



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 05:01 AM EST

PDB ID : 3GW6
Title : Intramolecular Chaperone
Authors : Schulz, E.C.; Dickmanns, A.; Ficner, R.
Deposited on : 2009-03-31
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

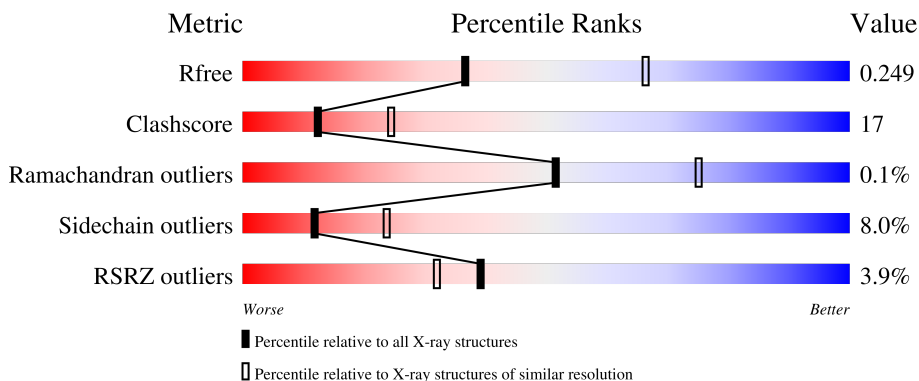
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	275	 4% 67% 21% 5% 7%
1	B	275	 4% 60% 29% • 7%
1	C	275	 3% 65% 24% • 8%
1	D	275	 5% 61% 27% • 8%
1	E	275	 4% 66% 23% • 7%

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Mol	Chain	Length	Quality of chain
1	F	275	

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
2	PEG	A	2	-	-	X	-
2	PEG	C	29	-	-	X	-
2	PEG	E	21	-	-	X	-
2	PEG	F	30	-	-	X	-
2	PEG	F	34	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12617 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 Endo-N-acetylneuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	Total 2028	C 1270	N 351	O 400	S 7	16	0	0
1	B	255	Total 2020	C 1267	N 349	O 397	S 7	24	0	0
1	E	257	Total 2032	C 1272	N 351	O 402	S 7	27	0	0
1	C	254	Total 2011	C 1262	N 349	O 393	S 7	11	0	0
1	D	252	Total 1996	C 1253	N 346	O 390	S 7	34	0	0
1	F	257	Total 2035	C 1274	N 352	O 402	S 7	24	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	911	ALA	SER	conflict	UNP Q858B1
B	911	ALA	SER	conflict	UNP Q858B1
E	911	ALA	SER	conflict	UNP Q858B1
C	911	ALA	SER	conflict	UNP Q858B1
D	911	ALA	SER	conflict	UNP Q858B1
F	911	ALA	SER	conflict	UNP Q858B1

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



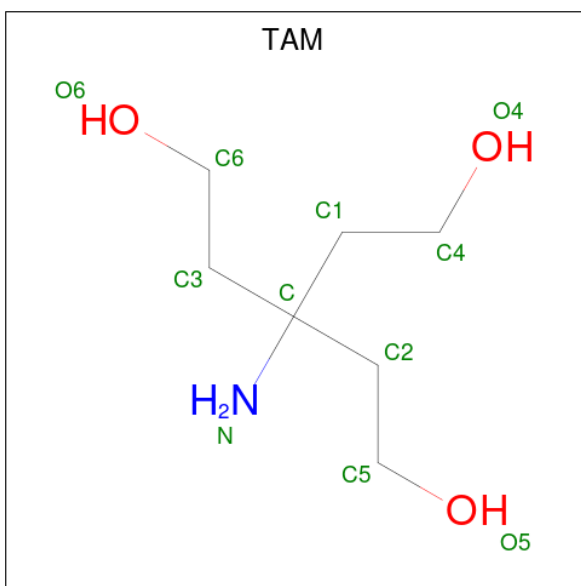
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 4 3	0	0
2	A	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	E	1	Total C O 7 4 3	0	0
2	E	1	Total C O 7 4 3	0	0
2	E	1	Total C O 7 4 3	0	0
2	E	1	Total C O 7 4 3	0	0
2	E	1	Total C O 7 4 3	0	0
2	E	1	Total C O 7 4 3	0	0
2	E	1	Total C O 7 4 3	0	0
2	C	1	Total C O 7 4 3	0	0
2	C	1	Total C O 7 4 3	0	0
2	C	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: C₇H₁₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	1	0
			11	7	1	3		
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	C	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	2	Total Cl 2 2	0	0
4	D	2	Total Cl 2 2	0	0

- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br).

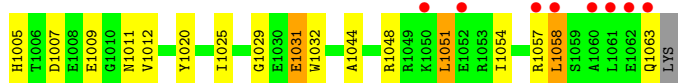
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total Br 3 3	0	0
5	E	1	Total Br 1 1	0	0
5	C	1	Total Br 1 1	0	0
5	F	1	Total Br 1 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

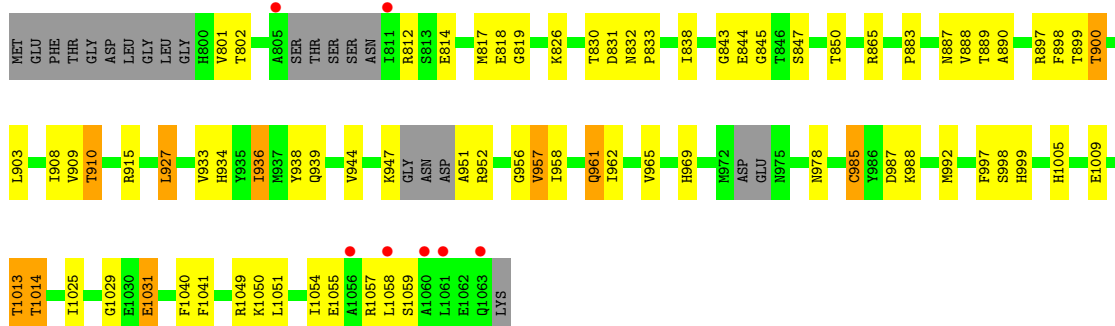
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Ca 1 1	0	0

- Molecule 7 is water.

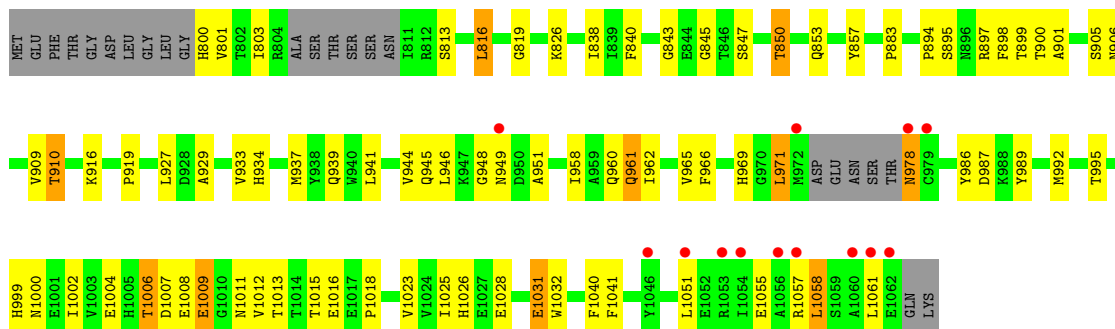
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	63	Total O 63 63	0	0
7	B	47	Total O 47 47	0	0
7	E	45	Total O 45 45	0	0
7	C	61	Total O 61 61	0	0
7	D	52	Total O 52 52	0	0
7	F	55	Total O 55 55	0	0



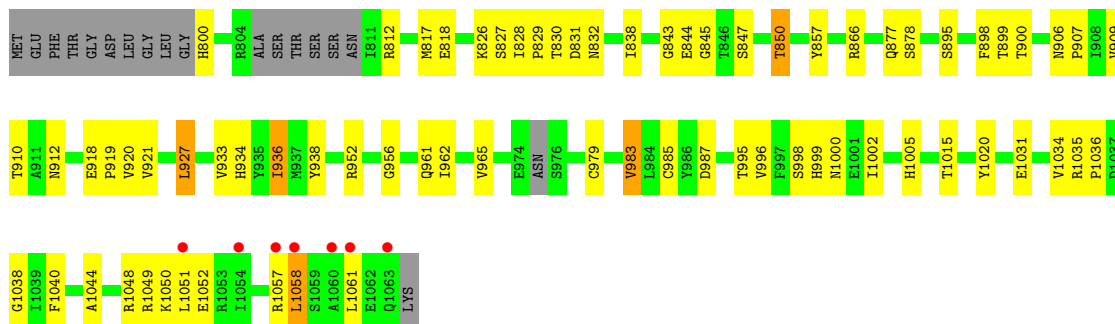
- Molecule 1: Endo-N-acetylneuraminidase



- Molecule 1: Endo-N-acetylneuraminidase



- Molecule 1: Endo-N-acetylneuraminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.65Å 79.95Å 109.58Å 81.71° 76.53° 87.11°	Depositor
Resolution (Å)	27.63 – 2.60 48.21 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.4 (27.63-2.60) 95.4 (48.21-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.61Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.209 , 0.255 0.204 , 0.249	Depositor DCC
R_{free} test set	3000 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtrriage
Anisotropy	0.521	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12617	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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: BR, TAM, CL, CA, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/2071	0.43	0/2810
1	B	0.24	0/2062	0.44	0/2797
1	C	0.24	0/2053	0.43	0/2785
1	D	0.25	0/2039	0.47	0/2767
1	E	0.23	0/2074	0.45	0/2815
1	F	0.23	0/2078	0.43	0/2820
All	All	0.24	0/12377	0.44	0/16794

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	2028	0	1916	82	0
1	B	2020	0	1914	100	0
1	C	2011	0	1910	78	0
1	D	1996	0	1893	81	0
1	E	2032	0	1922	72	0
1	F	2035	0	1923	88	0
2	A	14	0	20	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	7	0	10	0	0
2	C	21	0	30	5	0
2	D	7	0	10	0	0
2	E	49	0	70	13	0
2	F	28	0	40	19	0
3	A	22	0	34	3	0
3	C	11	0	17	1	0
4	A	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
5	B	3	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	F	1	0	0	0	0
7	A	63	0	0	4	0
7	B	47	0	0	1	0
7	C	61	0	0	4	0
7	D	52	0	0	2	0
7	E	45	0	0	1	0
7	F	55	0	0	4	0
All	All	12617	0	11709	402	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 17.

All (402) 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:845:GLY:H	1:B:850:THR:HG21	1.10	1.13
1:A:845:GLY:H	1:A:850:THR:HG21	1.18	1.06
1:F:845:GLY:H	1:F:850:THR:HG21	1.18	1.04
1:D:845:GLY:H	1:D:850:THR:HG21	1.23	1.04
1:F:934:HIS:H	1:F:961:GLN:NE2	1.66	0.93
1:B:980:ARG:HG3	1:B:980:ARG:HH11	1.34	0.93
1:F:934:HIS:H	1:F:961:GLN:HE22	1.18	0.91
1:F:830:THR:H	2:F:34:PEG:H22	1.37	0.90
1:A:934:HIS:H	1:A:961:GLN:NE2	1.73	0.86
1:F:831:ASP:H	2:F:34:PEG:H41	1.43	0.83
1:C:934:HIS:H	1:C:961:GLN:NE2	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:979:CYS:HB3	7:F:223:HOH:O	1.81	0.80
1:E:934:HIS:H	1:E:961:GLN:NE2	1.80	0.80
1:B:1051:LEU:HD23	1:F:1050:LYS:HD3	1.63	0.78
1:D:934:HIS:H	1:D:961:GLN:NE2	1.82	0.77
1:B:976:SER:N	1:B:977:THR:HA	1.98	0.77
3:A:35:TAM:H61	7:A:241:HOH:O	1.83	0.77
1:E:844:GLU:HG2	1:E:850:THR:HG21	1.66	0.77
1:A:910:THR:HG23	1:B:897:ARG:HD3	1.67	0.76
1:A:973:ASP:OD1	1:A:975:ASN:ND2	2.16	0.76
1:B:845:GLY:N	1:B:850:THR:HG21	1.95	0.75
1:A:957:VAL:HG21	1:A:962:ILE:HD11	1.68	0.74
2:C:29:PEG:H41	1:D:819:GLY:H	1.52	0.74
1:A:1051:LEU:HD23	1:B:1050:LYS:HG2	1.70	0.73
1:B:1006:THR:HG22	1:B:1012:VAL:HG13	1.68	0.73
1:C:831:ASP:H	2:C:29:PEG:H21	1.52	0.73
1:D:1008:GLU:HG3	1:D:1009:GLU:H	1.53	0.73
1:E:954:HIS:HE1	2:E:21:PEG:C3	2.01	0.72
1:F:985:CYS:HB3	7:F:212:HOH:O	1.87	0.72
1:E:934:HIS:H	1:E:961:GLN:HE22	1.36	0.72
1:C:934:HIS:H	1:C:961:GLN:HE21	1.35	0.71
1:A:840:PHE:HE2	1:A:856:LEU:HD22	1.54	0.71
1:A:1051:LEU:HD12	1:F:1051:LEU:HD21	1.72	0.71
1:F:830:THR:H	2:F:34:PEG:C2	2.04	0.70
1:C:1005:HIS:HB2	1:C:1013:THR:HG23	1.72	0.70
1:B:947:LYS:HD3	1:B:951:ALA:N	2.05	0.70
1:E:954:HIS:HE1	2:E:21:PEG:H32	1.56	0.70
1:B:1061:LEU:HD21	1:F:1061:LEU:HD22	1.72	0.70
1:A:974:GLU:OE2	1:A:974:GLU:C	2.29	0.70
1:E:910:THR:OG1	1:D:1031:GLU:HG3	1.92	0.69
1:B:1061:LEU:HD11	1:F:1061:LEU:HD21	1.74	0.69
1:F:927:LEU:HD23	1:F:1049:ARG:HD3	1.73	0.69
1:C:957:VAL:HG21	1:C:962:ILE:HD11	1.75	0.69
1:E:890:ALA:HB2	1:D:899:THR:OG1	1.93	0.68
1:D:933:VAL:HA	1:D:961:GLN:HE22	1.57	0.68
1:A:934:HIS:H	1:A:961:GLN:HE22	1.39	0.68
1:D:995:THR:HG23	7:D:253:HOH:O	1.93	0.68
1:F:878:SER:HA	2:F:30:PEG:H41	1.76	0.68
1:A:936:ILE:HD12	1:F:919:PRO:HB3	1.76	0.67
1:C:843:GLY:HA3	1:C:850:THR:HG22	1.75	0.67
1:B:847:SER:O	1:B:850:THR:HB	1.94	0.67
1:A:897:ARG:HD3	1:F:910:THR:HG23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:900:THR:HG23	1:D:905:SER:OG	1.94	0.67
1:E:940:TRP:HD1	2:E:21:PEG:H32	1.59	0.67
1:A:844:GLU:HG2	1:F:828:ILE:HG13	1.77	0.66
1:F:934:HIS:N	1:F:961:GLN:HE22	1.90	0.66
1:C:936:ILE:HD12	1:D:919:PRO:HB3	1.78	0.66
1:D:987:ASP:HB2	1:D:1031:GLU:OE1	1.96	0.65
1:D:1006:THR:HG22	1:D:1012:VAL:HG22	1.78	0.65
1:A:845:GLY:N	1:A:850:THR:HG21	2.02	0.64
1:C:898:PHE:CE1	1:D:883:PRO:HG3	2.31	0.64
1:F:987:ASP:HB2	1:F:1031:GLU:OE1	1.97	0.64
1:F:878:SER:H	2:F:30:PEG:H41	1.63	0.64
1:B:980:ARG:HG3	1:B:980:ARG:NH1	2.03	0.64
1:A:1058:LEU:HB3	1:B:1057:ARG:HH21	1.61	0.64
1:C:826:LYS:HB2	1:C:838:ILE:HG13	1.80	0.63
1:D:1057:ARG:O	1:D:1061:LEU:HG	1.99	0.63
1:C:961:GLN:HG2	7:C:64:HOH:O	1.97	0.63
1:D:900:THR:HG22	1:D:901:ALA:H	1.64	0.63
1:D:900:THR:HG22	1:D:901:ALA:N	2.13	0.63
1:C:909:VAL:HG21	1:D:906:ASN:OD1	1.99	0.63
1:F:845:GLY:H	1:F:850:THR:CG2	2.04	0.63
1:F:1005:HIS:NE2	1:F:1015:THR:HG22	2.13	0.63
1:A:844:GLU:HB3	1:F:827:SER:HA	1.81	0.63
1:A:1005:HIS:HE1	1:A:1015:THR:HG22	1.64	0.63
1:C:898:PHE:CD1	1:D:883:PRO:HG3	2.35	0.62
1:E:844:GLU:HG2	1:E:850:THR:CG2	2.29	0.62
1:B:960:GLN:HE22	1:B:963:ARG:HH11	1.47	0.62
1:F:845:GLY:N	1:F:850:THR:HG21	2.02	0.62
1:B:890:ALA:HB2	1:F:899:THR:OG1	2.00	0.62
1:A:909:VAL:HG21	1:F:906:ASN:OD1	1.99	0.62
1:B:977:THR:HG23	1:B:978:ASN:ND2	2.15	0.61
2:E:22:PEG:O1	1:C:818:GLU:HB3	2.01	0.61
1:C:1057:ARG:HB3	1:D:1058:LEU:HD12	1.83	0.61
1:E:1058:LEU:HD12	1:D:1057:ARG:HH21	1.65	0.61
1:B:883:PRO:HG3	1:F:898:PHE:CD1	2.35	0.61
1:E:941:LEU:HD12	1:C:915:ARG:HE	1.66	0.61
1:B:1058:LEU:HD11	1:F:1058:LEU:HD12	1.81	0.61
1:C:998:SER:OG	1:C:999:HIS:HD2	1.84	0.61
1:F:829:PRO:HB3	2:F:34:PEG:H42	1.83	0.61
1:B:960:GLN:HE22	1:B:963:ARG:NH1	1.99	0.61
1:B:977:THR:HG23	1:B:978:ASN:HD22	1.66	0.60
1:F:847:SER:O	1:F:850:THR:HB	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:957:VAL:HB	1:B:962:ILE:HD11	1.83	0.60
1:A:1058:LEU:HD21	1:B:1058:LEU:HD21	1.84	0.60
1:B:885:ASN:HB2	1:B:888:VAL:HG21	1.83	0.60
1:C:843:GLY:HA3	1:C:850:THR:CG2	2.32	0.60
1:B:960:GLN:NE2	1:B:963:ARG:HD3	2.16	0.60
1:A:1058:LEU:HD11	1:B:1058:LEU:HD22	1.82	0.60
1:B:888:VAL:HG23	1:B:889:THR:HG23	1.84	0.59
1:F:831:ASP:N	2:F:34:PEG:H41	2.16	0.59
1:B:1058:LEU:HB3	1:F:1057:ARG:NH2	2.18	0.59
1:D:941:LEU:O	1:D:944:VAL:HG22	2.03	0.59
1:A:900:THR:HG23	1:B:905:SER:OG	2.01	0.59
1:D:847:SER:O	1:D:850:THR:HB	2.03	0.59
1:B:906:ASN:OD1	1:F:909:VAL:HG21	2.02	0.59
1:B:1058:LEU:HD11	1:F:1058:LEU:CD1	2.33	0.59
1:E:992:MET:HE2	1:E:1025:ILE:HG21	1.86	0.58
1:C:899:THR:O	1:C:900:THR:HG23	2.04	0.58
1:C:933:VAL:HG22	1:C:962:ILE:HD13	1.85	0.58
1:D:986:TYR:HB2	1:D:1032:TRP:CZ3	2.38	0.58
1:A:952:ARG:H	2:A:2:PEG:H12	1.68	0.58
1:A:919:PRO:HB3	1:B:936:ILE:HD12	1.85	0.58
1:B:934:HIS:N	1:B:961:GLN:HE21	2.02	0.58
1:B:976:SER:HB2	1:B:977:THR:C	2.23	0.58
1:A:906:ASN:OD1	1:B:909:VAL:HG21	2.04	0.58
1:E:841:CYS:HB2	1:E:853:GLN:HG2	1.85	0.58
1:E:940:TRP:CD1	2:E:21:PEG:H32	2.38	0.57
1:C:1055:GLU:O	1:C:1059:SER:HB2	2.04	0.57
1:A:943:ALA:HB2	2:A:2:PEG:H21	1.87	0.57
1:C:1050:LYS:HD3	1:D:1051:LEU:HD23	1.85	0.57
1:E:1005:HIS:O	1:E:1012:VAL:HA	2.05	0.57
1:B:936:ILE:CD1	1:B:958:ILE:HG12	2.34	0.57
1:A:936:ILE:CD1	1:A:958:ILE:HG12	2.34	0.57
1:A:955:PHE:CE2	1:F:983:VAL:HG21	2.40	0.57
1:E:1007:ASP:HB2	1:E:1011:ASN:H	1.69	0.57
1:C:844:GLU:N	1:C:850:THR:HG21	2.19	0.57
1:E:1007:ASP:HB3	1:E:1009:GLU:H	1.70	0.56
1:C:1051:LEU:HD11	1:D:1051:LEU:HD11	1.86	0.56
1:B:1055:GLU:OE2	1:F:1050:LYS:HE2	2.05	0.56
1:E:934:HIS:N	1:E:961:GLN:HE22	2.02	0.56
1:A:843:GLY:HA3	1:A:850:THR:HG23	1.87	0.56
1:E:898:PHE:CD1	1:C:883:PRO:HG3	2.41	0.56
1:E:888:VAL:HG23	2:E:6:PEG:H11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:906:ASN:OD1	1:D:909:VAL:HG21	2.06	0.56
1:A:1057:ARG:O	1:A:1061:LEU:HD22	2.06	0.55
1:C:1040:PHE:CZ	1:D:1040:PHE:HB2	2.40	0.55
1:B:883:PRO:HG3	1:F:898:PHE:CE1	2.40	0.55
1:C:1057:ARG:HH21	1:D:1058:LEU:HB3	1.71	0.55
1:F:920:VAL:HG12	1:F:921:VAL:O	2.07	0.55
1:A:992:MET:HE2	1:A:1025:ILE:HG13	1.89	0.55
1:C:897:ARG:HD3	1:D:910:THR:HG23	1.89	0.55
1:C:845:GLY:H	1:C:850:THR:HG21	1.71	0.55
1:A:812:ARG:HD3	1:B:821:TYR:OH	2.07	0.54
1:A:936:ILE:HG12	1:A:956:GLY:O	2.07	0.54
1:A:973:ASP:OD2	1:A:975:ASN:ND2	2.37	0.54
1:A:974:GLU:CG	1:A:974:GLU:O	2.54	0.54
1:B:954:HIS:HD2	7:F:202:HOH:O	1.90	0.54
1:A:952:ARG:HB3	2:A:2:PEG:H32	1.89	0.54
7:A:251:HOH:O	1:F:800:HIS:HD2	1.90	0.54
1:C:992:MET:HE2	1:C:1025:ILE:HG21	1.90	0.54
1:E:922:PHE:HB3	1:E:927:LEU:HD21	1.89	0.54
1:C:988:LYS:HD2	1:C:1029:GLY:O	2.08	0.54
1:F:878:SER:CA	2:F:30:PEG:H41	2.38	0.54
1:E:831:ASP:H	2:E:22:PEG:H41	1.73	0.54
1:F:878:SER:N	2:F:30:PEG:H41	2.23	0.54
1:E:821:TYR:OH	1:C:812:ARG:HD3	2.08	0.53
1:A:899:THR:O	1:A:900:THR:HG23	2.07	0.53
1:B:845:GLY:H	1:B:850:THR:CG2	2.02	0.53
1:B:922:PHE:HB3	1:B:927:LEU:HD21	1.90	0.53
1:C:936:ILE:CD1	1:C:958:ILE:HG12	2.39	0.53
1:A:1031:GLU:HB2	1:F:912:ASN:HD22	1.73	0.53
1:C:938:TYR:CE1	1:D:916:LYS:HE2	2.43	0.53
1:E:986:TYR:HB2	1:E:1032:TRP:CZ3	2.43	0.53
1:D:944:VAL:O	1:D:948:GLY:N	2.42	0.53
1:D:966:PHE:O	1:D:971:LEU:HD22	2.09	0.53
1:C:927:LEU:HD23	1:C:1049:ARG:HD3	1.91	0.53
1:F:826:LYS:HB2	1:F:838:ILE:CG1	2.39	0.53
1:A:847:SER:O	1:A:850:THR:HB	2.09	0.53
1:E:888:VAL:HG22	1:E:889:THR:HG23	1.89	0.53
1:D:958:ILE:O	1:D:962:ILE:HG12	2.09	0.53
1:D:1008:GLU:HG3	1:D:1009:GLU:N	2.23	0.53
1:C:888:VAL:HG23	1:C:889:THR:HG23	1.91	0.52
1:A:1061:LEU:HG	1:F:1061:LEU:CD2	2.39	0.52
1:A:1057:ARG:HH11	1:F:1058:LEU:HB3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:943:ALA:CB	2:A:2:PEG:H21	2.39	0.52
1:B:819:GLY:CA	2:F:34:PEG:H11	2.38	0.52
1:E:954:HIS:CE1	2:E:21:PEG:C3	2.88	0.52
1:D:894:PRO:HB3	1:D:1031:GLU:OE1	2.10	0.52
1:E:810:ASN:N	1:E:810:ASN:HD22	2.07	0.52
1:F:826:LYS:HB2	1:F:838:ILE:HG13	1.91	0.52
1:A:1051:LEU:CD1	1:F:1051:LEU:HD21	2.39	0.52
1:C:956:GLY:HA2	1:D:1041:PHE:CD1	2.45	0.52
1:E:846:THR:HG1	1:E:1020:TYR:HH	1.54	0.52
1:E:905:SER:OG	1:C:900:THR:HG23	2.10	0.52
1:C:985:CYS:HB2	7:C:77:HOH:O	2.09	0.52
1:D:961:GLN:O	1:D:965:VAL:HG23	2.09	0.52
1:C:814:GLU:HB3	1:D:800:HIS:HD2	1.75	0.52
1:B:934:HIS:H	1:B:961:GLN:HE21	1.56	0.51
1:C:847:SER:HB2	1:C:997:PHE:CE2	2.45	0.51
1:D:803:ILE:HG22	1:D:813:SER:HB2	1.91	0.51
1:D:978:ASN:OD1	1:D:978:ASN:N	2.43	0.51
1:C:830:THR:N	2:C:29:PEG:H21	2.25	0.51
1:C:1057:ARG:HH21	1:D:1058:LEU:CB	2.24	0.51
1:D:929:ALA:HA	1:D:969:HIS:CD2	2.46	0.51
1:B:803:ILE:HB	1:F:817:MET:HE2	1.93	0.51
1:B:936:ILE:HD11	1:B:958:ILE:HG12	1.93	0.51
1:A:910:THR:OG1	1:B:1031:GLU:HG3	2.11	0.51
1:A:1040:PHE:CZ	1:F:1040:PHE:HB2	2.46	0.51
1:A:1050:LYS:O	1:A:1054:ILE:HG12	2.11	0.51
1:C:934:HIS:N	1:C:961:GLN:NE2	2.55	0.51
1:F:843:GLY:HA3	1:F:850:THR:HG23	1.93	0.51
1:F:933:VAL:HA	1:F:961:GLN:HE22	1.76	0.51
1:B:912:ASN:HA	1:F:1031:GLU:HB3	1.93	0.50
1:F:961:GLN:O	1:F:965:VAL:HG23	2.11	0.50
1:E:912:ASN:HA	1:D:1031:GLU:HB2	1.92	0.50
1:E:1031:GLU:HG3	1:C:910:THR:OG1	2.11	0.50
1:B:936:ILE:HG12	1:B:956:GLY:O	2.11	0.50
1:E:898:PHE:CE1	1:C:883:PRO:HG3	2.47	0.50
1:A:1061:LEU:HG	1:F:1061:LEU:HD21	1.92	0.50
1:B:1061:LEU:HD21	1:F:1061:LEU:CD2	2.39	0.50
1:B:978:ASN:HD22	1:B:978:ASN:H	1.59	0.50
1:E:844:GLU:H	1:E:850:THR:CG2	2.25	0.50
1:B:819:GLY:HA2	2:F:34:PEG:H11	1.93	0.50
1:E:952:ARG:HB3	2:E:21:PEG:H31	1.92	0.50
1:A:974:GLU:OE2	1:A:974:GLU:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:ARG:NH1	1:F:1058:LEU:HB3	2.27	0.49
1:B:1061:LEU:HD23	1:B:1062:GLU:N	2.27	0.49
1:B:819:GLY:H	2:F:34:PEG:H11	1.77	0.49
1:B:972:MET:HE1	1:B:976:SER:HB3	1.94	0.49
1:B:976:SER:N	1:B:977:THR:CA	2.73	0.49
1:C:956:GLY:HA2	1:D:1041:PHE:CE1	2.47	0.49
1:E:1051:LEU:HD11	1:C:1051:LEU:HD11	1.94	0.49
1:B:804:ARG:HG2	1:F:818:GLU:OE1	2.11	0.49
1:E:957:VAL:HG21	1:E:962:ILE:HD11	1.94	0.49
1:F:832:ASN:H	2:F:34:PEG:C4	2.25	0.49
7:A:134:HOH:O	1:F:1052:GLU:HA	2.12	0.49
1:F:877:GLN:HG2	1:F:878:SER:OG	2.13	0.49
1:C:1031:GLU:HG3	1:D:910:THR:OG1	2.12	0.49
1:F:1000:ASN:N	1:F:1000:ASN:HD22	2.10	0.48
1:E:1057:ARG:CZ	1:C:1058:LEU:HD23	2.44	0.48
1:F:878:SER:HA	2:F:30:PEG:H22	1.95	0.48
1:F:933:VAL:HG22	1:F:962:ILE:HG12	1.94	0.48
1:E:988:LYS:HD2	1:E:1029:GLY:O	2.13	0.48
1:A:936:ILE:HD11	1:A:958:ILE:HG12	1.95	0.48
1:E:1007:ASP:OD2	1:E:1011:ASN:HB2	2.12	0.48
1:B:900:THR:HG22	1:B:901:ALA:H	1.79	0.48
1:B:972:MET:CE	1:B:976:SER:HB3	2.43	0.48
1:E:954:HIS:HE1	2:E:21:PEG:H31	1.78	0.48
1:A:890:ALA:HB2	1:B:899:THR:OG1	2.13	0.48
1:A:1051:LEU:HD23	1:B:1050:LYS:CG	2.42	0.48
1:B:921:VAL:HB	7:B:182:HOH:O	2.13	0.48
1:B:988:LYS:NZ	1:B:1028:GLU:HG3	2.29	0.48
1:C:1040:PHE:CE2	1:D:1040:PHE:HB2	2.49	0.48
1:D:1031:GLU:HG2	1:D:1032:TRP:N	2.26	0.48
1:B:916:LYS:HD3	1:F:938:TYR:CG	2.48	0.48
1:B:1005:HIS:NE2	1:B:1015:THR:HG22	2.29	0.48
1:B:1036:PRO:HA	1:B:1039:ILE:HD12	1.96	0.48
1:C:939:GLN:HG2	1:C:952:ARG:O	2.14	0.48
1:B:843:GLY:HA3	1:B:850:THR:CG2	2.44	0.47
1:E:936:ILE:CD1	1:E:958:ILE:HG12	2.44	0.47
1:F:878:SER:H	2:F:30:PEG:C4	2.27	0.47
1:A:1058:LEU:HD21	1:F:1058:LEU:HD11	1.96	0.47
1:B:998:SER:HB2	1:B:1021:THR:HG22	1.96	0.47
1:D:949:ASN:C	1:D:951:ALA:H	2.17	0.47
1:D:948:GLY:HA2	1:D:949:ASN:HA	1.42	0.47
1:D:969:HIS:O	1:D:971:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1015:THR:HG22	1:D:1016:GLU:N	2.28	0.47
1:D:992:MET:HB3	1:D:1026:HIS:CD2	2.49	0.47
1:A:1058:LEU:HA	1:A:1061:LEU:HD23	1.95	0.47
1:F:998:SER:OG	1:F:999:HIS:CD2	2.67	0.47
1:A:1060:ALA:O	1:A:1061:LEU:HD13	2.14	0.47
1:E:1054:ILE:O	1:E:1058:LEU:HB2	2.14	0.47
1:D:961:GLN:HG2	7:D:257:HOH:O	2.13	0.47
1:A:1051:LEU:HD21	1:B:1051:LEU:CD1	2.44	0.47
1:E:872:ASP:OD1	1:C:865:ARG:NH1	2.48	0.47
1:A:877:GLN:HG2	1:A:878:SER:OG	2.15	0.46
1:A:927:LEU:HD12	1:A:927:LEU:HA	1.77	0.46
1:A:1063:GLN:N	1:A:1063:GLN:HE21	2.12	0.46
1:B:885:ASN:HB2	1:B:888:VAL:CG2	2.43	0.46
1:B:930:TRP:HZ2	1:B:1039:ILE:HG23	1.80	0.46
1:D:999:HIS:HD2	1:D:1000:ASN:O	1.98	0.46
1:B:915:ARG:HA	1:B:915:ARG:HD2	1.44	0.46
1:E:843:GLY:HA3	1:E:850:THR:HG22	1.97	0.46
1:E:1007:ASP:C	1:E:1009:GLU:H	2.17	0.46
1:A:843:GLY:HA3	1:A:850:THR:CG2	2.45	0.46
1:F:936:ILE:HD13	1:F:956:GLY:O	2.15	0.46
1:A:1045:ALA:HA	2:A:17:PEG:H22	1.98	0.46
1:E:899:THR:OG1	1:C:890:ALA:HB2	2.16	0.46
1:C:903:LEU:HA	1:D:898:PHE:O	2.15	0.46
1:A:1058:LEU:HD21	1:B:1058:LEU:CD2	2.44	0.46
1:C:832:ASN:N	1:C:833:PRO:HD3	2.32	0.45
1:F:1020:TYR:HE1	2:F:5:PEG:H21	1.81	0.45
1:F:1044:ALA:O	1:F:1048:ARG:HG3	2.16	0.45
1:E:900:THR:HG23	1:D:905:SER:HG	1.80	0.45
1:C:961:GLN:O	1:C:965:VAL:HG23	2.17	0.45
1:B:932:ASP:OD2	1:B:969:HIS:HE1	1.99	0.45
1:B:978:ASN:ND2	1:B:978:ASN:N	2.64	0.45
1:C:978:ASN:HB3	7:C:239:HOH:O	2.16	0.45
1:A:1063:GLN:N	1:A:1063:GLN:NE2	2.64	0.45
1:E:910:THR:HG23	1:D:897:ARG:HD3	1.99	0.45
2:C:29:PEG:H41	1:D:819:GLY:N	2.26	0.45
1:D:971:LEU:HD22	1:D:971:LEU:H	1.81	0.45
1:D:945:GLN:HB2	1:D:946:LEU:HD12	1.98	0.45
1:A:857:TYR:HB2	1:A:866:ARG:N	2.32	0.45
1:B:819:GLY:H	2:F:34:PEG:C1	2.28	0.45
1:E:810:ASN:N	1:E:810:ASN:ND2	2.64	0.44
1:C:961:GLN:HG3	1:C:962:ILE:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:GLU:O	1:B:826:LYS:HE2	2.17	0.44
1:A:823:PHE:CE1	1:B:846:THR:HA	2.53	0.44
1:B:813:SER:OG	1:F:817:MET:HB3	2.17	0.44
1:B:877:GLN:O	1:B:878:SER:HB2	2.17	0.44
1:F:1020:TYR:CE1	2:F:5:PEG:H21	2.52	0.44
1:F:1034:VAL:O	1:F:1036:PRO:HD3	2.18	0.44
1:B:932:ASP:OD2	1:B:969:HIS:CE1	2.71	0.44
1:E:944:VAL:HG13	1:E:948:GLY:HA2	2.00	0.44
1:C:817:MET:HB3	1:D:813:SER:OG	2.18	0.44
1:A:1005:HIS:HE1	1:A:1015:THR:CG2	2.28	0.44
1:E:956:GLY:HA2	1:C:1041:PHE:CE1	2.53	0.44
1:C:844:GLU:N	1:C:850:THR:CG2	2.80	0.44
1:B:843:GLY:HA3	1:B:850:THR:HG22	2.00	0.44
1:E:857:TYR:HD2	1:E:866:ARG:O	2.00	0.43
1:A:992:MET:HB2	1:A:1026:HIS:NE2	2.33	0.43
1:E:844:GLU:N	1:E:850:THR:HG21	2.34	0.43
1:C:1013:THR:OG1	1:C:1014:THR:N	2.51	0.43
1:C:1057:ARG:NH2	1:D:1058:LEU:HB3	2.33	0.43
1:B:934:HIS:O	1:B:957:VAL:HG12	2.18	0.43
1:C:969:HIS:HD2	7:C:106:HOH:O	2.01	0.43
1:E:820:GLU:HB2	2:E:18:PEG:H41	2.00	0.43
1:E:896:ASN:HB3	1:C:883:PRO:HD2	2.01	0.43
1:D:933:VAL:HA	1:D:961:GLN:NE2	2.30	0.43
1:F:895:SER:HB3	7:F:282:HOH:O	2.18	0.43
1:A:1001:GLU:HB3	1:A:1019:VAL:HG23	2.01	0.43
1:B:836:GLN:O	1:B:837:ARG:HB3	2.19	0.43
1:C:927:LEU:HD12	1:C:927:LEU:HA	1.85	0.43
1:C:908:ILE:HG13	1:D:900:THR:HG21	1.99	0.42
1:D:840:PHE:O	1:D:853:GLN:HA	2.18	0.42
1:D:944:VAL:O	1:D:948:GLY:HA3	2.19	0.42
1:A:821:TYR:OH	1:F:812:ARG:HD3	2.19	0.42
1:A:961:GLN:HG2	7:A:148:HOH:O	2.18	0.42
1:B:1058:LEU:O	1:B:1062:GLU:HG3	2.19	0.42
1:D:1000:ASN:HD22	1:D:1018:PRO:HA	1.84	0.42
1:A:999:HIS:HD2	1:A:1000:ASN:O	2.02	0.42
1:E:1007:ASP:C	1:E:1009:GLU:N	2.72	0.42
1:B:919:PRO:HB3	1:F:936:ILE:HG13	2.01	0.42
1:A:936:ILE:HD12	1:F:919:PRO:CB	2.47	0.42
1:B:996:VAL:CG2	1:B:997:PHE:N	2.82	0.42
1:B:1018:PRO:HG2	1:F:812:ARG:NH2	2.35	0.42
1:F:918:GLU:HA	1:F:919:PRO:HD2	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1002:ILE:O	1:E:1002:ILE:HG12	2.19	0.42
1:D:1007:ASP:OD1	1:D:1009:GLU:O	2.36	0.42
1:B:819:GLY:N	2:F:34:PEG:H11	2.33	0.42
1:B:972:MET:HE1	1:B:1032:TRP:HH2	1.84	0.42
1:D:843:GLY:HA3	1:D:850:THR:HG23	2.02	0.42
1:A:1047:GLN:O	1:A:1051:LEU:HD13	2.20	0.42
3:A:35:TAM:H11	3:A:35:TAM:O6	2.19	0.42
1:C:831:ASP:HB2	2:C:29:PEG:H11	2.02	0.42
1:D:1007:ASP:OD1	1:D:1007:ASP:N	2.52	0.42
1:A:900:THR:HG21	1:F:1035:ARG:HH12	1.84	0.42
1:A:1054:ILE:HG21	1:B:1054:ILE:HD13	2.02	0.42
1:B:927:LEU:HD12	1:B:1046:TYR:HA	2.01	0.42
1:E:922:PHE:HA	1:D:937:MET:SD	2.60	0.42
1:E:954:HIS:CE1	2:E:21:PEG:H31	2.54	0.42
1:A:883:PRO:HD3	1:B:898:PHE:CE2	2.55	0.41
1:C:1051:LEU:O	1:C:1055:GLU:HG3	2.19	0.41
1:C:1054:ILE:HD11	1:D:1055:GLU:CG	2.50	0.41
3:A:35:TAM:H52	3:A:35:TAM:H12	1.72	0.41
1:D:949:ASN:C	1:D:951:ALA:N	2.74	0.41
1:F:983:VAL:HG13	1:F:1038:GLY:HA3	2.02	0.41
1:A:857:TYR:HB2	1:A:866:ARG:H	1.84	0.41
1:E:802:THR:HA	1:D:816:LEU:O	2.19	0.41
1:D:1023:VAL:HG12	1:D:1025:ILE:HD13	2.00	0.41
1:E:924:ASP:O	1:E:928:ASP:OD1	2.38	0.41
1:E:936:ILE:HD12	1:E:958:ILE:HG12	2.01	0.41
1:D:826:LYS:HB2	1:D:838:ILE:HG13	2.01	0.41
1:F:844:GLU:OE2	1:F:844:GLU:N	2.50	0.41
1:E:886:ASP:O	1:E:888:VAL:HG12	2.20	0.41
2:E:22:PEG:H21	1:C:819:GLY:HA2	2.02	0.41
1:C:992:MET:HG2	1:C:1025:ILE:HB	2.02	0.41
1:C:1050:LYS:O	1:C:1054:ILE:HD13	2.19	0.41
1:F:983:VAL:O	1:F:1034:VAL:HA	2.20	0.41
1:F:998:SER:OG	1:F:999:HIS:HD2	2.03	0.41
1:A:963:ARG:O	1:A:967:ILE:HG13	2.21	0.41
1:E:803:ILE:CG2	7:E:207:HOH:O	2.67	0.41
1:E:956:GLY:HA2	1:C:1041:PHE:CD1	2.56	0.41
1:B:1034:VAL:HB	1:B:1039:ILE:HD11	2.03	0.41
1:A:989:TYR:HA	1:A:990:PRO:HD3	1.78	0.41
1:E:961:GLN:O	1:E:965:VAL:HG23	2.21	0.41
1:B:976:SER:OG	1:B:1032:TRP:CH2	2.69	0.41
1:B:982:ALA:O	1:B:985:CYS:SG	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1028:GLU:HG2	1:B:1029:GLY:N	2.35	0.41
1:E:992:MET:CE	1:E:1025:ILE:HG21	2.51	0.41
1:C:887:ASN:O	3:C:28:TAM:H61	2.21	0.41
1:C:936:ILE:HD11	1:C:958:ILE:HG12	2.03	0.41
1:D:857:TYR:N	1:D:857:TYR:CD2	2.89	0.41
1:D:900:THR:CG2	1:D:901:ALA:N	2.82	0.41
1:D:941:LEU:HD23	1:D:941:LEU:HA	1.92	0.41
1:F:857:TYR:HD2	1:F:866:ARG:O	2.03	0.41
1:A:973:ASP:OD1	1:A:973:ASP:N	2.54	0.41
1:C:947:LYS:HD3	1:C:951:ALA:HB3	2.03	0.41
1:B:947:LYS:O	1:B:947:LYS:HG2	2.21	0.40
1:B:978:ASN:HD22	1:B:978:ASN:N	2.19	0.40
1:E:829:PRO:HB2	1:E:833:PRO:HA	2.03	0.40
1:A:900:THR:HG21	1:F:1035:ARG:NH1	2.36	0.40
1:E:845:GLY:H	1:E:850:THR:HG21	1.87	0.40
1:D:934:HIS:H	1:D:961:GLN:HE22	1.61	0.40
1:A:900:THR:CG2	1:B:905:SER:OG	2.68	0.40
1:E:1044:ALA:O	1:E:1048:ARG:HG3	2.22	0.40
1:C:944:VAL:HA	1:C:951:ALA:HB2	2.02	0.40
1:F:906:ASN:HA	1:F:907:PRO:HD3	1.94	0.40
1:D:989:TYR:O	1:D:1028:GLU:HG2	2.22	0.40
1:F:843:GLY:HA3	1:F:850:THR:CG2	2.52	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	250/275 (91%)	237 (95%)	12 (5%)	1 (0%)	34 57
1	B	247/275 (90%)	237 (96%)	10 (4%)	0	100 100
1	C	246/275 (90%)	237 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	246/275 (90%)	238 (97%)	8 (3%)	0	100	100
1	E	251/275 (91%)	241 (96%)	10 (4%)	0	100	100
1	F	251/275 (91%)	244 (97%)	7 (3%)	0	100	100
All	All	1491/1650 (90%)	1434 (96%)	56 (4%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	975	ASN

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	215/230 (94%)	194 (90%)	21 (10%)	8	15
1	B	214/230 (93%)	194 (91%)	20 (9%)	9	17
1	C	213/230 (93%)	199 (93%)	14 (7%)	16	33
1	D	211/230 (92%)	192 (91%)	19 (9%)	9	18
1	E	215/230 (94%)	196 (91%)	19 (9%)	10	19
1	F	216/230 (94%)	206 (95%)	10 (5%)	27	51
All	All	1284/1380 (93%)	1181 (92%)	103 (8%)	12	24

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	802	THR
1	A	844	GLU
1	A	850	THR
1	A	856	LEU
1	A	900	THR
1	A	920	VAL
1	A	927	LEU

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Mol	Chain	Res	Type
1	A	942	ASP
1	A	961	GLN
1	A	974	GLU
1	A	995	THR
1	A	1001	GLU
1	A	1006	THR
1	A	1013	THR
1	A	1014	THR
1	A	1015	THR
1	A	1031	GLU
1	A	1055	GLU
1	A	1058	LEU
1	A	1061	LEU
1	A	1063	GLN
1	B	850	THR
1	B	900	THR
1	B	910	THR
1	B	915	ARG
1	B	920	VAL
1	B	936	ILE
1	B	942	ASP
1	B	946	LEU
1	B	974	GLU
1	B	976	SER
1	B	977	THR
1	B	978	ASN
1	B	980	ARG
1	B	993	THR
1	B	995	THR
1	B	996	VAL
1	B	1000	ASN
1	B	1021	THR
1	B	1031	GLU
1	B	1061	LEU
1	E	810	ASN
1	E	888	VAL
1	E	900	THR
1	E	910	THR
1	E	923	ASP
1	E	927	LEU
1	E	936	ILE
1	E	942	ASP

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Mol	Chain	Res	Type
1	E	961	GLN
1	E	971	LEU
1	E	992	MET
1	E	995	THR
1	E	996	VAL
1	E	1000	ASN
1	E	1002	ILE
1	E	1031	GLU
1	E	1051	LEU
1	E	1058	LEU
1	E	1063	GLN
1	C	801	VAL
1	C	802	THR
1	C	900	THR
1	C	910	THR
1	C	927	LEU
1	C	936	ILE
1	C	957	VAL
1	C	961	GLN
1	C	985	CYS
1	C	987	ASP
1	C	1009	GLU
1	C	1013	THR
1	C	1014	THR
1	C	1031	GLU
1	D	801	VAL
1	D	816	LEU
1	D	850	THR
1	D	895	SER
1	D	910	THR
1	D	927	LEU
1	D	939	GLN
1	D	960	GLN
1	D	961	GLN
1	D	971	LEU
1	D	978	ASN
1	D	1002	ILE
1	D	1004	GLU
1	D	1006	THR
1	D	1009	GLU
1	D	1011	ASN
1	D	1013	THR

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Mol	Chain	Res	Type
1	D	1031	GLU
1	D	1058	LEU
1	F	850	THR
1	F	900	THR
1	F	927	LEU
1	F	936	ILE
1	F	952	ARG
1	F	983	VAL
1	F	995	THR
1	F	996	VAL
1	F	1002	ILE
1	F	1058	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	860	ASN
1	A	885	ASN
1	A	912	ASN
1	A	954	HIS
1	A	961	GLN
1	A	969	HIS
1	A	1005	HIS
1	A	1063	GLN
1	B	896	ASN
1	B	912	ASN
1	B	934	HIS
1	B	954	HIS
1	B	960	GLN
1	B	961	GLN
1	B	969	HIS
1	B	978	ASN
1	E	832	ASN
1	E	912	ASN
1	E	954	HIS
1	E	961	GLN
1	C	961	GLN
1	C	975	ASN
1	C	999	HIS
1	C	1011	ASN
1	D	800	HIS
1	D	860	ASN

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Mol	Chain	Res	Type
1	D	912	ASN
1	D	945	GLN
1	D	961	GLN
1	D	978	ASN
1	D	1000	ASN
1	D	1026	HIS
1	F	853	GLN
1	F	877	GLN
1	F	912	ASN
1	F	961	GLN
1	F	1000	ASN
1	F	1026	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 13 are monoatomic - leaving 21 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	$\# Z > 2$
2	PEG	C	29	-	6,6,6	0.49	0	5,5,5	1.43	0
2	PEG	A	2	-	6,6,6	0.50	0	5,5,5	1.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TAM	A	35	-	7,10,10	0.65	0	9,12,12	1.66	3 (33%)
3	TAM	C	28	-	7,10,10	0.60	0	9,12,12	1.68	2 (22%)
3	TAM	A	32	-	7,10,10	0.61	0	9,12,12	1.41	3 (33%)
2	PEG	A	17	-	6,6,6	0.48	0	5,5,5	1.50	0
2	PEG	F	24	-	6,6,6	0.49	0	5,5,5	1.55	0
2	PEG	E	6	-	6,6,6	0.50	0	5,5,5	1.50	0
2	PEG	E	27	-	6,6,6	0.49	0	5,5,5	1.39	0
2	PEG	E	21	-	6,6,6	0.51	0	5,5,5	1.44	0
2	PEG	E	18	-	6,6,6	0.49	0	5,5,5	1.39	0
2	PEG	F	5	-	6,6,6	0.51	0	5,5,5	1.50	0
2	PEG	E	33	-	6,6,6	0.49	0	5,5,5	1.44	0
2	PEG	C	14	-	6,6,6	0.48	0	5,5,5	1.41	0
2	PEG	F	30	-	6,6,6	0.49	0	5,5,5	1.48	0
2	PEG	B	13	-	6,6,6	0.49	0	5,5,5	1.48	0
2	PEG	E	22	-	6,6,6	0.50	0	5,5,5	1.39	0
2	PEG	D	15	-	6,6,6	0.49	0	5,5,5	1.43	0
2	PEG	F	34	-	6,6,6	0.49	0	5,5,5	1.54	1 (20%)
2	PEG	C	3	-	6,6,6	0.50	0	5,5,5	1.45	0
2	PEG	E	16	-	6,6,6	0.50	0	5,5,5	1.41	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
2	PEG	C	29	-	-	2/4/4/4	-
2	PEG	A	2	-	-	2/4/4/4	-
3	TAM	A	35	-	-	7/12/12/12	-
3	TAM	C	28	-	-	4/12/12/12	-
3	TAM	A	32	-	-	6/12/12/12	-
2	PEG	A	17	-	-	2/4/4/4	-
2	PEG	F	24	-	-	2/4/4/4	-
2	PEG	E	6	-	-	2/4/4/4	-
2	PEG	E	27	-	-	2/4/4/4	-
2	PEG	E	21	-	-	1/4/4/4	-
2	PEG	E	18	-	-	1/4/4/4	-
2	PEG	F	5	-	-	2/4/4/4	-
2	PEG	E	33	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	C	14	-	-	2/4/4/4	-
2	PEG	F	30	-	-	1/4/4/4	-
2	PEG	B	13	-	-	2/4/4/4	-
2	PEG	E	22	-	-	0/4/4/4	-
2	PEG	D	15	-	-	2/4/4/4	-
2	PEG	F	34	-	-	3/4/4/4	-
2	PEG	C	3	-	-	4/4/4/4	-
2	PEG	E	16	-	-	2/4/4/4	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	28	TAM	O5-C5-C2	3.17	119.86	111.39
3	A	35	TAM	O6-C6-C3	2.82	118.91	111.39
3	C	28	TAM	O6-C6-C3	2.71	118.63	111.39
3	A	35	TAM	O5-C5-C2	2.40	117.81	111.39
3	A	32	TAM	O6-C6-C3	2.34	117.63	111.39
3	A	32	TAM	O4-C4-C1	2.26	117.44	111.39
3	A	32	TAM	O5-C5-C2	2.24	117.39	111.39
2	F	34	PEG	O2-C2-C1	2.09	119.24	110.07
3	A	35	TAM	O4-C4-C1	2.07	116.93	111.39

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	32	TAM	N-C-C1-C4
3	A	32	TAM	C1-C-C2-C5
3	A	32	TAM	C3-C-C2-C5
3	A	32	TAM	N-C-C2-C5
3	A	32	TAM	C-C3-C6-O6
3	A	35	TAM	C2-C-C1-C4
3	A	35	TAM	C3-C-C1-C4
3	A	35	TAM	N-C-C1-C4
3	A	35	TAM	N-C-C3-C6
3	C	28	TAM	C2-C-C1-C4
3	C	28	TAM	C3-C-C1-C4
3	C	28	TAM	N-C-C1-C4
3	C	28	TAM	C-C2-C5-O5

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Mol	Chain	Res	Type	Atoms
2	A	2	PEG	C1-C2-O2-C3
2	E	16	PEG	O2-C3-C4-O4
2	C	29	PEG	O2-C3-C4-O4
2	F	24	PEG	O1-C1-C2-O2
2	F	24	PEG	O2-C3-C4-O4
2	A	17	PEG	O2-C3-C4-O4
2	E	21	PEG	O2-C3-C4-O4
2	C	14	PEG	O2-C3-C4-O4
2	B	13	PEG	C4-C3-O2-C2
3	A	35	TAM	C1-C-C3-C6
3	A	35	TAM	C2-C-C3-C6
2	E	27	PEG	O1-C1-C2-O2
2	E	27	PEG	O2-C3-C4-O4
2	F	30	PEG	O2-C3-C4-O4
2	F	34	PEG	O1-C1-C2-O2
3	A	32	TAM	C-C1-C4-O4
2	F	5	PEG	O1-C1-C2-O2
2	B	13	PEG	O2-C3-C4-O4
2	C	14	PEG	O1-C1-C2-O2
2	F	5	PEG	O2-C3-C4-O4
2	E	33	PEG	C4-C3-O2-C2
2	E	6	PEG	C4-C3-O2-C2
2	E	18	PEG	O1-C1-C2-O2
2	E	16	PEG	C1-C2-O2-C3
3	A	35	TAM	C-C1-C4-O4
2	A	2	PEG	C4-C3-O2-C2
2	E	6	PEG	C1-C2-O2-C3
2	F	34	PEG	C4-C3-O2-C2
2	D	15	PEG	C4-C3-O2-C2
2	A	17	PEG	O1-C1-C2-O2
2	C	3	PEG	O1-C1-C2-O2
2	E	33	PEG	O1-C1-C2-O2
2	E	33	PEG	C1-C2-O2-C3
2	C	3	PEG	C1-C2-O2-C3
2	D	15	PEG	O2-C3-C4-O4
2	C	3	PEG	O2-C3-C4-O4
2	C	29	PEG	C1-C2-O2-C3
2	F	34	PEG	O2-C3-C4-O4
2	C	3	PEG	C4-C3-O2-C2

There are no ring outliers.

12 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	29	PEG	5	0
2	A	2	PEG	4	0
3	A	35	TAM	3	0
3	C	28	TAM	1	0
2	A	17	PEG	1	0
2	E	6	PEG	1	0
2	E	21	PEG	8	0
2	E	18	PEG	1	0
2	F	5	PEG	2	0
2	F	30	PEG	6	0
2	E	22	PEG	3	0
2	F	34	PEG	11	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	256/275 (93%)	0.07	10 (3%) 39 32	24, 49, 81, 147	26 (10%)
1	B	255/275 (92%)	0.18	11 (4%) 35 28	25, 50, 95, 143	41 (16%)
1	C	254/275 (92%)	-0.06	7 (2%) 53 46	26, 47, 79, 123	14 (5%)
1	D	252/275 (91%)	0.18	13 (5%) 27 21	23, 55, 90, 116	44 (17%)
1	E	257/275 (93%)	0.08	11 (4%) 35 28	24, 53, 93, 131	44 (17%)
1	F	257/275 (93%)	0.04	7 (2%) 54 48	26, 52, 82, 127	34 (13%)
All	All	1531/1650 (92%)	0.08	59 (3%) 39 32	23, 51, 88, 147	203 (13%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1056	ALA	7.8
1	D	1061	LEU	7.3
1	A	1058	LEU	5.1
1	E	1061	LEU	4.9
1	F	1061	LEU	4.6
1	A	1061	LEU	4.4
1	C	1061	LEU	4.4
1	B	1058	LEU	4.3
1	E	1058	LEU	4.2
1	D	1062	GLU	4.1
1	F	1054	ILE	4.0
1	C	1063	GLN	4.0
1	B	1055	GLU	3.9
1	A	1054	ILE	3.7
1	F	1063	GLN	3.7
1	E	1003	VAL	3.7
1	B	1060	ALA	3.6
1	D	1051	LEU	3.5
1	A	1062	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	1057	ARG	3.4
1	F	1058	LEU	3.4
1	B	1054	ILE	3.4
1	D	1056	ALA	3.3
1	B	1059	SER	3.2
1	A	1063	GLN	3.2
1	A	1056	ALA	3.1
1	E	977	THR	3.1
1	C	1060	ALA	3.1
1	A	1057	ARG	3.0
1	D	1046	TYR	3.0
1	F	1057	ARG	2.9
1	D	1060	ALA	2.9
1	E	1062	GLU	2.9
1	A	1060	ALA	2.9
1	C	1058	LEU	2.9
1	B	1061	LEU	2.8
1	C	805	ALA	2.7
1	E	1057	ARG	2.7
1	E	1060	ALA	2.6
1	D	1054	ILE	2.6
1	B	1052	GLU	2.6
1	B	1062	GLU	2.6
1	C	811	ILE	2.5
1	D	972	MET	2.5
1	E	1063	GLN	2.5
1	D	1053	ARG	2.5
1	C	1056	ALA	2.4
1	A	1051	LEU	2.4
1	B	1057	ARG	2.4
1	A	1055	GLU	2.4
1	B	929	ALA	2.3
1	E	1050	LYS	2.3
1	D	979	CYS	2.3
1	E	1002	ILE	2.3
1	E	1052	GLU	2.2
1	F	1060	ALA	2.2
1	F	1051	LEU	2.1
1	D	978	ASN	2.1
1	D	949	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PEG	E	16	7/7	0.49	0.22	94,97,98,99	0
3	TAM	A	32	11/11	0.69	0.24	71,74,75,76	2
2	PEG	C	3	7/7	0.70	0.33	71,75,79,80	0
2	PEG	F	24	7/7	0.74	0.22	86,87,88,88	0
2	PEG	D	15	7/7	0.74	0.30	63,67,68,68	0
2	PEG	E	33	7/7	0.76	0.36	80,81,83,83	3
2	PEG	B	13	7/7	0.78	0.25	75,78,80,80	2
2	PEG	A	17	7/7	0.81	0.38	52,60,71,72	0
2	PEG	E	27	7/7	0.82	0.42	78,78,79,79	5
3	TAM	A	35	11/11	0.82	0.26	56,61,64,66	0
2	PEG	F	30	7/7	0.83	0.29	29,47,55,57	0
3	TAM	C	28	11/11	0.83	0.24	59,64,66,66	0
2	PEG	C	29	7/7	0.86	0.37	66,73,78,79	0
2	PEG	C	14	7/7	0.87	0.16	66,69,72,73	0
2	PEG	E	6	7/7	0.89	0.23	73,73,75,75	5
2	PEG	A	2	7/7	0.90	0.18	42,48,57,60	0
2	PEG	E	21	7/7	0.91	0.20	43,48,56,59	0
2	PEG	F	5	7/7	0.92	0.41	50,57,58,58	0
2	PEG	E	22	7/7	0.92	0.31	59,60,62,63	0
4	CL	C	12	1/1	0.93	0.20	66,66,66,66	0
2	PEG	E	18	7/7	0.94	0.41	45,48,52,52	0
4	CL	D	41	1/1	0.94	0.11	45,45,45,45	0
2	PEG	F	34	7/7	0.96	0.21	51,52,60,62	0
5	BR	B	39	1/1	0.96	0.07	77,77,77,77	1
4	CL	E	42	1/1	0.97	0.07	61,61,61,61	0
5	BR	B	11	1/1	0.98	0.06	78,78,78,78	0
4	CL	A	40	1/1	0.98	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	BR	C	8	1/1	0.98	0.06	64,64,64,64	0
5	BR	F	37	1/1	0.98	0.11	68,68,68,68	0
5	BR	E	36	1/1	0.99	0.09	61,61,61,61	0
5	BR	B	38	1/1	0.99	0.06	66,66,66,66	0
4	CL	D	10	1/1	0.99	0.17	42,42,42,42	0
6	CA	F	1	1/1	0.99	0.21	44,44,44,44	0
4	CL	C	9	1/1	1.00	0.11	41,41,41,41	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.