:A:395[A]:VAL:HG13	1:A:527:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:MET:HE3	1:B:588:LEU:HB2	1.92	0.51
1:C:815:LYS:HE2	7:C:1128:HOH:O	2.10	0.51
1:B:67:GLU:O	1:B:71:ILE:HD13	2.11	0.51
5:C:903:PEG:H12	7:C:1017:HOH:O	2.11	0.51
1:D:590:TRP:O	1:D:593:ARG:HG2	2.11	0.51
1:C:602:ASP:HB2	7:C:1064:HOH:O	2.11	0.50
1:C:113:LEU:HB3	1:C:127:GLN:HE21	1.76	0.50
1:B:485[A]:GLU:OE2	7:B:1002:HOH:O	2.19	0.50
1:C:153:ILE:HD12	1:C:345:ILE:CD1	2.41	0.50
1:D:164:GLU:HG3	1:D:165:LYS:N	2.27	0.50
1:B:386:ASP:N	1:B:386:ASP:OD1	2.43	0.50
1:A:201:GLN:HB2	7:A:1542:HOH:O	2.09	0.50
1:B:187:TRP:CG	1:B:188:TYR:H	2.29	0.50
1:A:395[A]:VAL:HG21	1:A:530:TRP:HB2	1.93	0.50
1:B:503:PRO:HB3	1:B:507:ILE:HD13	1.92	0.50
1:A:256:ARG:HG2	7:A:1079:HOH:O	2.12	0.50
1:A:371:MET:HE3	1:A:588:LEU:HB2	1.94	0.50
1:B:5:GLN:O	1:B:155:LYS:HD2	2.12	0.50
1:B:485[A]:GLU:HG2	7:B:1002:HOH:O	2.11	0.50
1:B:562:SER:OG	1:B:564[B]:ASN:OD1	2.22	0.50
1:A:153:ILE:HD12	1:A:345:ILE:CD1	2.42	0.49
5:C:903:PEG:H41	7:C:1014:HOH:O	2.11	0.49
1:B:62:GLY:HA2	1:B:64:VAL:N	2.28	0.49
1:A:24:LYS:HE3	7:A:1628:HOH:O	2.13	0.49
1:C:113:LEU:HB3	1:C:127:GLN:NE2	2.28	0.49
1:B:163:VAL:HG23	1:B:164:GLU:N	2.27	0.49
1:A:101:VAL:HG11	1:A:135:VAL:HG22	1.93	0.49
1:C:562:SER:HB3	1:C:568:LEU:HD11	1.95	0.49
6:D:903:EDO:H12	7:D:1384:HOH:O	2.11	0.49
1:B:562:SER:HB3	1:B:568:LEU:HD11	1.94	0.49
1:C:560:LYS:HB2	7:C:1698:HOH:O	2.13	0.49
1:A:214:ARG:NH2	7:A:1031:HOH:O	2.46	0.49
1:B:101:VAL:HG13	1:B:102:PRO:HD2	1.95	0.49
1:B:673:ILE:HD12	1:B:674:PRO:HA	1.94	0.49
1:C:696:TRP:HB3	1:C:697:TNQ:CE3	2.42	0.49
1:B:214:ARG:NH2	7:B:1008:HOH:O	2.30	0.48
1:B:590:TRP:O	1:B:593:ARG:HG2	2.13	0.48
1:D:483:LYS:NZ	7:D:1028:HOH:O	2.46	0.48
1:A:514:VAL:HG12	1:A:514:VAL:O	2.14	0.48
1:D:787:ALA:HB1	1:D:809:ALA:HB1	1.95	0.48
1:D:706[A]:LEU:C	1:D:706[A]:LEU:CD1	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:ALA:HB2	1:A:807:TYR:CE2	2.49	0.48
1:C:739:GLU:CD	1:C:739:GLU:H	2.22	0.48
1:D:172:ASP:OD1	1:D:338:LYS:HG2	2.13	0.48
1:A:228[A]:VAL:HG21	1:A:237:LEU:HD11	1.95	0.48
1:B:347:ASP:OD1	1:B:350[A]:SER:HB3	2.14	0.48
1:B:539:GLN:NE2	7:B:1029:HOH:O	2.47	0.48
1:C:346:GLN:HB3	7:C:1613:HOH:O	2.13	0.48
1:D:757:HIS:HA	1:D:763:PHE:CZ	2.49	0.48
1:A:696:TRP:HB3	1:A:697:TNQ:CE3	2.44	0.47
1:D:99:HIS:H	1:D:99:HIS:HD2	1.62	0.47
1:B:757:HIS:HA	1:B:763:PHE:CZ	2.49	0.47
1:A:110:LEU:HD21	1:A:128:ILE:HG23	1.97	0.47
1:C:64:VAL:CG1	1:C:94:LEU:HD23	2.45	0.47
1:D:164:GLU:CG	1:D:165:LYS:N	2.77	0.47
1:B:101:VAL:HG11	1:B:135:VAL:CG1	2.45	0.47
1:C:606[A]:SER:HB2	1:C:608:THR:O	2.14	0.47
1:A:45:TYR:CD2	1:A:790:MET:HG2	2.50	0.47
1:B:428:GLU:OE1	1:B:428:GLU:HA	2.14	0.47
1:C:41:THR:HB	1:C:793:PRO:HD3	1.97	0.47
1:A:320[B]:SER:OG	1:B:484:ASP:HB3	2.15	0.47
1:D:706[A]:LEU:HD13	1:D:706[A]:LEU:O	2.14	0.47
1:A:395[A]:VAL:HG13	1:A:527:LEU:CD1	2.45	0.47
1:A:606:SER:HB2	1:A:612[A]:ASN:HA	1.96	0.47
1:C:756:LEU:O	1:C:761[A]:LEU:HD12	2.15	0.46
1:D:90:THR:O	1:D:94:LEU:HG	2.15	0.46
1:A:747:GLU:OE1	7:A:1001:HOH:O	2.20	0.46
1:A:290:ASP:CG	1:A:294:VAL:HG13	2.40	0.46
1:B:78:ARG:HD2	1:B:78:ARG:O	2.15	0.46
1:C:316:PHE:HE1	5:C:903:PEG:H32	1.80	0.46
1:A:562:SER:HB3	1:A:568:LEU:HD11	1.96	0.46
1:B:169:THR:OG1	1:B:172:ASP:OD2	2.31	0.46
1:D:423[B]:ARG:HH11	1:D:423[B]:ARG:CG	2.28	0.46
1:C:680:ALA:HB3	1:C:776:LEU:HD22	1.97	0.46
1:D:564[A]:ASN:ND2	1:D:567:LEU:HD22	2.30	0.46
1:A:560:LYS:HB2	7:A:1684:HOH:O	2.16	0.46
1:C:756:LEU:HD12	1:C:761[A]:LEU:CD1	2.45	0.46
5:C:903:PEG:H21	7:C:1387:HOH:O	2.15	0.46
1:D:504:ASN:CG	1:D:505:ASP:H	2.23	0.46
1:C:72:LYS:HD3	1:C:124:ILE:HG21	1.98	0.46
1:D:71:ILE:C	1:D:71:ILE:HD12	2.41	0.46
1:D:696:TRP:HB3	1:D:697:TNQ:CE3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ILE:O	1:C:132:LEU:HG	2.16	0.46
1:D:60:PHE:CE1	1:D:129:LYS:HD3	2.51	0.46
1:A:590:TRP:O	1:A:593:ARG:HG2	2.16	0.46
1:A:169:THR:OG1	1:A:338:LYS:HE2	2.16	0.45
1:D:423[B]:ARG:HH11	1:D:423[B]:ARG:HG3	1.80	0.45
1:D:761:LEU:HD21	1:D:786:MET:SD	2.56	0.45
1:B:336:GLU:HG3	1:B:342:THR:HG22	1.98	0.45
1:C:101:VAL:CG2	1:C:106:LEU:HD21	2.46	0.45
1:B:82:LYS:CG	1:B:83:PHE:H	2.29	0.45
1:B:696:TRP:HB3	1:B:697:TNQ:CE3	2.46	0.45
1:B:23:ILE:HD13	1:B:100:LEU:HD21	1.99	0.45
1:B:153:ILE:HD12	1:B:345:ILE:HD12	1.99	0.45
1:C:600:GLN:HG2	7:C:1064:HOH:O	2.16	0.45
1:D:61:GLY:HA2	1:D:62:GLY:HA2	1.55	0.45
1:A:71:ILE:HG22	1:A:71:ILE:O	2.17	0.44
1:B:760:ASP:O	1:B:782:GLN:HG3	2.17	0.44
1:C:423[A]:ARG:CG	1:C:423[A]:ARG:NH1	2.81	0.44
1:C:262:ASN:C	1:C:262:ASN:OD1	2.59	0.44
1:C:504:ASN:CG	1:C:505:ASP:H	2.26	0.44
1:D:72:LYS:HE2	1:D:76:ASP:OD2	2.17	0.44
1:D:503:PRO:HB3	1:D:507:ILE:HD13	1.99	0.44
1:A:290:ASP:OD2	1:A:294:VAL:HG13	2.17	0.44
1:D:707:PRO:HG2	1:D:710:ARG:HG2	1.99	0.44
1:A:761[B]:LEU:HD11	1:A:786:MET:SD	2.58	0.44
1:D:514:VAL:HG12	1:D:514:VAL:O	2.18	0.44
1:B:534:ASP:OD1	7:B:1004:HOH:O	2.21	0.44
1:D:70:GLN:O	1:D:73:THR:OG1	2.27	0.44
1:A:413:PHE:CD2	1:A:414:THR:HG23	2.53	0.44
1:B:66:ASN:OD1	1:B:70:GLN:NE2	2.49	0.44
1:B:278:GLU:O	1:B:279:ARG:HB2	2.17	0.44
1:D:308:SER:OG	7:D:1003:HOH:O	2.21	0.44
1:D:178:VAL:HG21	1:D:255:LEU:HD11	1.99	0.43
1:B:179:GLU:O	1:B:329:GLY:HA3	2.18	0.43
1:C:398[B]:ILE:HD11	1:C:523:MET:CE	2.47	0.43
1:C:736:MET:SD	1:C:744:LEU:HD12	2.58	0.43
1:D:564[B]:ASN:ND2	1:D:564[B]:ASN:H	2.15	0.43
1:A:504:ASN:CG	1:A:505:ASP:H	2.26	0.43
1:C:344:GLU:CG	1:C:346:GLN:NE2	2.80	0.43
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.19	0.43
1:B:82:LYS:CG	1:B:83:PHE:N	2.80	0.43
1:D:67:GLU:CG	1:D:94:LEU:CD1	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LYS:O	1:A:134:LYS:HD3	2.19	0.43
1:B:348:GLU:HG2	7:B:1538:HOH:O	2.18	0.43
1:B:523[A]:MET:HE3	1:B:523[A]:MET:HA	2.01	0.43
1:D:423[B]:ARG:CG	1:D:423[B]:ARG:NH1	2.81	0.43
1:C:64:VAL:HG12	1:C:94:LEU:CD2	2.48	0.43
1:D:92:THR:HA	1:D:95:LEU:CD1	2.49	0.43
1:C:45:TYR:CD2	1:C:790:MET:HG2	2.53	0.42
1:B:504:ASN:CG	1:B:505:ASP:H	2.27	0.42
1:C:590:TRP:O	1:C:593:ARG:HG2	2.19	0.42
1:D:179:GLU:O	1:D:329:GLY:HA3	2.19	0.42
1:B:756:LEU:HD12	1:B:761:LEU:CD1	2.50	0.42
1:C:462:ASP:HB2	7:C:1005:HOH:O	2.18	0.42
1:D:696:TRP:HB3	1:D:697:TNQ:CD2	2.49	0.42
1:A:173:LYS:HE3	1:A:248:ASP:OD2	2.19	0.42
1:C:182:ASN:HB2	1:C:326:ILE:O	2.19	0.42
1:C:696:TRP:HB3	1:C:697:TNQ:CD2	2.49	0.42
1:A:462:ASP:OD1	7:A:1002:HOH:O	2.21	0.42
1:A:696:TRP:HB3	1:A:697:TNQ:CD2	2.50	0.42
1:B:736:MET:HE2	1:C:424:GLU:HB2	2.01	0.42
1:C:787:ALA:HB1	1:C:809:ALA:HB1	2.01	0.42
1:D:695[A]:SER:HB2	1:D:703:VAL:HG21	2.02	0.42
1:B:45:TYR:CD2	1:B:790:MET:HG2	2.55	0.42
1:C:108:ARG:HA	1:C:111:ASP:HB2	2.01	0.42
1:C:590:TRP:CG	1:C:591:PRO:HD3	2.55	0.42
1:D:45:TYR:CD2	1:D:790:MET:HG2	2.55	0.42
1:D:83:PHE:CZ	1:D:124:ILE:HD11	2.34	0.42
1:A:349:GLN:CD	1:A:349:GLN:H	2.28	0.42
1:A:717:SER:HB2	7:A:1435:HOH:O	2.20	0.42
1:A:766:TYR:OH	1:D:697:TNQ:O3	2.37	0.42
1:C:208:LYS:HB2	1:C:208:LYS:HE3	1.30	0.42
1:D:92:THR:HA	1:D:95:LEU:HD11	2.02	0.42
1:A:500:PRO:HB2	1:A:502:TYR:CE2	2.55	0.42
1:B:696:TRP:HB3	1:B:697:TNQ:CD2	2.50	0.42
1:C:509:TYR:CD1	1:D:639:HIS:HB3	2.55	0.42
1:D:60:PHE:CD1	1:D:129:LYS:HD3	2.54	0.42
1:A:560:LYS:NZ	7:A:1009:HOH:O	2.33	0.41
1:A:596:LEU:CD1	1:A:650:ILE:HD12	2.49	0.41
1:C:695:SER:HB2	1:C:703:VAL:HG21	2.02	0.41
1:C:152:TYR:CE1	1:C:165:LYS:HE2	2.55	0.41
1:C:608:THR:HB	1:C:611:ILE:HB	2.02	0.41
1:D:386:ASP:OD1	1:D:386:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:ARG:HA	1:B:752:ARG:HD3	1.88	0.41
1:D:152:TYR:CD1	1:D:165:LYS:HD3	2.55	0.41
1:D:562:SER:HB3	1:D:568:LEU:HD11	2.02	0.41
1:D:678:ASP:CG	7:D:1018:HOH:O	2.64	0.41
1:A:104:GLN:HB3	1:A:108:ARG:NE	2.36	0.41
1:A:154:TYR:HH	1:A:565[A]:SER:HB2	1.85	0.41
1:B:84:LYS:O	1:B:85:GLN:C	2.63	0.41
1:B:14:ILE:HG21	1:B:577:LEU:HD11	2.03	0.41
1:B:72:LYS:HE2	1:B:124:ILE:CG2	2.49	0.41
1:B:101:VAL:HG11	1:B:135:VAL:HG11	2.03	0.41
1:B:504:ASN:HB2	1:B:516:TRP:C	2.46	0.41
1:C:84:LYS:O	1:C:87:GLU:N	2.53	0.41
1:D:153:ILE:HD12	1:D:345:ILE:CD1	2.51	0.41
1:D:491:LYS:HD3	7:D:1449:HOH:O	2.20	0.41
1:D:797:PRO:HB3	1:D:802:ILE:O	2.21	0.41
1:A:424:GLU:HB2	1:D:736:MET:HE2	2.03	0.41
1:B:580:GLY:HA2	1:B:581:GLY:C	2.45	0.41
1:B:787:ALA:HB1	1:B:809:ALA:HB1	2.03	0.41
1:C:84:LYS:HD3	1:C:85:GLN:H	1.86	0.41
1:B:71:ILE:O	1:B:75:LEU:HD23	2.20	0.40
1:B:84:LYS:H	1:B:87:GLU:CG	2.33	0.40
1:C:316:PHE:CZ	5:C:903:PEG:H32	2.56	0.40
1:B:82:LYS:HE2	1:B:111:ASP:O	2.21	0.40
1:B:108:ARG:HG2	1:B:112:ASN:OD1	2.22	0.40
1:C:711:TYR:HA	1:C:714:PHE:CE2	2.56	0.40
1:D:157:ASP:OD1	1:D:161:ASN:HB3	2.21	0.40
1:C:71:ILE:O	1:C:75:LEU:HD23	2.20	0.40
1:B:367:PRO:O	1:B:401:ARG:HD3	2.22	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	771/816 (94%)	747 (97%)	23 (3%)	1 (0%)	48	38
1	B	785/816 (96%)	764 (97%)	19 (2%)	2 (0%)	36	26
1	C	771/816 (94%)	750 (97%)	20 (3%)	1 (0%)	48	38
1	D	778/816 (95%)	754 (97%)	22 (3%)	2 (0%)	36	26
All	All	3105/3264 (95%)	3015 (97%)	84 (3%)	6 (0%)	43	33

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	GLY
1	B	85	GLN
1	B	279	ARG
1	D	96	GLY
1	D	279	ARG
1	C	279	ARG

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	679/711 (96%)	663 (98%)	16 (2%)	43	27
1	B	693/711 (98%)	682 (98%)	11 (2%)	55	44
1	C	682/711 (96%)	657 (96%)	25 (4%)	30	12
1	D	686/711 (96%)	665 (97%)	21 (3%)	35	17
All	All	2740/2844 (96%)	2667 (97%)	73 (3%)	42	22

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	95	LEU
1	A	164	GLU
1	A	174	VAL
1	A	228[A]	VAL

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Mol	Chain	Res	Type
1	A	228[B]	VAL
1	A	294	VAL
1	A	424	GLU
1	A	471	ASN
1	A	540	VAL
1	A	567	LEU
1	A	569	CYS
1	A	574	LEU
1	A	625	LEU
1	A	667	LEU
1	A	756	LEU
1	B	98	SER
1	B	485[A]	GLU
1	B	485[B]	GLU
1	B	569	CYS
1	B	574	LEU
1	B	575	ASP
1	B	596	LEU
1	B	608	THR
1	B	628	LEU
1	B	746	LEU
1	B	756	LEU
1	C	64	VAL
1	C	75	LEU
1	C	95	LEU
1	C	126	GLN
1	C	208	LYS
1	C	215	LEU
1	C	278	GLU
1	C	344	GLU
1	C	346	GLN
1	C	423[A]	ARG
1	C	423[B]	ARG
1	C	424	GLU
1	C	461	ILE
1	C	540	VAL
1	C	553	LEU
1	C	567	LEU
1	C	569	CYS
1	C	575	ASP
1	C	606[A]	SER
1	C	606[B]	SER

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Mol	Chain	Res	Type
1	C	612[A]	ASN
1	C	612[B]	ASN
1	C	678	ASP
1	C	756	LEU
1	C	776	LEU
1	D	58	GLU
1	D	70	GLN
1	D	95	LEU
1	D	173	LYS
1	D	215	LEU
1	D	278	GLU
1	D	279	ARG
1	D	294	VAL
1	D	346	GLN
1	D	424	GLU
1	D	471	ASN
1	D	553	LEU
1	D	567	LEU
1	D	574	LEU
1	D	575	ASP
1	D	596	LEU
1	D	608	THR
1	D	628	LEU
1	D	678	ASP
1	D	746	LEU
1	D	756	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	103	GLN
1	A	236	GLN
1	A	252	GLN
1	A	349	GLN
1	A	433	GLN
1	A	471	ASN
1	A	525	GLN
1	A	561	ASN
1	A	683	GLN
1	A	743	HIS
1	A	751	GLN

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Mol	Chain	Res	Type
1	B	99	HIS
1	B	127	GLN
1	B	213	HIS
1	B	284	GLN
1	B	349	GLN
1	B	410	GLN
1	B	433	GLN
1	B	459	GLN
1	B	525	GLN
1	B	600	GLN
1	B	626	GLN
1	B	635	GLN
1	B	683	GLN
1	B	785	ASN
1	B	812	GLN
1	C	127	GLN
1	C	142	HIS
1	C	231	ASN
1	C	242	GLN
1	C	339	ASN
1	C	346	GLN
1	C	406	GLN
1	C	468	GLN
1	C	525	GLN
1	C	626	GLN
1	C	635	GLN
1	C	751	GLN
1	C	778	GLN
1	C	785	ASN
1	D	49	GLN
1	D	54	GLN
1	D	213	HIS
1	D	236	GLN
1	D	284	GLN
1	D	346	GLN
1	D	410	GLN
1	D	468	GLN
1	D	525	GLN
1	D	626	GLN
1	D	635	GLN
1	D	683	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	TNQ	A	697	1	20,21,22	3.33	7 (35%)	21,29,31	2.93	8 (38%)
1	TNQ	B	697	1	20,21,22	3.25	6 (30%)	21,29,31	2.75	5 (23%)
1	TNQ	C	697	1	20,21,22	3.23	6 (30%)	21,29,31	2.97	5 (23%)
1	TNQ	D	697	1	20,21,22	3.25	6 (30%)	21,29,31	2.69	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TNQ	A	697	1	-	4/10/11/13	0/2/2/2
1	TNQ	B	697	1	-	4/10/11/13	0/2/2/2
1	TNQ	C	697	1	-	4/10/11/13	0/2/2/2
1	TNQ	D	697	1	-	4/10/11/13	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	697	TNQ	C2-N1	-11.27	1.27	1.45
1	B	697	TNQ	C2-N1	-11.27	1.27	1.45
1	D	697	TNQ	C2-N1	-11.19	1.28	1.45
1	A	697	TNQ	C2-N1	-11.15	1.28	1.45
1	B	697	TNQ	CH2-CZ2	5.97	1.48	1.40
1	A	697	TNQ	CH2-CZ2	5.93	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	697	TNQ	CH2-CZ2	5.57	1.48	1.40
1	A	697	TNQ	CD2-CE2	5.42	1.48	1.41
1	C	697	TNQ	CH2-CZ2	4.88	1.47	1.40
1	C	697	TNQ	CD2-CE2	4.74	1.47	1.41
1	D	697	TNQ	CD2-CE2	4.37	1.47	1.41
1	B	697	TNQ	CD2-CE2	4.09	1.46	1.41
1	D	697	TNQ	CD2-CG	2.95	1.48	1.44
1	C	697	TNQ	CD2-CG	2.81	1.48	1.44
1	D	697	TNQ	CE2-CZ2	2.73	1.48	1.40
1	B	697	TNQ	CE2-CZ2	2.73	1.48	1.40
1	B	697	TNQ	CD1-CG	2.59	1.40	1.36
1	A	697	TNQ	CD2-CG	2.50	1.48	1.44
1	C	697	TNQ	CE2-CZ2	2.46	1.47	1.40
1	D	697	TNQ	CD1-CG	2.37	1.40	1.36
1	A	697	TNQ	CE2-CZ2	2.37	1.47	1.40
1	B	697	TNQ	CD2-CG	2.31	1.47	1.44
1	A	697	TNQ	CE2-NE1	-2.27	1.34	1.37
1	C	697	TNQ	CE2-NE1	-2.19	1.34	1.37
1	A	697	TNQ	CD1-CG	2.11	1.39	1.36

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	697	TNQ	C2-N1-CH2	-8.67	111.11	123.94
1	C	697	TNQ	C2-N1-CH2	-8.46	111.42	123.94
1	D	697	TNQ	C1-C2-N1	8.38	126.15	110.77
1	B	697	TNQ	C1-C2-N1	8.02	125.49	110.77
1	C	697	TNQ	C1-C2-N1	7.76	125.00	110.77
1	A	697	TNQ	C1-C2-N1	7.46	124.45	110.77
1	D	697	TNQ	C2-N1-CH2	-7.39	113.01	123.94
1	B	697	TNQ	C2-N1-CH2	-6.99	113.59	123.94
1	C	697	TNQ	CZ2-CH2-N1	-5.18	116.07	119.52
1	B	697	TNQ	O3-C1-C2	3.35	125.54	112.81
1	B	697	TNQ	CD2-CE2-CZ2	-3.23	117.02	121.41
1	A	697	TNQ	O3-C1-C2	3.14	124.75	112.81
1	C	697	TNQ	CD2-CE2-CZ2	-3.05	117.26	121.41
1	A	697	TNQ	CD2-CE2-CZ2	-2.73	117.69	121.41
1	D	697	TNQ	CD2-CE2-CZ2	-2.72	117.71	121.41
1	A	697	TNQ	CZ2-CH2-N1	-2.42	117.91	119.52
1	A	697	TNQ	O2-C1-C2	-2.26	113.28	122.66
1	A	697	TNQ	CG-CD1-NE1	2.19	112.71	110.31
1	B	697	TNQ	O2-C1-C2	-2.13	113.81	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	697	TNQ	CE3-CD2-CE2	2.13	121.54	119.14
1	C	697	TNQ	CE3-CD2-CE2	2.08	121.48	119.14
1	D	697	TNQ	CE2-NE1-CD1	2.07	110.72	108.93
1	D	697	TNQ	CB-CG-CD2	2.06	130.66	126.70

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	D	697	TNQ	CZ2-CH2-N1-C2
1	B	697	TNQ	CZ3-CH2-N1-C2
1	D	697	TNQ	CZ3-CH2-N1-C2
1	B	697	TNQ	O2-C1-C2-N1
1	B	697	TNQ	O3-C1-C2-N1
1	D	697	TNQ	O3-C1-C2-N1
1	C	697	TNQ	O2-C1-C2-N1
1	D	697	TNQ	O2-C1-C2-N1
1	C	697	TNQ	CZ2-CH2-N1-C2
1	A	697	TNQ	O2-C1-C2-N1
1	C	697	TNQ	O3-C1-C2-N1
1	A	697	TNQ	CZ3-CH2-N1-C2
1	A	697	TNQ	O3-C1-C2-N1
1	C	697	TNQ	CZ3-CH2-N1-C2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 8 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	$\# Z > 2$
4	PGE	A	903	-	9,9,9	0.41	0	8,8,8	0.51	0
6	EDO	D	903	-	3,3,3	0.49	0	2,2,2	0.14	0
5	PEG	C	903	-	6,6,6	0.43	0	5,5,5	0.45	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
4	PGE	A	903	-	-	3/7/7/7	-
6	EDO	D	903	-	-	0/1/1/1	-
5	PEG	C	903	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	903	PEG	O1-C1-C2-O2
4	A	903	PGE	O2-C3-C4-O3
4	A	903	PGE	O1-C1-C2-O2
4	A	903	PGE	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	903	EDO	3	0
5	C	903	PEG	8	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	767/816 (93%)	0.06	39 (5%)	33	38	8, 21, 71, 120	14 (1%)
1	B	785/816 (96%)	0.14	41 (5%)	33	37	8, 26, 72, 117	10 (1%)
1	C	776/816 (95%)	0.06	40 (5%)	33	37	10, 22, 72, 122	7 (0%)
1	D	783/816 (95%)	0.20	36 (4%)	37	43	8, 25, 75, 125	5 (0%)
All	All	3111/3264 (95%)	0.12	156 (5%)	34	40	8, 24, 73, 125	36 (1%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	71	ILE	5.8
1	C	124	ILE	5.6
1	A	88	ILE	5.2
1	C	73	THR	4.9
1	C	83	PHE	4.8
1	A	102	PRO	4.6
1	C	678	ASP	4.6
1	D	124	ILE	4.6
1	A	95	LEU	4.5
1	A	113	LEU	4.5
1	B	124	ILE	4.5
1	D	83	PHE	4.5
1	A	71	ILE	4.3
1	A	59	ALA	4.2
1	C	125	VAL	4.1
1	D	113	LEU	4.1
1	D	75	LEU	4.0
1	D	73	THR	3.9
1	D	163	VAL	3.8
1	C	75	LEU	3.8
1	C	61	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	64	VAL	3.8
1	C	262	ASN	3.7
1	C	110	LEU	3.6
1	A	68	ILE	3.5
1	A	64	VAL	3.5
1	C	113	LEU	3.5
1	A	62	GLY	3.4
1	B	4	CYS	3.3
1	C	65	ILE	3.3
1	D	68	ILE	3.3
1	A	60	PHE	3.3
1	A	94	LEU	3.3
1	D	90	THR	3.3
1	A	90	THR	3.3
1	B	75	LEU	3.3
1	A	65	ILE	3.2
1	D	469	SER	3.2
1	D	71	ILE	3.2
1	A	106	LEU	3.2
1	B	115	LEU	3.1
1	D	64	VAL	3.1
1	A	99	HIS	3.1
1	A	126	GLN	3.1
1	C	161	ASN	3.1
1	B	68	ILE	3.1
1	C	278	GLU	3.0
1	C	4	CYS	3.0
1	C	91	ILE	3.0
1	D	262	ASN	3.0
1	A	467	GLY	3.0
1	C	106	LEU	3.0
1	B	83	PHE	3.0
1	C	63	ASN	3.0
1	B	157	ASP	2.9
1	A	161	ASN	2.9
1	A	69	SER	2.9
1	D	99	HIS	2.9
1	A	101	VAL	2.8
1	C	199	HIS	2.8
1	A	156	CYS	2.8
1	A	128	ILE	2.8
1	D	61	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	127	GLN	2.8
1	A	92	THR	2.8
1	B	92	THR	2.8
1	C	90	THR	2.8
1	A	63	ASN	2.8
1	C	99	HIS	2.8
1	B	128	ILE	2.8
1	A	346	GLN	2.7
1	D	4	CYS	2.7
1	B	278	GLU	2.7
1	C	68	ILE	2.7
1	A	678	ASP	2.7
1	D	65	ILE	2.7
1	B	94	LEU	2.6
1	C	66	ASN	2.6
1	C	94	LEU	2.6
1	D	62	GLY	2.6
1	D	157	ASP	2.6
1	B	79	LYS	2.6
1	C	74	LYS	2.6
1	D	74	LYS	2.6
1	C	95	LEU	2.6
1	B	116	LYS	2.6
1	B	98	SER	2.6
1	D	161	ASN	2.6
1	A	4	CYS	2.5
1	A	61	GLY	2.5
1	B	62	GLY	2.5
1	A	91	ILE	2.5
1	C	128	ILE	2.5
1	B	99	HIS	2.5
1	D	69	SER	2.5
1	B	65	ILE	2.5
1	B	78	ARG	2.4
1	A	110	LEU	2.4
1	C	60	PHE	2.4
1	D	114	GLU	2.4
1	C	102	PRO	2.4
1	B	469	SER	2.4
1	D	122	ASP	2.4
1	C	87	GLU	2.4
1	D	87	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	56	LEU	2.4
1	A	278	GLU	2.4
1	A	262	ASN	2.4
1	D	467	GLY	2.4
1	B	470	SER	2.4
1	B	82	LYS	2.4
1	B	467	GLY	2.3
1	C	109	SER	2.3
1	B	111	ASP	2.3
1	C	156	CYS	2.3
1	B	113	LEU	2.3
1	D	95	LEU	2.3
1	B	106	LEU	2.3
1	D	278	GLU	2.3
1	A	163	VAL	2.3
1	B	71	ILE	2.2
1	D	70	GLN	2.2
1	B	93	GLY	2.2
1	B	76	ASP	2.2
1	B	123	ASP	2.2
1	C	88	ILE	2.2
1	D	63	ASN	2.2
1	D	111	ASP	2.2
1	B	66	ASN	2.2
1	B	471	ASN	2.2
1	C	739	GLU	2.2
1	B	73	THR	2.2
1	A	157	ASP	2.2
1	D	76	ASP	2.2
1	D	92	THR	2.1
1	D	470	SER	2.1
1	C	467	GLY	2.1
1	B	161	ASN	2.1
1	C	112	ASN	2.1
1	D	127	GLN	2.1
1	B	61	GLY	2.1
1	D	88	ILE	2.1
1	B	104	GLN	2.1
1	B	678	ASP	2.1
1	B	343	PHE	2.0
1	C	84	LYS	2.0
1	B	125	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	102	PRO	2.0
1	B	86	GLU	2.0
1	C	469	SER	2.0
1	A	199	HIS	2.0
1	B	88	ILE	2.0
1	A	96	GLY	2.0
1	A	103	GLN	2.0
1	C	104	GLN	2.0
1	B	112	ASN	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	TNQ	A	697	20/21	0.95	0.07	11,16,25,25	0
1	TNQ	B	697	20/21	0.95	0.07	13,17,26,30	0
1	TNQ	C	697	20/21	0.95	0.07	12,17,25,28	0
1	TNQ	D	697	20/21	0.96	0.06	14,18,28,30	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(Å ²)	Q<0.9
4	PGE	A	903	10/10	0.67	0.18	51,65,74,76	0
5	PEG	C	903	7/7	0.72	0.18	41,54,67,67	0
6	EDO	D	903	4/4	0.80	0.25	34,42,50,60	0
3	NA	C	902	1/1	0.96	0.12	41,41,41,41	0
3	NA	B	902	1/1	0.96	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	902	1/1	0.97	0.08	38,38,38,38	0
3	NA	D	902	1/1	0.98	0.07	37,37,37,37	0
2	MG	D	901	1/1	0.98	0.06	23,23,23,23	0
2	MG	C	901	1/1	0.99	0.03	18,18,18,18	0
2	MG	A	901	1/1	0.99	0.03	15,15,15,15	0
2	MG	B	901	1/1	0.99	0.05	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.