Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 06:33 PM EDT

PDB ID	:	6EER
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 (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:

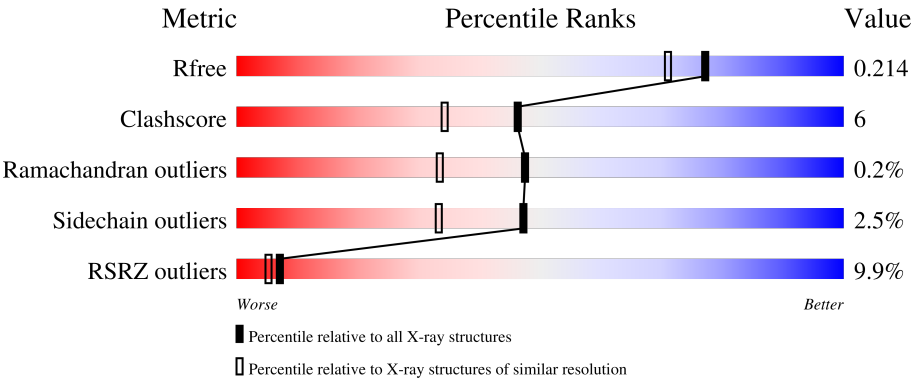
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 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}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	8% 83% 10% • 6%
1	B	816	11% 83% 13% •
1	C	816	8% 82% 12% • 5%
1	D	816	11% 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 6161	C 3891	N 1049	O 1201	S 20	0	14	0
1	B	786	Total 6298	C 3976	N 1073	O 1228	S 21	0	10	0
1	C	777	Total 6202	C 3921	N 1057	O 1204	S 20	0	7	0
1	D	784	Total 6241	C 3941	N 1062	O 1218	S 20	0	5	0

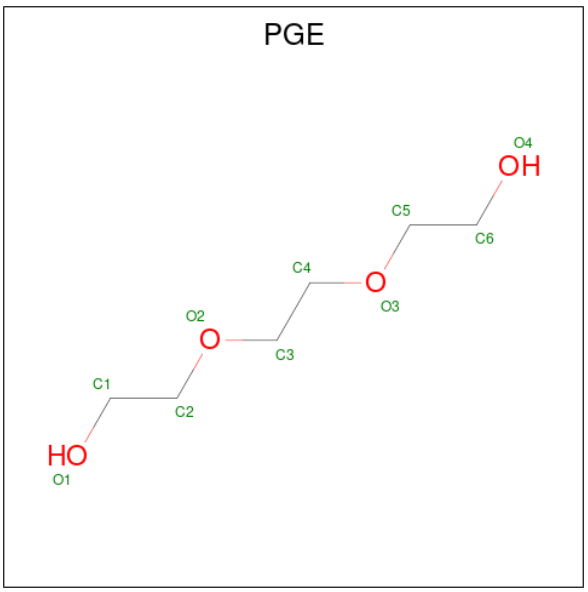
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

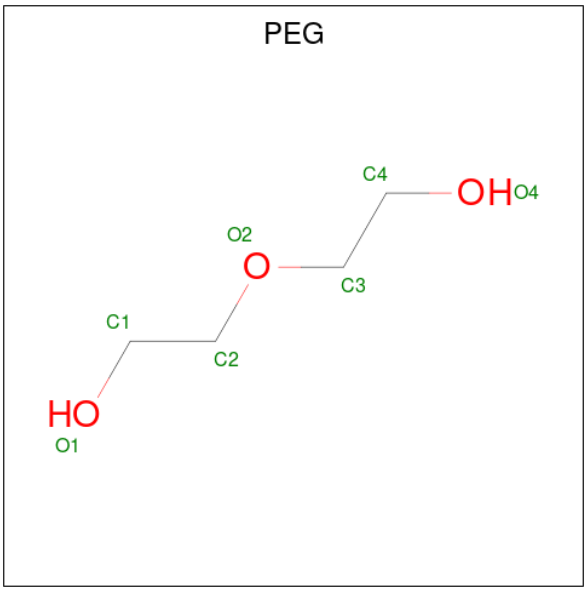
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0
3	D	1	Total 1	Na 1	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



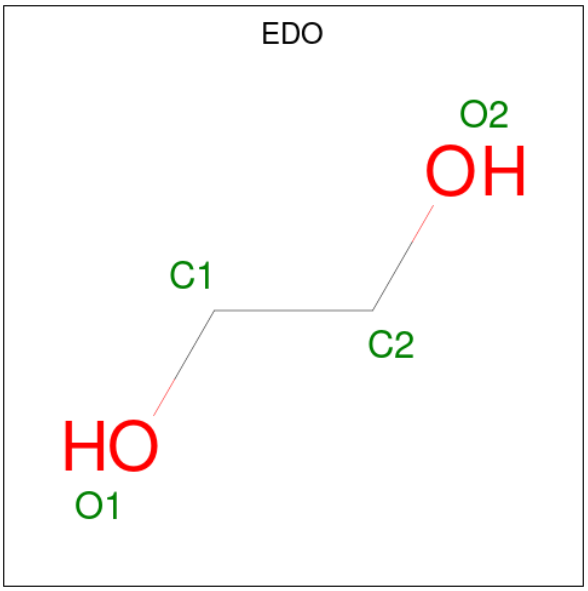
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: 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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is water.

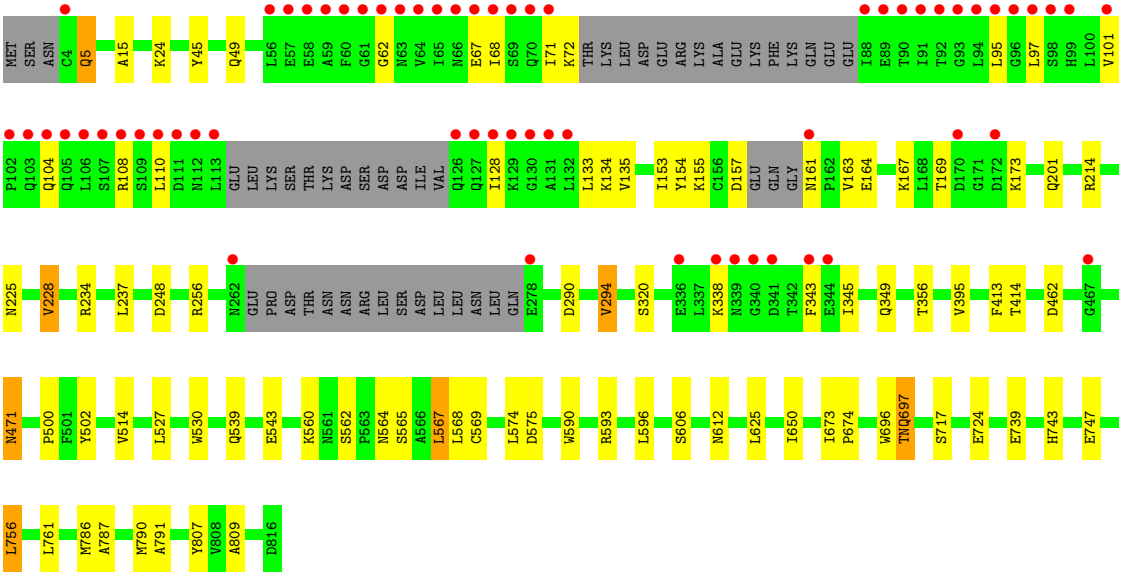
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	776	Total O 781 781	0	5
7	B	699	Total O 704 704	0	5
7	C	772	Total O 775 775	0	3
7	D	705	Total O 714 714	0	9

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.

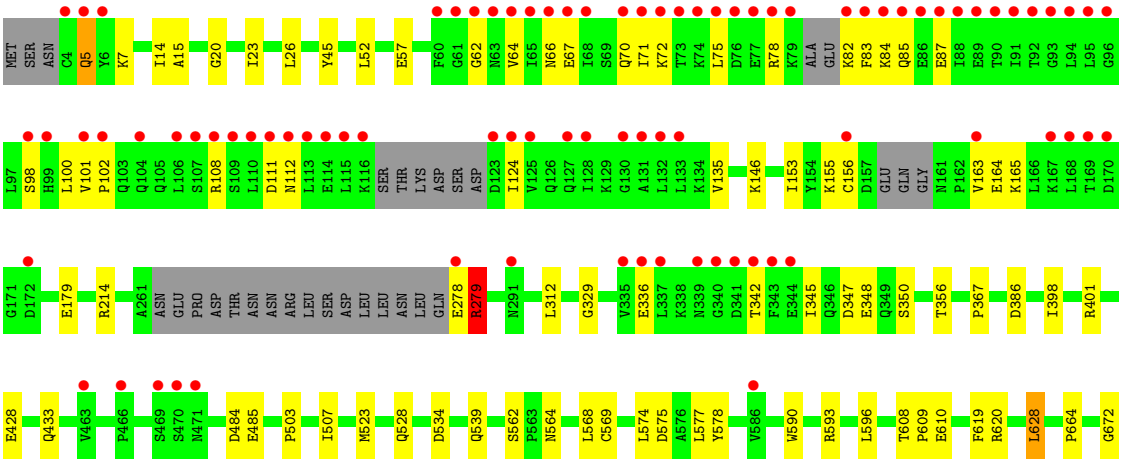
- Molecule 1: GoxA

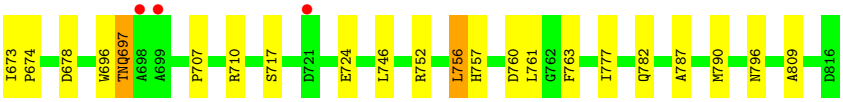
Chain A:



- Molecule 1: GoxA

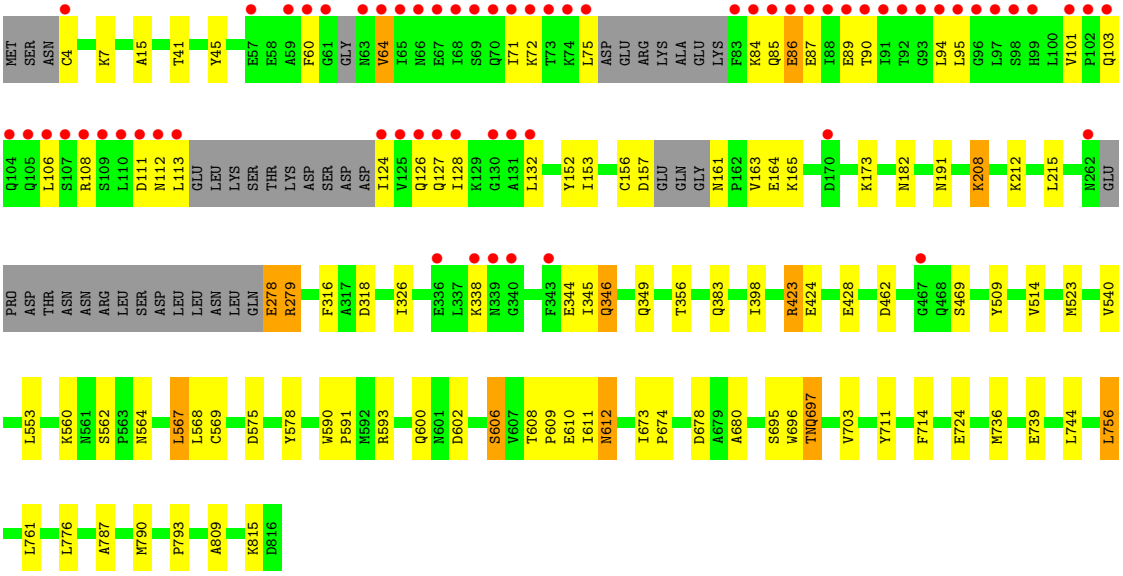
Chain B:





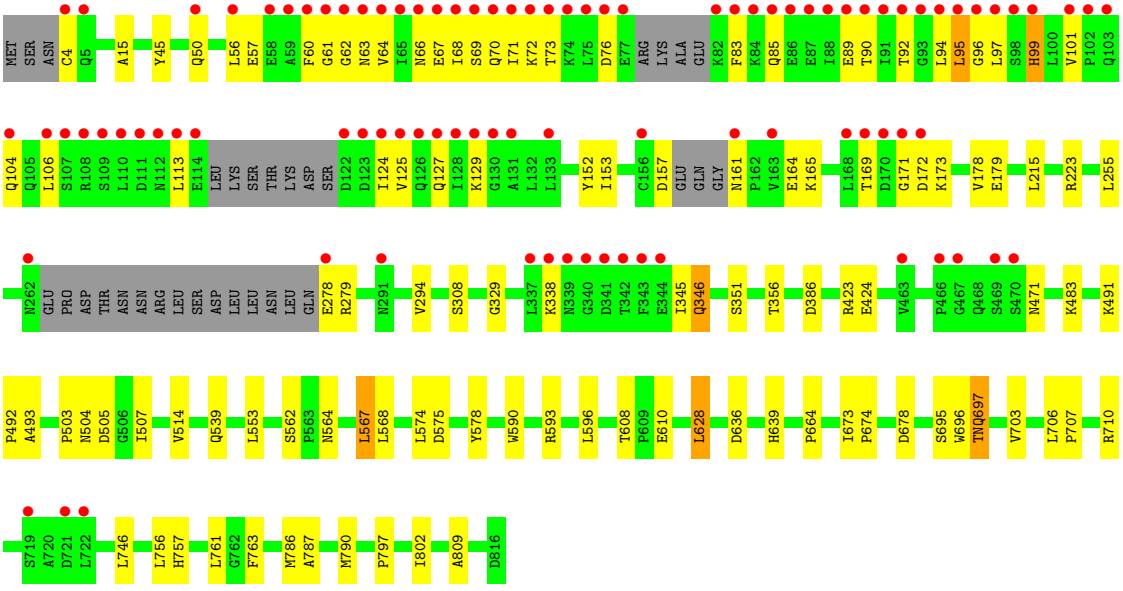
• Molecule 1: GoxA

Chain C:



• Molecule 1: GoxA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	110.24Å 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
$< I/\sigma(I) >$ [1]	2.39 (at 1.82Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.175 , 0.213 0.177 , 0.214	Depositor DCC
R_{free} test set	17055 reflections (5.05%)	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 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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: PGE, NA, EDO, MG, PEG, TNQ

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	0.38	0/6287	0.56	0/8563
1	B	0.35	0/6425	0.54	0/8739
1	C	0.38	0/6328	0.57	0/8612
1	D	0.36	0/6368	0.55	0/8667
All	All	0.37	0/25408	0.56	0/34581

There are no bond length outliers.

There are no bond angle outliers.

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	59	0
1	B	6298	0	6048	82	0
1	C	6202	0	5957	83	0
1	D	6241	0	5984	83	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	11	0
7	B	704	0	0	12	0
7	C	775	0	0	13	0
7	D	714	0	0	8	0
All	All	27905	30	23922	308	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (308) 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:345:ILE:HG23	1:B:350[A]:SER:OG	1.86	0.74
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:A:225:ASN:O	1:A:228[A]:VAL:HG23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:706[A]:LEU:HD13	1:D:706[A]:LEU:C	2.17	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:B:398:ILE:HD11	1:B:523[A]:MET:CE	2.27	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: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: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
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:B:398:ILE:HD11	1:B:523[A]:MET:HE2	1.83	0.59
1:B:672:GLY:HA3	1:B:678:ASP:CG	2.23	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:485[A]:GLU:CD	1:B:485[A]:GLU:H	2.07	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: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:D:57:GLU:OE1	1:D:57:GLU:HA	2.06	0.56
1:C:208:LYS:HE2	1:C:212:LYS:HB2	1.88	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:173:LYS:NZ	7:C:1015:HOH:O	2.39	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: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: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: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:104:GLN:CD	1:D:104:GLN:H	2.13	0.52
1:B:20:GLY:O	1:B:146:LYS:HE2	2.11	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:C:349:GLN:H	1:C:349:GLN:CD	2.13	0.51
1:A:395[A]:VAL:HG13	1:A:527:LEU:HD12	1.91	0.51
1:B:164:GLU:CD	1:B:165:LYS:H	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:HG2	7:A:1079:HOH:O	2.12	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:A:791:ALA:HB2	1:A:807:TYR:CE2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:72:LYS:HD3	1:C:124:ILE:HG21	1.98	0.46
1:D:696:TRP:HB3	1:D:697:TNQ:CE3	2.46	0.46
1:B:398:ILE:HD11	1:B:523[A]:MET:HE3	1.97	0.46
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:C:398[B]:ILE:HD11	1:C:523:MET:CE	2.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:156:CYS:HG	1:C:161:ASN:N	2.16	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: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:D:706[A]:LEU:C	1:D:706[A]:LEU:CD1	2.86	0.43
1:C:344:GLU:CG	1:C:346:GLN:NE2	2.80	0.43
1:C:739:GLU:CD	1:C:739:GLU:H	2.22	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
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: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: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:A:154:TYR:HH	1:A:565[A]:SER:HB2	1.82	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:A:290:ASP:CG	1:A:294:VAL:HG13	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:717:SER:HB2	7:A:1435:HOH:O	2.20	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: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
1:D:504:ASN:CG	1:D:505:ASP:H	2.23	0.41
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:71:ILE:C	1:D:71:ILE:HD12	2.41	0.41
1:A:104:GLN:HB3	1:A:108:ARG:NE	2.36	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: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: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%)	51	37
1	B	785/816 (96%)	764 (97%)	19 (2%)	2 (0%)	41	27
1	C	771/816 (94%)	750 (97%)	20 (3%)	1 (0%)	51	37
1	D	778/816 (95%)	754 (97%)	22 (3%)	2 (0%)	41	27
All	All	3105/3264 (95%)	3015 (97%)	84 (3%)	6 (0%)	47	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 (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	679/711 (96%)	664 (98%)	15 (2%)	52	39
1	B	693/711 (98%)	682 (98%)	11 (2%)	62	53
1	C	682/711 (96%)	658 (96%)	24 (4%)	36	20
1	D	686/711 (96%)	664 (97%)	22 (3%)	39	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2740/2844 (96%)	2668 (97%)	72 (3%)	47 32

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	67	GLU
1	A	164	GLU
1	A	167	LYS
1	A	228[A]	VAL
1	A	228[B]	VAL
1	A	294	VAL
1	A	349	GLN
1	A	471	ASN
1	A	567	LEU
1	A	569	CYS
1	A	574	LEU
1	A	575	ASP
1	A	625	LEU
1	A	756	LEU
1	B	5	GLN
1	B	98	SER
1	B	279	ARG
1	B	569	CYS
1	B	574	LEU
1	B	575	ASP
1	B	578	TYR
1	B	596	LEU
1	B	628	LEU
1	B	746	LEU
1	B	756	LEU
1	C	64	VAL
1	C	86	GLU
1	C	95	LEU
1	C	126	GLN
1	C	208	LYS
1	C	215	LEU
1	C	278	GLU
1	C	338	LYS
1	C	346	GLN
1	C	423[A]	ARG
1	C	423[B]	ARG

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Mol	Chain	Res	Type
1	C	424	GLU
1	C	540	VAL
1	C	553	LEU
1	C	567	LEU
1	C	569	CYS
1	C	575	ASP
1	C	578	TYR
1	C	606[A]	SER
1	C	606[B]	SER
1	C	612[A]	ASN
1	C	612[B]	ASN
1	C	678	ASP
1	C	756	LEU
1	D	4	CYS
1	D	50	GLN
1	D	70	GLN
1	D	95	LEU
1	D	99	HIS
1	D	173	LYS
1	D	215	LEU
1	D	278	GLU
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	578	TYR
1	D	596	LEU
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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	C	127	GLN
1	C	346	GLN

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Mol	Chain	Res	Type
1	D	99	HIS

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	2.97	3 (16%)	16,29,31	3.06	6 (37%)
1	TNQ	A	697	1	18,21,22	2.94	4 (22%)	16,29,31	3.22	5 (31%)
1	TNQ	D	697	1	18,21,22	2.95	3 (16%)	16,29,31	3.07	5 (31%)
1	TNQ	C	697	1	18,21,22	2.93	4 (22%)	16,29,31	3.07	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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	697	TNQ	C2-N1	-11.14	1.27	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	697	TNQ	C2-N1	-11.13	1.27	1.45
1	D	697	TNQ	C2-N1	-11.06	1.28	1.45
1	A	697	TNQ	C2-N1	-11.02	1.28	1.45
1	D	697	TNQ	CZ2-CE2	3.31	1.48	1.42
1	B	697	TNQ	CZ2-CE2	3.30	1.48	1.42
1	B	697	TNQ	CH2-CZ2	2.91	1.48	1.40
1	A	697	TNQ	CH2-CZ2	2.89	1.48	1.40
1	C	697	TNQ	CZ2-CE2	2.84	1.47	1.42
1	D	697	TNQ	CH2-CZ2	2.70	1.48	1.40
1	A	697	TNQ	CZ2-CE2	2.69	1.47	1.42
1	C	697	TNQ	CH2-CZ2	2.35	1.47	1.40
1	A	697	TNQ	CE3-CZ3	2.08	1.41	1.36
1	C	697	TNQ	CE3-CZ3	2.07	1.41	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	697	TNQ	C2-N1-CH2	-8.98	111.11	123.98
1	C	697	TNQ	C2-N1-CH2	-8.77	111.42	123.98
1	D	697	TNQ	C1-C2-N1	8.28	126.15	110.96
1	B	697	TNQ	C1-C2-N1	7.92	125.49	110.96
1	D	697	TNQ	C2-N1-CH2	-7.65	113.01	123.98
1	C	697	TNQ	C1-C2-N1	7.65	125.00	110.96
1	A	697	TNQ	C1-C2-N1	7.35	124.45	110.96
1	B	697	TNQ	C2-N1-CH2	-7.25	113.59	123.98
1	B	697	TNQ	O3-C1-C2	3.68	125.54	112.74
1	A	697	TNQ	O3-C1-C2	3.46	124.75	112.74
1	D	697	TNQ	CB-CG-CD2	2.83	130.66	126.25
1	D	697	TNQ	CB-CG-CD1	-2.74	124.58	127.97
1	A	697	TNQ	O2-C1-C2	-2.33	113.28	122.68
1	C	697	TNQ	CG-CB-CA	-2.27	111.02	114.53
1	B	697	TNQ	CG-CB-CA	-2.26	111.04	114.53
1	B	697	TNQ	O2-C1-C2	-2.19	113.81	122.68
1	A	697	TNQ	CB-CG-CD2	2.04	129.42	126.25
1	D	697	TNQ	CG-CB-CA	-2.01	111.42	114.53
1	B	697	TNQ	CB-CG-CD2	2.00	129.36	126.25

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	697	TNQ	CZ3-CH2-N1-C2

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

There are no ring outliers.

4 monomers are involved in 8 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\|>2$
5	PEG	C	903	-	6,6,6	0.42	0	5,5,5	0.46	0
4	PGE	A	903	-	9,9,9	0.40	0	8,8,8	0.52	0
6	EDO	D	903	-	3,3,3	0.54	0	2,2,2	0.20	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
5	PEG	C	903	-	-	1/4/4/4	-
4	PGE	A	903	-	-	3/7/7/7	-
6	EDO	D	903	-	-	0/1/1/1	-

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
5	C	903	PEG	8	0
6	D	903	EDO	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	767/816 (93%)	0.30	62 (8%)	12	9	12, 22, 71, 120	0
1	B	785/816 (96%)	0.40	89 (11%)	5	3	15, 26, 72, 117	0
1	C	776/816 (95%)	0.29	64 (8%)	11	9	13, 22, 72, 122	0
1	D	783/816 (95%)	0.47	93 (11%)	4	3	14, 26, 75, 125	0
All	All	3111/3264 (95%)	0.37	308 (9%)	7	5	12, 24, 73, 125	0

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	71	ILE	11.9
1	D	124	ILE	10.7
1	A	71	ILE	10.2
1	A	64	VAL	9.9
1	B	115	LEU	9.7
1	D	75	LEU	9.5
1	D	83	PHE	9.4
1	D	62	GLY	9.3
1	A	62	GLY	9.2
1	D	113	LEU	8.9
1	C	83	PHE	8.8
1	A	68	ILE	8.7
1	C	110	LEU	8.7
1	B	124	ILE	8.4
1	D	73	THR	8.2
1	D	68	ILE	8.0
1	A	65	ILE	7.9
1	A	94	LEU	7.8
1	C	113	LEU	7.8
1	C	68	ILE	7.8
1	A	61	GLY	7.7

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Mol	Chain	Res	Type	RSRZ
1	B	83	PHE	7.7
1	A	60	PHE	7.4
1	D	71	ILE	7.4
1	D	90	THR	7.3
1	D	61	GLY	7.2
1	B	75	LEU	7.2
1	D	122	ASP	7.1
1	A	110	LEU	7.1
1	A	90	THR	7.0
1	C	91	ILE	6.9
1	C	128	ILE	6.9
1	A	59	ALA	6.8
1	A	91	ILE	6.7
1	C	65	ILE	6.6
1	A	113	LEU	6.5
1	A	95	LEU	6.5
1	B	128	ILE	6.4
1	A	63	ASN	6.4
1	B	116	LYS	6.3
1	A	128	ILE	6.3
1	B	71	ILE	6.3
1	C	64	VAL	6.2
1	D	65	ILE	6.2
1	C	61	GLY	6.1
1	A	127	GLN	6.0
1	D	69	SER	6.0
1	C	127	GLN	6.0
1	C	73	THR	6.0
1	B	68	ILE	5.9
1	A	66	ASN	5.9
1	D	72	LYS	5.9
1	D	74	LYS	5.8
1	C	94	LEU	5.8
1	A	69	SER	5.8
1	A	70	GLN	5.7
1	C	124	ILE	5.7
1	A	109	SER	5.7
1	A	102	PRO	5.6
1	D	128	ILE	5.6
1	C	88	ILE	5.5
1	D	77	GLU	5.5
1	A	106	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	123	ASP	5.5
1	D	66	ASN	5.5
1	C	125	VAL	5.5
1	B	111	ASP	5.5
1	D	91	ILE	5.5
1	B	113	LEU	5.5
1	B	343	PHE	5.5
1	D	92	THR	5.4
1	D	76	ASP	5.3
1	C	112	ASN	5.3
1	B	78	ARG	5.3
1	D	86	GLU	5.3
1	C	75	LEU	5.2
1	C	107	SER	5.2
1	D	95	LEU	5.2
1	B	88	ILE	5.2
1	D	127	GLN	5.1
1	C	86	GLU	5.1
1	D	60	PHE	5.1
1	D	114	GLU	5.1
1	D	63	ASN	5.0
1	D	112	ASN	5.0
1	A	92	THR	5.0
1	C	89	GLU	5.0
1	C	72	LYS	4.9
1	B	86	GLU	4.9
1	C	95	LEU	4.9
1	C	85	GLN	4.9
1	C	109	SER	4.9
1	B	92	THR	4.8
1	D	4	CYS	4.7
1	C	111	ASP	4.7
1	D	111	ASP	4.7
1	B	110	LEU	4.7
1	A	88	ILE	4.7
1	C	84	LYS	4.7
1	C	60	PHE	4.7
1	B	90	THR	4.6
1	B	125	VAL	4.6
1	D	125	VAL	4.6
1	D	67	GLU	4.6
1	B	85	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	108	ARG	4.5
1	B	114	GLU	4.5
1	D	88	ILE	4.5
1	B	73	THR	4.5
1	B	77	GLU	4.5
1	D	87	GLU	4.5
1	D	126	GLN	4.4
1	C	74	LYS	4.4
1	D	85	GLN	4.4
1	B	60	PHE	4.4
1	B	112	ASN	4.4
1	D	70	GLN	4.4
1	B	63	ASN	4.4
1	B	89	GLU	4.4
1	D	89	GLU	4.4
1	A	96	GLY	4.4
1	C	126	GLN	4.4
1	C	4	CYS	4.4
1	C	97	LEU	4.4
1	B	340	GLY	4.3
1	B	84	LYS	4.3
1	A	97	LEU	4.3
1	B	106	LEU	4.3
1	D	59	ALA	4.3
1	B	66	ASN	4.2
1	D	343	PHE	4.2
1	D	341	ASP	4.2
1	C	106	LEU	4.2
1	A	112	ASN	4.1
1	A	126	GLN	4.1
1	C	66	ASN	4.1
1	D	82	LYS	4.1
1	C	92	THR	4.1
1	B	82	LYS	4.1
1	A	98	SER	4.0
1	D	133	LEU	4.0
1	B	79	LYS	4.0
1	B	91	ILE	4.0
1	D	131	ALA	4.0
1	D	64	VAL	4.0
1	D	84	LYS	3.9
1	A	104	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	262	ASN	3.8
1	B	127	GLN	3.7
1	A	111	ASP	3.7
1	A	467	GLY	3.7
1	A	4	CYS	3.7
1	C	90	THR	3.7
1	C	132	LEU	3.7
1	A	132	LEU	3.7
1	B	93	GLY	3.7
1	B	341	ASP	3.7
1	A	67	GLU	3.7
1	B	99	HIS	3.6
1	D	337	LEU	3.6
1	C	108	ARG	3.6
1	A	103	GLN	3.6
1	A	93	GLY	3.6
1	C	70	GLN	3.6
1	B	4	CYS	3.6
1	A	105	GLN	3.5
1	B	98	SER	3.5
1	B	123	ASP	3.5
1	B	169	THR	3.5
1	D	94	LEU	3.5
1	A	108	ARG	3.5
1	D	169	THR	3.5
1	A	170	ASP	3.5
1	D	170	ASP	3.5
1	B	76	ASP	3.5
1	B	65	ILE	3.4
1	C	104	GLN	3.4
1	C	340	GLY	3.4
1	D	110	LEU	3.3
1	D	104	GLN	3.3
1	D	469	SER	3.3
1	A	89	GLU	3.3
1	A	130	GLY	3.3
1	D	338	LYS	3.3
1	B	104	GLN	3.3
1	C	59	ALA	3.3
1	B	72	LYS	3.2
1	C	102	PRO	3.2
1	B	107	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	96	GLY	3.2
1	D	130	GLY	3.1
1	D	99	HIS	3.1
1	D	340	GLY	3.1
1	D	109	SER	3.1
1	B	62	GLY	3.1
1	D	129	LYS	3.1
1	B	64	VAL	3.0
1	B	96	GLY	3.0
1	A	107	SER	3.0
1	A	338	LYS	3.0
1	C	105	GLN	3.0
1	D	106	LEU	3.0
1	B	109	SER	3.0
1	D	172	ASP	3.0
1	A	343	PHE	3.0
1	A	339	ASN	3.0
1	A	278	GLU	3.0
1	A	129	LYS	3.0
1	A	101	VAL	3.0
1	B	95	LEU	2.9
1	C	131	ALA	2.9
1	C	63	ASN	2.9
1	B	342	THR	2.9
1	D	56	LEU	2.9
1	B	167	LYS	2.9
1	B	131	ALA	2.9
1	C	170	ASP	2.9
1	B	94	LEU	2.8
1	D	5	GLN	2.8
1	B	102	PRO	2.8
1	A	340	GLY	2.8
1	A	99	HIS	2.8
1	C	130	GLY	2.8
1	C	99	HIS	2.8
1	D	467	GLY	2.7
1	B	70	GLN	2.7
1	A	57	GLU	2.7
1	D	98	SER	2.7
1	B	335	VAL	2.7
1	B	5	GLN	2.7
1	A	131	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	470	SER	2.7
1	B	336	GLU	2.7
1	D	108	ARG	2.6
1	D	291	ASN	2.6
1	D	97	LEU	2.6
1	D	102	PRO	2.6
1	C	69	SER	2.6
1	D	470	SER	2.6
1	D	342	THR	2.6
1	C	262	ASN	2.6
1	D	96	GLY	2.6
1	C	343	PHE	2.6
1	D	101	VAL	2.6
1	B	471	ASN	2.5
1	D	156	CYS	2.5
1	C	101	VAL	2.5
1	D	107	SER	2.5
1	D	721	ASP	2.5
1	B	132	LEU	2.5
1	B	337	LEU	2.5
1	C	467	GLY	2.5
1	D	93	GLY	2.5
1	C	103	GLN	2.5
1	B	698	ALA	2.5
1	A	58	GLU	2.5
1	D	58	GLU	2.5
1	B	172	ASP	2.5
1	C	87	GLU	2.5
1	C	338	LYS	2.5
1	B	168	LEU	2.5
1	B	67	GLU	2.5
1	C	98	SER	2.4
1	B	344	GLU	2.4
1	D	171	GLY	2.4
1	B	469	SER	2.4
1	C	57	GLU	2.4
1	B	101	VAL	2.4
1	B	163	VAL	2.4
1	B	170	ASP	2.4
1	D	339	ASN	2.4
1	D	103	GLN	2.4
1	B	339	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	722	LEU	2.3
1	C	93	GLY	2.3
1	B	466	PRO	2.3
1	A	161	ASN	2.3
1	A	56	LEU	2.3
1	B	61	GLY	2.2
1	B	463	VAL	2.2
1	D	463	VAL	2.2
1	B	87	GLU	2.2
1	A	262	ASN	2.2
1	D	466	PRO	2.2
1	D	50	GLN	2.2
1	B	721	ASP	2.2
1	B	133	LEU	2.2
1	C	67	GLU	2.2
1	B	74	LYS	2.2
1	A	344	GLU	2.2
1	C	339	ASN	2.2
1	D	719	SER	2.1
1	A	341	ASP	2.1
1	B	291	ASN	2.1
1	D	161	ASN	2.1
1	B	130	GLY	2.1
1	B	6	TYR	2.1
1	B	278	GLU	2.1
1	B	699	ALA	2.1
1	A	172	ASP	2.0
1	D	163	VAL	2.0
1	D	344	GLU	2.0
1	B	156	CYS	2.0
1	B	586	VAL	2.0
1	D	168	LEU	2.0
1	A	336	GLU	2.0
1	C	336	GLU	2.0
1	D	278	GLU	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	B	697	20/21	0.93	0.12	13,17,26,30	0
1	TNQ	C	697	20/21	0.94	0.12	12,17,25,28	0
1	TNQ	A	697	20/21	0.95	0.10	11,16,25,25	0
1	TNQ	D	697	20/21	0.96	0.11	14,18,28,30	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
4	PGE	A	903	10/10	0.67	0.25	51,65,74,76	0
5	PEG	C	903	7/7	0.71	0.27	41,54,67,67	0
6	EDO	D	903	4/4	0.74	0.39	34,42,50,60	0
3	NA	A	902	1/1	0.96	0.18	38,38,38,38	0
3	NA	B	902	1/1	0.96	0.14	45,45,45,45	0
3	NA	C	902	1/1	0.96	0.23	41,41,41,41	0
2	MG	D	901	1/1	0.98	0.08	23,23,23,23	0
2	MG	B	901	1/1	0.98	0.08	24,24,24,24	0
3	NA	D	902	1/1	0.98	0.07	37,37,37,37	0
2	MG	A	901	1/1	0.99	0.08	15,15,15,15	0
2	MG	C	901	1/1	0.99	0.12	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.