Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:43 pm GMT

PDB ID	:	1TEX
Title	:	Mycobacterium smegmatis Stf0 Sulfotransferase with Trehalose
Authors	:	Mougous, J.D.; Petzold, C.J.; Senaratne, R.H.; Lee, D.H.; Akey, D.L.; Lin, F.L.; Munchel, S.E.; Pratt, M.R.; Riley, L.W.; Leary, J.A.; Berger, J.M.; Bertozzi, C.R.
Deposited on	:	2004-05-25
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

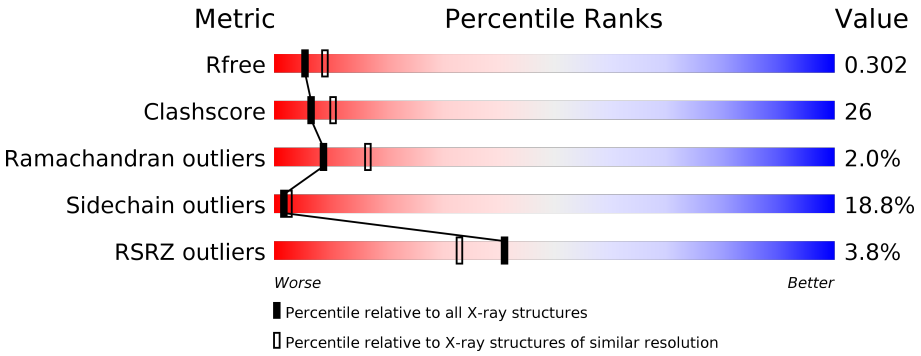
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	287	7% 43% 30% 11% 17%
1	B	287	2% 44% 30% 10% 15%
1	C	287	% 54% 24% 7% 15%
1	D	287	2% 53% 28% 6% 14%

2 Entry composition

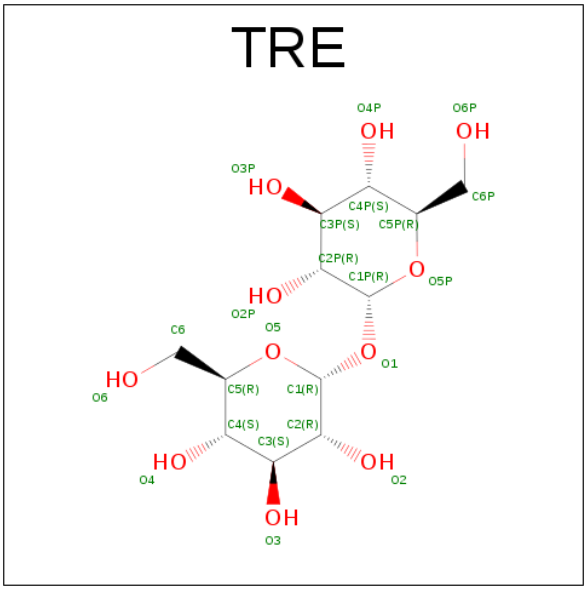
There are 3 unique types of molecules in this entry. The entry contains 7919 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Stf0 Sulfotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1794	1145	312	334	3			
1	B	243	Total	C	N	O	S	0	0	0
			1853	1183	327	340	3			
1	C	244	Total	C	N	O	S	0	0	0
			1883	1205	326	349	3			
1	D	247	Total	C	N	O	S	0	0	0
			1887	1212	329	343	3			

- Molecule 2 is TREHALOSE (three-letter code: TRE) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 23 12 11	0	0
2	D	1	Total C O 23 12 11	0	0

- Molecule 3 is water.

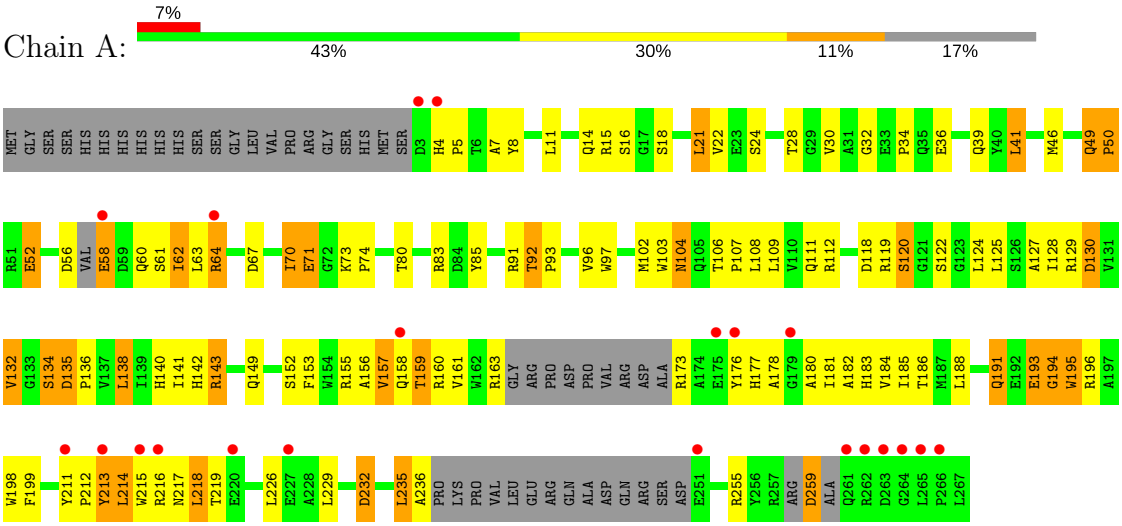
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	63	Total O 63 63	0	0
3	B	113	Total O 113 113	0	0
3	C	138	Total O 138 138	0	0
3	D	96	Total O 96 96	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

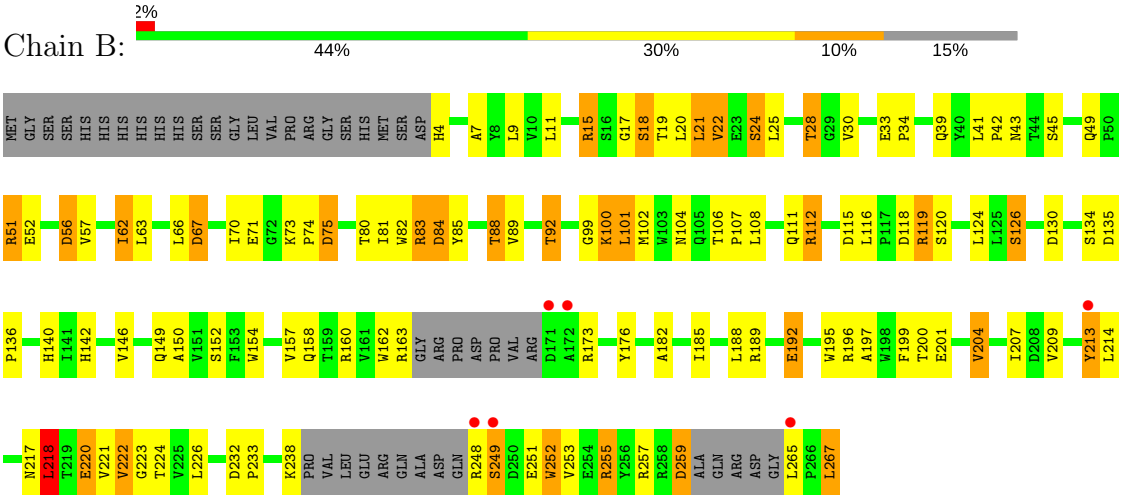
• Molecule 1: Stf0 Sulfotransferase

Chain A:



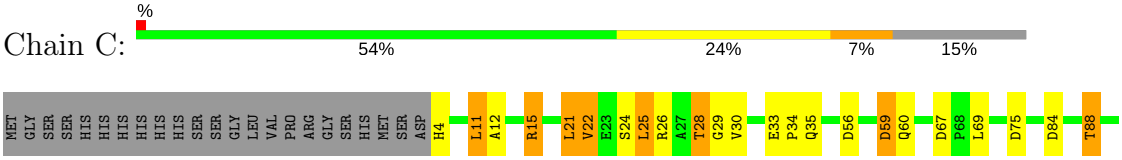
• Molecule 1: Stf0 Sulfotransferase

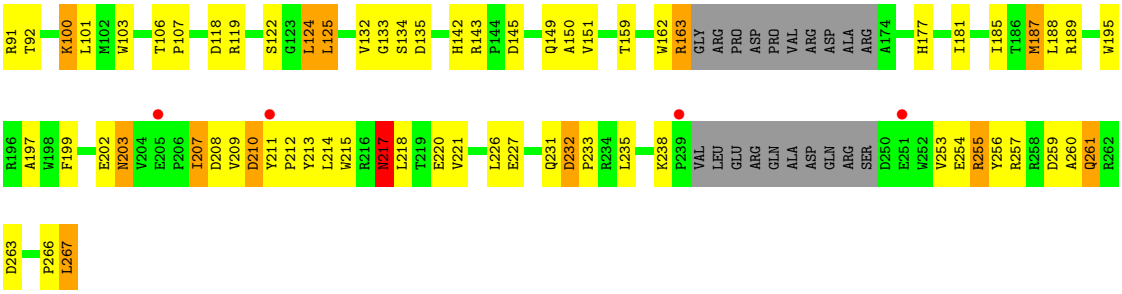
Chain B:



• Molecule 1: Stf0 Sulfotransferase

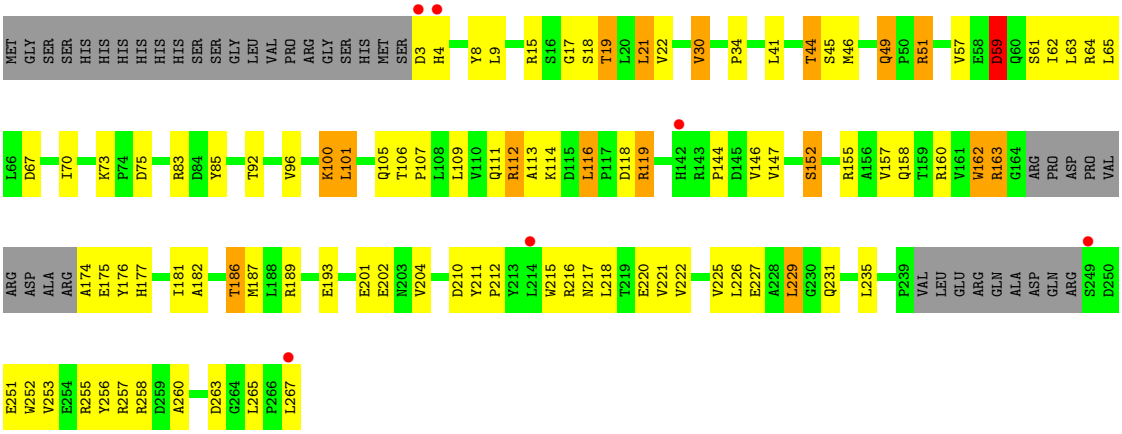
Chain C:





• Molecule 1: Stf0 Sulfotransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	101.93Å 101.93Å 228.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.60 14.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.60) 97.6 (14.99-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.218 , 0.274 0.254 , 0.302	Depositor DCC
R_{free} test set	2104 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7919	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TRE

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	0.75	0/1839	0.83	5/2520 (0.2%)
1	B	0.85	1/1899 (0.1%)	0.89	4/2601 (0.2%)
1	C	0.91	0/1933	1.01	11/2650 (0.4%)
1	D	0.86	2/1939 (0.1%)	0.90	4/2662 (0.2%)
All	All	0.85	3/7610 (0.0%)	0.91	24/10433 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	85	TYR	CD2-CE2	5.44	1.47	1.39
1	B	252	TRP	CB-CG	5.43	1.60	1.50
1	D	162	TRP	CB-CG	-5.24	1.40	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	75	ASP	CB-CG-OD2	10.32	127.58	118.30
1	B	84	ASP	CB-CG-OD2	7.61	125.15	118.30
1	D	59	ASP	CB-CG-OD2	7.30	124.87	118.30
1	C	84	ASP	CB-CG-OD2	6.96	124.57	118.30
1	C	259	ASP	CB-CG-OD2	6.84	124.46	118.30
1	D	67	ASP	CB-CG-OD2	6.64	124.27	118.30
1	B	67	ASP	CB-CG-OD2	6.59	124.23	118.30
1	C	75	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	A	259	ASP	CB-CG-OD2	6.04	123.74	118.30
1	C	263	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	67	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	56	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	135	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	59	ASP	CB-CG-OD2	5.62	123.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	124	LEU	CB-CG-CD2	5.59	120.51	111.00
1	D	75	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	135	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	145	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	56	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	67	ASP	CB-CG-OD2	5.43	123.19	118.30
1	D	263	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	232	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	75	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	130	ASP	CB-CG-OD2	5.13	122.92	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1794	0	1647	93	0
1	B	1853	0	1765	121	0
1	C	1883	0	1801	101	0
1	D	1887	0	1805	74	0
2	A	23	0	22	5	0
2	B	23	0	22	2	0
2	C	23	0	22	1	0
2	D	23	0	22	0	0
3	A	63	0	0	24	0
3	B	113	0	0	38	0
3	C	138	0	0	29	0
3	D	96	0	0	18	0
All	All	7919	0	7106	384	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 26.

All (384) 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:C:122:SER:HB3	3:C:580:HOH:O	1.29	1.28
1:D:44:THR:CG2	1:D:46:MET:HB2	1.75	1.16
1:C:15:ARG:HG3	1:C:15:ARG:HH11	1.06	1.11
1:C:28:THR:HG22	1:C:30:VAL:H	1.18	1.07
1:B:249:SER:HA	3:B:513:HOH:O	1.53	1.06
1:B:257:ARG:NH1	1:C:197:ALA:HB2	1.75	1.00
1:B:74:PRO:HD2	3:B:557:HOH:O	1.64	0.97
1:B:49:GLN:HE22	1:B:70:ILE:H	1.13	0.95
1:D:158:GLN:HE22	1:D:175:GLU:H	0.97	0.94
1:B:51:ARG:HG3	1:B:51:ARG:HH11	1.29	0.94
1:A:156:ALA:HA	1:A:159:THR:CG2	1.96	0.94
1:A:104:ASN:HB3	1:A:191:GLN:HE21	1.30	0.94
1:D:44:THR:HG22	1:D:46:MET:HB2	1.51	0.91
1:B:238:LYS:HA	3:B:508:HOH:O	1.69	0.91
1:C:217:ASN:HD22	1:C:217:ASN:N	1.68	0.90
1:A:85:TYR:CE2	3:A:524:HOH:O	2.26	0.88
1:B:207:ILE:HG22	1:B:207:ILE:O	1.73	0.88
1:C:15:ARG:NH1	1:C:15:ARG:HG3	1.89	0.87
1:C:25:LEU:O	1:C:28:THR:HB	1.75	0.87
1:C:91:ARG:HD3	3:C:540:HOH:O	1.73	0.85
1:D:19:THR:HG22	1:D:100:LYS:HE3	1.57	0.84
1:C:28:THR:HG23	1:C:30:VAL:HB	1.60	0.83
1:D:44:THR:HG21	1:D:46:MET:HB2	1.58	0.83
1:C:15:ARG:HH11	1:C:15:ARG:CG	1.91	0.83
1:C:142:HIS:HE1	1:C:208:ASP:OD2	1.62	0.82
1:A:103:TRP:HB3	1:A:191:GLN:HG2	1.61	0.81
1:A:156:ALA:HA	1:A:159:THR:HG22	1.62	0.81
1:B:73:LYS:HB2	3:B:557:HOH:O	1.79	0.81
1:C:266:PRO:HA	3:C:606:HOH:O	1.81	0.81
1:B:20:LEU:O	1:B:24:SER:HB2	1.81	0.80
1:B:119:ARG:HH12	1:B:126:SER:HB2	1.48	0.79
1:B:118:ASP:O	1:B:119:ARG:C	2.20	0.79
1:A:122:SER:HB3	3:A:549:HOH:O	1.83	0.79
1:A:91:ARG:CB	3:A:563:HOH:O	2.30	0.78
1:B:49:GLN:NE2	1:B:70:ILE:H	1.80	0.78
1:B:257:ARG:HH11	1:C:197:ALA:HB2	1.48	0.78
1:D:44:THR:HG22	1:D:46:MET:N	1.98	0.78
1:C:21:LEU:HD22	1:C:25:LEU:HD22	1.66	0.77
1:A:85:TYR:HB2	3:A:547:HOH:O	1.83	0.77
1:D:30:VAL:HG13	1:D:231:GLN:HG3	1.66	0.77
1:B:22:VAL:HG11	1:B:100:LYS:HZ2	1.50	0.76
1:C:28:THR:HG22	1:C:30:VAL:N	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:PRO:HD2	3:D:565:HOH:O	1.85	0.75
1:B:51:ARG:HH11	1:B:51:ARG:CG	1.99	0.75
1:B:259:ASP:C	3:B:610:HOH:O	2.25	0.75
1:D:158:GLN:HE22	1:D:175:GLU:N	1.81	0.75
1:B:115:ASP:HB2	3:B:549:HOH:O	1.86	0.75
1:B:57:VAL:HG11	1:B:62:ILE:HG12	1.69	0.74
1:B:25:LEU:O	1:B:28:THR:HG23	1.88	0.74
1:B:80:THR:HG23	3:B:564:HOH:O	1.87	0.74
1:B:118:ASP:C	1:B:119:ARG:O	2.24	0.74
1:B:108:LEU:HA	3:B:562:HOH:O	1.88	0.73
1:C:217:ASN:ND2	1:C:217:ASN:N	2.34	0.73
2:A:501:TRE:C6P	3:A:521:HOH:O	2.37	0.73
1:C:142:HIS:CE1	1:C:208:ASP:OD2	2.42	0.72
1:C:163:ARG:HG3	1:C:163:ARG:NH1	2.05	0.72
1:C:202:GLU:HB3	3:C:598:HOH:O	1.90	0.72
1:B:257:ARG:NH2	3:B:524:HOH:O	2.22	0.72
1:D:22:VAL:HG13	1:D:34:PRO:HG2	1.72	0.72
1:D:160:ARG:CB	3:D:600:HOH:O	2.37	0.71
1:A:155:ARG:O	1:A:159:THR:HG22	1.90	0.71
1:A:143:ARG:HG3	1:A:211:TYR:CD2	2.24	0.71
1:C:227:GLU:HG2	1:C:233:PRO:HG3	1.70	0.71
1:B:118:ASP:O	1:B:119:ARG:O	2.09	0.70
1:B:43:ASN:CB	3:B:517:HOH:O	2.39	0.70
1:B:217:ASN:O	1:B:218:LEU:C	2.29	0.69
1:C:125:LEU:HD11	3:C:583:HOH:O	1.92	0.69
1:A:158:GLN:HA	3:A:519:HOH:O	1.93	0.69
1:C:100:LYS:CE	3:C:539:HOH:O	2.40	0.69
1:C:207:ILE:H	1:C:207:ILE:CD1	2.06	0.68
1:A:5:PRO:HD2	3:A:506:HOH:O	1.93	0.68
1:B:112:ARG:NE	3:B:529:HOH:O	2.27	0.68
1:C:266:PRO:HB3	3:C:588:HOH:O	1.93	0.68
1:B:176:TYR:HD1	1:B:252:TRP:CD1	2.12	0.67
1:D:252:TRP:CZ2	3:D:519:HOH:O	2.46	0.67
1:C:163:ARG:HG3	1:C:163:ARG:HH11	1.59	0.66
1:A:62:ILE:O	1:A:64:ARG:N	2.29	0.66
1:C:28:THR:CG2	1:C:30:VAL:H	2.02	0.66
1:B:140:HIS:CE1	3:B:615:HOH:O	2.48	0.66
1:C:261:GLN:HG2	3:C:633:HOH:O	1.95	0.65
1:B:62:ILE:HG13	1:B:63:LEU:N	2.12	0.65
1:B:83:ARG:HD3	3:B:613:HOH:O	1.97	0.65
1:C:4:HIS:CB	3:C:513:HOH:O	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLN:NE2	1:B:188:LEU:HD13	2.12	0.65
1:C:177:HIS:O	1:C:181:ILE:HD12	1.97	0.64
1:C:215:TRP:CB	3:C:586:HOH:O	2.45	0.64
2:A:501:TRE:H6P1	3:A:521:HOH:O	1.95	0.64
1:C:28:THR:CG2	1:C:30:VAL:HB	2.28	0.64
1:B:100:LYS:HE2	3:B:561:HOH:O	1.98	0.64
1:B:207:ILE:O	1:B:207:ILE:CG2	2.44	0.64
1:C:151:VAL:CB	3:C:630:HOH:O	2.44	0.64
1:B:146:VAL:HG21	1:B:189:ARG:CZ	2.27	0.64
3:A:547:HOH:O	1:B:85:TYR:CE1	2.50	0.63
1:D:44:THR:HG22	1:D:46:MET:CB	2.25	0.63
1:A:85:TYR:CZ	3:A:524:HOH:O	2.50	0.63
1:C:11:LEU:HG	1:C:195:TRP:CH2	2.34	0.63
1:A:62:ILE:CG2	1:A:180:ALA:HB2	2.30	0.62
1:C:210:ASP:HB3	3:C:613:HOH:O	1.99	0.62
1:B:112:ARG:HD3	3:B:608:HOH:O	1.99	0.62
1:D:51:ARG:HG2	1:D:51:ARG:HH11	1.63	0.62
1:B:22:VAL:HG11	1:B:100:LYS:NZ	2.15	0.62
1:C:125:LEU:CD1	3:C:583:HOH:O	2.47	0.62
1:C:217:ASN:ND2	1:C:217:ASN:H	1.96	0.62
1:A:11:LEU:HB3	1:A:195:TRP:CZ2	2.35	0.62
1:D:112:ARG:NH1	3:D:598:HOH:O	2.31	0.62
1:D:155:ARG:CZ	3:D:519:HOH:O	2.47	0.62
1:B:82:TRP:CE2	1:B:112:ARG:HD2	2.34	0.61
1:A:41:LEU:HB3	3:A:532:HOH:O	2.00	0.61
1:C:100:LYS:HE3	3:C:539:HOH:O	2.00	0.61
2:A:501:TRE:HC2P	3:A:511:HOH:O	1.99	0.61
1:D:44:THR:HG22	1:D:46:MET:H	1.63	0.61
1:A:153:PHE:O	1:A:157:VAL:HB	2.01	0.60
1:A:143:ARG:HG3	1:A:211:TYR:HB3	1.84	0.60
1:D:158:GLN:NE2	1:D:175:GLU:H	1.82	0.60
1:A:120:SER:HB3	1:A:130:ASP:OD2	2.02	0.60
1:B:18:SER:HB2	1:B:100:LYS:HD3	1.82	0.60
1:B:19:THR:HG21	1:B:163:ARG:HD3	1.83	0.60
1:C:260:ALA:HB1	1:C:267:LEU:HD21	1.84	0.60
1:B:21:LEU:HB2	1:B:214:LEU:HD21	1.82	0.60
1:C:226:LEU:CD2	1:C:231:GLN:HB2	2.32	0.59
1:C:253:VAL:HB	3:C:632:HOH:O	2.02	0.59
1:B:257:ARG:HH12	1:C:197:ALA:HB2	1.63	0.59
1:B:119:ARG:NH1	1:B:126:SER:HB2	2.18	0.59
1:C:132:VAL:O	1:C:132:VAL:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:THR:HG22	3:C:533:HOH:O	2.02	0.59
1:A:156:ALA:HA	1:A:159:THR:HG23	1.81	0.59
1:B:238:LYS:HA	3:B:530:HOH:O	2.01	0.59
1:B:56:ASP:HB3	3:B:551:HOH:O	2.03	0.59
1:C:212:PRO:HA	3:C:566:HOH:O	2.03	0.59
1:D:260:ALA:HA	1:D:265:LEU:HB2	1.85	0.59
1:A:218:LEU:HD12	1:A:218:LEU:C	2.22	0.59
1:B:253:VAL:O	1:B:257:ARG:HG3	2.02	0.59
1:B:49:GLN:HE22	1:B:70:ILE:N	1.93	0.58
1:A:49:GLN:O	1:A:52:GLU:HB2	2.03	0.58
1:C:26:ARG:NH2	1:C:35:GLN:OE1	2.36	0.58
1:A:140:HIS:C	1:A:140:HIS:CD2	2.76	0.58
1:B:160:ARG:NH1	3:B:506:HOH:O	2.36	0.58
1:C:133:GLY:O	1:C:134:SER:HB3	2.04	0.57
1:D:210:ASP:CB	3:D:561:HOH:O	2.52	0.57
1:A:7:ALA:O	1:A:136:PRO:HA	2.04	0.57
1:D:252:TRP:CH2	3:D:519:HOH:O	2.58	0.57
3:A:547:HOH:O	1:B:85:TYR:CD1	2.58	0.57
1:C:33:GLU:HG2	3:D:553:HOH:O	2.04	0.57
1:C:187:MET:HE2	3:C:575:HOH:O	2.05	0.57
1:D:113:ALA:HA	1:D:116:LEU:HD22	1.86	0.57
1:A:125:LEU:O	1:A:129:ARG:HG2	2.04	0.56
1:A:22:VAL:HG13	1:A:34:PRO:HB2	1.87	0.56
1:A:62:ILE:C	1:A:64:ARG:H	2.08	0.56
1:D:19:THR:HG21	3:D:574:HOH:O	2.05	0.56
1:C:118:ASP:OD2	1:C:118:ASP:N	2.34	0.56
1:D:15:ARG:NH1	1:D:152:SER:OG	2.38	0.56
1:A:143:ARG:HG3	1:A:211:TYR:CB	2.36	0.55
1:C:132:VAL:O	1:C:132:VAL:CG1	2.55	0.55
1:C:207:ILE:CD1	1:C:207:ILE:N	2.67	0.55
1:B:257:ARG:NH1	1:C:197:ALA:CB	2.60	0.55
1:B:56:ASP:HA	3:B:592:HOH:O	2.07	0.55
1:B:176:TYR:HB2	1:B:252:TRP:NE1	2.21	0.55
1:D:163:ARG:HG3	1:D:163:ARG:NH1	2.22	0.55
1:D:251:GLU:HG3	3:D:580:HOH:O	2.05	0.55
1:A:161:VAL:HG22	1:B:30:VAL:CG1	2.37	0.55
1:B:83:ARG:CD	3:B:613:HOH:O	2.54	0.55
1:A:118:ASP:HA	3:A:562:HOH:O	2.07	0.55
1:D:176:TYR:HB2	1:D:252:TRP:CE2	2.42	0.55
1:B:106:THR:N	1:B:107:PRO:CD	2.70	0.55
1:C:210:ASP:OD1	1:C:213:TYR:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TYR:OH	1:A:178:ALA:HB2	2.07	0.54
1:B:142:HIS:CB	3:B:609:HOH:O	2.55	0.54
1:D:220:GLU:CB	3:D:551:HOH:O	2.55	0.54
1:A:235:LEU:O	1:A:236:ALA:HB2	2.07	0.54
1:C:88:THR:HG21	1:D:45:SER:HB3	1.89	0.54
1:D:212:PRO:O	1:D:216:ARG:HD2	2.07	0.54
1:B:238:LYS:CA	3:B:508:HOH:O	2.39	0.54
1:B:176:TYR:CD1	1:B:252:TRP:CD1	2.96	0.54
1:C:163:ARG:HH11	1:C:163:ARG:CG	2.20	0.54
1:A:71:GLU:O	1:A:71:GLU:HG2	2.08	0.53
1:B:176:TYR:HB2	1:B:252:TRP:CD1	2.44	0.53
1:B:84:ASP:O	1:B:88:THR:HG23	2.08	0.53
1:C:207:ILE:N	1:C:207:ILE:HD12	2.23	0.53
1:D:182:ALA:O	1:D:186:THR:HG22	2.09	0.53
1:D:44:THR:HG21	3:D:509:HOH:O	2.08	0.53
1:B:49:GLN:O	1:B:52:GLU:HB2	2.09	0.52
1:C:59:ASP:C	1:C:59:ASP:OD2	2.47	0.52
1:B:221:VAL:C	1:B:223:GLY:N	2.63	0.52
1:D:62:ILE:HG13	1:D:177:HIS:CE1	2.45	0.52
1:D:19:THR:CG2	3:D:574:HOH:O	2.57	0.52
1:B:51:ARG:NH1	1:B:67:ASP:O	2.43	0.52
1:D:112:ARG:CZ	3:D:598:HOH:O	2.58	0.52
1:D:163:ARG:HH11	1:D:163:ARG:HG3	1.75	0.51
1:B:19:THR:HG23	3:B:573:HOH:O	2.09	0.51
1:D:49:GLN:HE22	1:D:70:ILE:H	1.57	0.51
1:B:259:ASP:N	1:B:259:ASP:OD1	2.44	0.51
1:B:217:ASN:HB3	1:B:220:GLU:HB2	1.93	0.51
1:D:46:MET:SD	3:D:576:HOH:O	2.59	0.51
1:A:106:THR:OG1	1:A:107:PRO:HD3	2.11	0.51
1:A:193:GLU:O	1:A:195:TRP:N	2.44	0.51
1:B:39:GLN:NE2	2:B:502:TRE:O4P	2.43	0.51
1:D:193:GLU:CB	3:D:558:HOH:O	2.59	0.50
1:C:4:HIS:N	3:C:513:HOH:O	2.43	0.50
1:D:118:ASP:OD1	1:D:118:ASP:N	2.42	0.50
1:A:62:ILE:HG21	1:A:180:ALA:HB2	1.94	0.50
1:B:7:ALA:O	1:B:136:PRO:HA	2.12	0.50
1:A:214:LEU:HD23	1:A:218:LEU:HB2	1.93	0.50
1:C:142:HIS:HB2	3:C:564:HOH:O	2.11	0.50
1:D:22:VAL:HG13	1:D:34:PRO:CG	2.41	0.50
1:A:104:ASN:HB3	1:A:191:GLN:NE2	2.12	0.50
1:A:140:HIS:HD1	1:A:199:PHE:HZ	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:THR:HB	1:A:124:LEU:HD13	1.94	0.50
1:D:22:VAL:CG1	1:D:34:PRO:HB2	2.42	0.50
1:B:192:GLU:HG3	3:B:595:HOH:O	2.11	0.49
1:C:211:TYR:HB3	1:C:212:PRO:HD3	1.94	0.49
1:B:199:PHE:HA	1:B:204:VAL:HG23	1.94	0.49
1:B:192:GLU:OE1	1:B:192:GLU:HA	2.03	0.49
1:C:210:ASP:OD1	1:C:213:TYR:CB	2.61	0.49
1:B:222:VAL:O	1:B:226:LEU:HD12	2.12	0.49
1:D:177:HIS:O	1:D:181:ILE:HD12	2.11	0.49
1:A:92:THR:HB	1:A:93:PRO:CD	2.43	0.49
1:A:124:LEU:O	1:A:127:ALA:HB3	2.12	0.49
1:D:62:ILE:O	1:D:65:LEU:HB2	2.13	0.49
1:A:134:SER:OG	1:A:135:ASP:N	2.45	0.48
1:D:218:LEU:O	1:D:221:VAL:N	2.45	0.48
1:A:193:GLU:HA	1:A:196:ARG:NH1	2.28	0.48
1:C:207:ILE:H	1:C:207:ILE:HD13	1.76	0.48
1:B:101:LEU:HD13	1:B:195:TRP:HH2	1.77	0.48
1:C:150:ALA:CB	1:C:185:ILE:HG13	2.43	0.48
1:B:112:ARG:NH2	3:B:529:HOH:O	2.47	0.48
1:B:267:LEU:C	3:B:527:HOH:O	2.51	0.48
1:C:119:ARG:O	3:C:629:HOH:O	2.20	0.48
1:A:125:LEU:HB2	1:A:198:TRP:HZ2	1.79	0.48
1:C:187:MET:HE3	1:C:187:MET:HB2	1.69	0.48
1:B:75:ASP:OD2	1:B:112:ARG:NH1	2.39	0.48
1:C:150:ALA:HB2	1:C:185:ILE:HG13	1.94	0.48
1:C:214:LEU:HD12	1:C:221:VAL:HG21	1.96	0.48
1:D:118:ASP:O	1:D:119:ARG:C	2.51	0.48
1:B:221:VAL:O	1:B:223:GLY:N	2.47	0.47
1:B:248:ARG:C	3:B:554:HOH:O	2.52	0.47
1:B:251:GLU:O	1:B:255:ARG:HB2	2.13	0.47
1:C:226:LEU:HD22	1:C:231:GLN:HB2	1.96	0.47
1:C:26:ARG:NH2	1:C:34:PRO:O	2.47	0.47
1:A:30:VAL:O	1:A:30:VAL:HG13	2.14	0.47
1:A:91:ARG:HA	1:A:96:VAL:O	2.14	0.47
1:C:142:HIS:CD2	3:C:564:HOH:O	2.68	0.47
1:D:101:LEU:HD23	1:D:105:GLN:HE21	1.79	0.47
1:A:70:ILE:CG2	1:A:71:GLU:N	2.76	0.47
1:B:182:ALA:HB2	1:B:265:LEU:HD22	1.96	0.47
1:B:42:PRO:O	1:B:74:PRO:HA	2.15	0.47
1:B:83:ARG:HH11	1:B:116:LEU:HD22	1.80	0.47
1:C:28:THR:HG22	1:C:29:GLY:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ASP:OD2	1:D:61:SER:OG	2.28	0.47
1:A:138:LEU:HA	1:A:138:LEU:HD12	1.67	0.47
1:A:36:GLU:O	1:A:39:GLN:HG2	2.14	0.47
1:B:221:VAL:C	1:B:223:GLY:H	2.16	0.47
1:D:96:VAL:HG11	1:D:229:LEU:HD13	1.96	0.47
1:B:146:VAL:HG12	1:B:185:ILE:HG12	1.97	0.47
1:B:189:ARG:HA	3:B:597:HOH:O	2.14	0.47
1:A:143:ARG:HG3	1:A:211:TYR:HD2	1.78	0.47
1:A:194:GLY:HA2	3:A:561:HOH:O	2.15	0.47
1:B:28:THR:OG1	1:B:30:VAL:HG22	2.15	0.47
1:A:70:ILE:HG22	1:A:71:GLU:N	2.30	0.46
1:B:34:PRO:C	3:B:598:HOH:O	2.53	0.46
1:B:162:TRP:CD2	2:B:502:TRE:HC1P	2.51	0.46
1:D:163:ARG:HA	1:D:163:ARG:HD2	1.50	0.46
1:B:213:TYR:CE2	1:B:217:ASN:HB2	2.50	0.46
1:B:21:LEU:HD12	3:B:539:HOH:O	2.14	0.46
1:C:142:HIS:HD2	3:C:564:HOH:O	1.98	0.46
1:A:14:GLN:O	1:A:15:ARG:HB2	2.15	0.46
1:A:73:LYS:HB2	1:A:74:PRO:CD	2.45	0.46
1:C:232:ASP:HA	1:C:233:PRO:HD3	1.67	0.46
1:D:51:ARG:HG2	1:D:51:ARG:NH1	2.30	0.46
1:D:59:ASP:HB3	1:D:62:ILE:HD12	1.98	0.46
1:A:16:SER:OG	1:A:18:SER:HB2	2.16	0.46
1:A:28:THR:HG21	1:A:226:LEU:HD21	1.96	0.46
1:C:28:THR:CG2	1:C:30:VAL:N	2.72	0.46
1:D:255:ARG:O	1:D:258:ARG:HB3	2.15	0.46
1:B:257:ARG:HH12	1:C:197:ALA:CB	2.25	0.46
3:C:634:HOH:O	1:D:73:LYS:HE3	2.16	0.46
1:A:11:LEU:HD11	1:A:138:LEU:HG	1.97	0.46
1:A:4:HIS:CB	3:A:506:HOH:O	2.63	0.46
1:D:176:TYR:OH	1:D:256:TYR:HA	2.16	0.46
1:C:238:LYS:HD2	1:C:238:LYS:HA	1.70	0.46
1:D:22:VAL:HG13	1:D:34:PRO:HB2	1.98	0.46
1:A:4:HIS:HA	3:A:506:HOH:O	2.14	0.45
1:B:82:TRP:CZ2	1:B:112:ARG:HD2	2.51	0.45
1:A:4:HIS:CA	3:A:506:HOH:O	2.64	0.45
1:B:17:GLY:O	1:B:18:SER:C	2.53	0.45
1:A:163:ARG:HA	1:A:163:ARG:HD2	1.80	0.45
1:D:147:VAL:HG12	1:D:253:VAL:HG13	1.99	0.45
1:A:11:LEU:HB3	1:A:195:TRP:CH2	2.52	0.45
2:A:501:TRE:C2P	3:A:511:HOH:O	2.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HD22	1:B:195:TRP:CH2	2.51	0.45
1:C:231:GLN:HB3	3:C:608:HOH:O	2.16	0.45
1:A:218:LEU:C	1:A:218:LEU:CD1	2.85	0.45
1:B:92:THR:HB	3:B:548:HOH:O	2.17	0.45
1:B:154:TRP:CE2	1:B:158:GLN:NE2	2.85	0.45
1:A:143:ARG:HG3	1:A:211:TYR:CG	2.50	0.45
1:A:157:VAL:HG13	1:A:157:VAL:O	2.17	0.45
1:D:22:VAL:HG13	1:D:34:PRO:CB	2.47	0.45
1:A:211:TYR:N	1:A:212:PRO:HD2	2.32	0.45
1:A:58:GLU:N	3:A:505:HOH:O	2.50	0.45
1:B:4:HIS:N	3:B:522:HOH:O	2.50	0.45
1:B:51:ARG:NH1	1:B:51:ARG:CG	2.66	0.44
1:C:21:LEU:HD22	1:C:25:LEU:CD2	2.43	0.44
1:A:61:SER:OG	1:A:177:HIS:NE2	2.49	0.44
1:B:150:ALA:CB	1:B:185:ILE:HG13	2.47	0.44
1:B:265:LEU:N	3:B:605:HOH:O	2.49	0.44
1:D:119:ARG:HA	1:D:119:ARG:HD2	1.71	0.44
1:C:233:PRO:C	1:C:235:LEU:H	2.19	0.44
1:C:261:GLN:CG	3:C:633:HOH:O	2.62	0.44
1:D:21:LEU:O	1:D:21:LEU:HD22	2.18	0.44
1:B:85:TYR:CE2	1:B:89:VAL:HG21	2.52	0.44
1:A:7:ALA:HA	1:A:97:TRP:O	2.18	0.44
1:A:92:THR:HB	1:A:93:PRO:HD2	2.00	0.44
1:C:188:LEU:HD23	1:C:188:LEU:HA	1.74	0.44
1:C:226:LEU:HD23	1:C:231:GLN:HB2	1.99	0.44
1:B:85:TYR:CZ	1:B:89:VAL:HG21	2.53	0.44
1:A:128:ILE:O	1:A:132:VAL:HG13	2.17	0.44
1:B:34:PRO:HA	1:B:99:GLY:HA2	2.00	0.44
1:C:103:TRP:CE3	1:C:106:THR:HG21	2.53	0.44
1:C:29:GLY:HA3	1:D:163:ARG:HB2	2.00	0.44
1:A:213:TYR:HD1	1:A:217:ASN:OD1	2.00	0.43
1:A:30:VAL:O	1:A:30:VAL:CG1	2.66	0.43
1:A:50:PRO:C	1:A:52:GLU:H	2.20	0.43
1:B:56:ASP:C	3:B:592:HOH:O	2.55	0.43
1:D:226:LEU:O	1:D:227:GLU:C	2.55	0.43
1:C:118:ASP:O	1:C:119:ARG:C	2.55	0.43
1:C:208:ASP:O	1:C:209:VAL:HG22	2.18	0.43
1:D:162:TRP:N	1:D:162:TRP:CD1	2.86	0.43
1:D:217:ASN:O	1:D:218:LEU:C	2.56	0.43
1:D:19:THR:HG23	3:D:533:HOH:O	2.18	0.43
1:B:104:ASN:HA	3:B:593:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ALA:CA	1:A:159:THR:HG22	2.40	0.43
1:A:32:GLY:HA2	1:A:92:THR:HG23	2.01	0.43
1:C:162:TRP:CD2	2:C:503:TRE:HC1	2.54	0.43
1:C:22:VAL:HG22	1:C:34:PRO:HG3	2.01	0.43
1:C:255:ARG:CB	3:C:530:HOH:O	2.67	0.43
1:B:15:ARG:O	1:B:149:GLN:HG3	2.19	0.43
1:C:106:THR:N	1:C:107:PRO:CD	2.82	0.43
1:B:120:SER:N	1:B:130:ASP:OD2	2.50	0.42
1:B:62:ILE:HD12	1:B:154:TRP:CH2	2.54	0.42
1:C:254:GLU:O	1:C:256:TYR:N	2.52	0.42
1:A:149:GLN:NE2	1:A:188:LEU:HD22	2.34	0.42
1:C:213:TYR:CE2	1:C:220:GLU:OE1	2.71	0.42
1:A:193:GLU:O	1:A:194:GLY:C	2.58	0.42
1:B:146:VAL:CG2	1:B:189:ARG:CZ	2.98	0.42
1:A:255:ARG:C	3:A:541:HOH:O	2.58	0.42
1:D:158:GLN:NE2	1:D:174:ALA:HA	2.35	0.42
1:D:17:GLY:O	1:D:18:SER:C	2.55	0.42
1:B:218:LEU:HD22	1:B:222:VAL:CG2	2.50	0.42
1:D:106:THR:N	1:D:107:PRO:CD	2.82	0.42
1:C:163:ARG:HD2	1:C:163:ARG:HA	1.49	0.42
1:D:3:ASP:O	1:D:4:HIS:C	2.58	0.42
1:A:191:GLN:HG3	3:A:551:HOH:O	2.20	0.42
1:A:143:ARG:CG	1:A:211:TYR:HB3	2.49	0.42
1:B:9:LEU:HD11	1:B:101:LEU:HB2	2.01	0.42
1:A:143:ARG:NH1	1:A:149:GLN:HA	2.34	0.42
1:A:8:TYR:CD2	1:A:229:LEU:HD11	2.55	0.42
1:B:100:LYS:HG3	1:B:100:LYS:HZ2	1.59	0.42
1:A:232:ASP:HB3	1:A:235:LEU:HD12	2.02	0.41
1:A:181:ILE:O	1:A:181:ILE:HG22	2.19	0.41
1:C:189:ARG:HH21	1:C:267:LEU:C	2.23	0.41
1:C:213:TYR:C	1:C:213:TYR:CD2	2.94	0.41
1:A:216:ARG:HH11	1:A:216:ARG:HG3	1.86	0.41
1:B:112:ARG:CZ	3:B:529:HOH:O	2.65	0.41
1:A:149:GLN:HG2	1:A:188:LEU:HD13	2.03	0.41
1:C:143:ARG:HG3	1:C:211:TYR:CD2	2.55	0.41
1:A:194:GLY:N	3:A:561:HOH:O	2.53	0.41
1:B:197:ALA:O	1:B:201:GLU:HB2	2.20	0.41
1:C:199:PHE:O	1:C:203:ASN:N	2.54	0.41
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.84	0.41
1:A:56:ASP:O	3:A:505:HOH:O	2.22	0.41
1:D:112:ARG:HA	3:D:544:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:GLN:HG2	1:C:188:LEU:HD13	2.03	0.41
1:C:60:GLN:CB	3:C:571:HOH:O	2.68	0.41
1:D:211:TYR:HB3	1:D:212:PRO:HD3	2.03	0.41
1:B:196:ARG:NH2	1:C:257:ARG:CZ	2.84	0.41
1:C:267:LEU:HB2	3:C:599:HOH:O	2.20	0.41
1:B:232:ASP:HA	1:B:233:PRO:HD3	1.96	0.41
1:B:51:ARG:HD2	3:B:575:HOH:O	2.21	0.41
1:D:229:LEU:HD12	1:D:231:GLN:HG2	2.03	0.40
1:B:15:ARG:HA	3:B:606:HOH:O	2.20	0.40
1:B:17:GLY:O	1:B:19:THR:N	2.55	0.40
1:D:8:TYR:N	1:D:8:TYR:CD2	2.90	0.40
1:A:21:LEU:HD12	1:A:141:ILE:HD11	2.04	0.40
2:A:501:TRE:HC4P	1:B:33:GLU:OE2	2.21	0.40
1:D:222:VAL:O	1:D:225:VAL:N	2.55	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	228/287 (79%)	181 (79%)	38 (17%)	9 (4%)	3 4
1	B	235/287 (82%)	217 (92%)	14 (6%)	4 (2%)	11 21
1	C	238/287 (83%)	222 (93%)	12 (5%)	4 (2%)	11 21
1	D	241/287 (84%)	220 (91%)	19 (8%)	2 (1%)	22 44
All	All	942/1148 (82%)	840 (89%)	83 (9%)	19 (2%)	9 17

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	LEU

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Mol	Chain	Res	Type
1	A	194	GLY
1	B	119	ARG
1	B	218	LEU
1	A	182	ALA
1	A	193	GLU
1	D	59	ASP
1	D	64	ARG
1	C	203	ASN
1	A	60	GLN
1	A	183	HIS
1	B	209	VAL
1	C	217	ASN
1	A	184	VAL
1	C	12	ALA
1	C	255	ARG
1	B	222	VAL
1	A	185	ILE
1	A	50	PRO

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	172/245 (70%)	131 (76%)	41 (24%)	1 1
1	B	185/245 (76%)	146 (79%)	39 (21%)	1 2
1	C	192/245 (78%)	168 (88%)	24 (12%)	5 10
1	D	190/245 (78%)	155 (82%)	35 (18%)	2 3
All	All	739/980 (75%)	600 (81%)	139 (19%)	2 2

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	24	SER
1	A	41	LEU

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Mol	Chain	Res	Type
1	A	46	MET
1	A	49	GLN
1	A	52	GLU
1	A	58	GLU
1	A	62	ILE
1	A	64	ARG
1	A	70	ILE
1	A	71	GLU
1	A	80	THR
1	A	83	ARG
1	A	92	THR
1	A	102	MET
1	A	104	ASN
1	A	109	LEU
1	A	111	GLN
1	A	112	ARG
1	A	119	ARG
1	A	120	SER
1	A	132	VAL
1	A	134	SER
1	A	138	LEU
1	A	142	HIS
1	A	143	ARG
1	A	152	SER
1	A	157	VAL
1	A	159	THR
1	A	160	ARG
1	A	173	ARG
1	A	186	THR
1	A	191	GLN
1	A	195	TRP
1	A	213	TYR
1	A	214	LEU
1	A	215	TRP
1	A	218	LEU
1	A	219	THR
1	A	235	LEU
1	A	259	ASP
1	B	15	ARG
1	B	18	SER
1	B	21	LEU
1	B	22	VAL

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Mol	Chain	Res	Type
1	B	24	SER
1	B	28	THR
1	B	41	LEU
1	B	45	SER
1	B	51	ARG
1	B	62	ILE
1	B	66	LEU
1	B	71	GLU
1	B	81	ILE
1	B	83	ARG
1	B	88	THR
1	B	92	THR
1	B	100	LYS
1	B	101	LEU
1	B	102	MET
1	B	111	GLN
1	B	112	ARG
1	B	124	LEU
1	B	126	SER
1	B	134	SER
1	B	135	ASP
1	B	152	SER
1	B	157	VAL
1	B	173	ARG
1	B	192	GLU
1	B	200	THR
1	B	204	VAL
1	B	213	TYR
1	B	218	LEU
1	B	220	GLU
1	B	224	THR
1	B	249	SER
1	B	255	ARG
1	B	259	ASP
1	B	267	LEU
1	C	11	LEU
1	C	15	ARG
1	C	21	LEU
1	C	22	VAL
1	C	24	SER
1	C	25	LEU
1	C	28	THR

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Mol	Chain	Res	Type
1	C	69	LEU
1	C	88	THR
1	C	92	THR
1	C	100	LYS
1	C	101	LEU
1	C	124	LEU
1	C	125	LEU
1	C	159	THR
1	C	163	ARG
1	C	187	MET
1	C	207	ILE
1	C	210	ASP
1	C	217	ASN
1	C	218	LEU
1	C	232	ASP
1	C	261	GLN
1	C	267	LEU
1	D	9	LEU
1	D	19	THR
1	D	21	LEU
1	D	30	VAL
1	D	41	LEU
1	D	44	THR
1	D	49	GLN
1	D	51	ARG
1	D	57	VAL
1	D	63	LEU
1	D	83	ARG
1	D	92	THR
1	D	100	LYS
1	D	101	LEU
1	D	109	LEU
1	D	111	GLN
1	D	112	ARG
1	D	114	LYS
1	D	116	LEU
1	D	119	ARG
1	D	146	VAL
1	D	152	SER
1	D	157	VAL
1	D	163	ARG
1	D	186	THR

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Mol	Chain	Res	Type
1	D	187	MET
1	D	189	ARG
1	D	201	GLU
1	D	202	GLU
1	D	204	VAL
1	D	215	TRP
1	D	229	LEU
1	D	235	LEU
1	D	257	ARG
1	D	267	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	105	GLN
1	A	149	GLN
1	A	191	GLN
1	B	39	GLN
1	B	49	GLN
1	B	87	GLN
1	B	111	GLN
1	B	149	GLN
1	B	183	HIS
1	C	105	GLN
1	C	142	HIS
1	C	217	ASN
1	D	35	GLN
1	D	39	GLN
1	D	49	GLN
1	D	105	GLN
1	D	158	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands 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	$\#\|Z\| > 2$
2	TRE	A	501	-	24,24,24	0.90	0	35,35,35	3.21	19 (54%)
2	TRE	B	502	-	24,24,24	0.82	0	35,35,35	3.32	23 (65%)
2	TRE	C	503	-	24,24,24	1.01	1 (4%)	35,35,35	3.39	24 (68%)
2	TRE	D	504	-	24,24,24	0.90	1 (4%)	35,35,35	3.22	21 (60%)

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	TRE	A	501	-	-	0/8/48/48	0/2/2/2
2	TRE	B	502	-	-	0/8/48/48	0/2/2/2
2	TRE	C	503	-	-	0/8/48/48	0/2/2/2
2	TRE	D	504	-	-	0/8/48/48	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	503	TRE	C4-C3	-2.06	1.47	1.52
2	D	504	TRE	C3P-C2P	-2.04	1.47	1.52

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	503	TRE	C6-C5-C4	-6.21	98.47	113.00
2	D	504	TRE	O1-C1P-O5P	-5.80	96.61	110.70
2	C	503	TRE	O1-C1P-O5P	-4.93	98.73	110.70
2	A	501	TRE	O1-C1P-O5P	-4.51	99.74	110.70
2	C	503	TRE	O1-C1-C2	-4.22	98.60	108.11
2	B	502	TRE	O1-C1-O5	-4.20	100.51	110.70
2	D	504	TRE	O1-C1-C2	-3.88	99.36	108.11
2	B	502	TRE	C6-C5-C4	-3.44	104.94	113.00
2	A	501	TRE	O1-C1P-C2P	-3.34	100.58	108.11
2	B	502	TRE	O1-C1P-C2P	-3.27	100.73	108.11
2	B	502	TRE	O5-C5-C6	-3.03	99.15	106.41
2	B	502	TRE	O1-C1P-O5P	-3.02	103.37	110.70
2	D	504	TRE	O1-C1-O5	-2.70	104.15	110.70
2	D	504	TRE	O1-C1P-C2P	-2.66	102.11	108.11
2	A	501	TRE	O3P-C3P-C2P	-2.63	104.64	110.36
2	C	503	TRE	O1-C1P-C2P	-2.32	102.88	108.11
2	D	504	TRE	O4-C4-C5	2.01	114.34	109.28
2	C	503	TRE	C1P-O1-C1	2.03	118.03	114.37
2	C	503	TRE	O5-C1-C2	2.06	114.28	110.30
2	D	504	TRE	O3P-C3P-C4P	2.16	115.06	110.36
2	B	502	TRE	O5P-C5P-C6P	2.19	111.65	106.41
2	C	503	TRE	O5P-C1P-C2P	2.21	114.56	110.30
2	D	504	TRE	O3-C3-C2	2.23	115.22	110.36
2	B	502	TRE	O5-C1-C2	2.30	114.74	110.30
2	B	502	TRE	O2-C2-C3	2.32	115.40	110.36
2	D	504	TRE	O2-C2-C3	2.37	115.51	110.36
2	B	502	TRE	O3P-C3P-C4P	2.40	115.59	110.36
2	C	503	TRE	O4P-C4P-C3P	2.58	115.98	110.36
2	B	502	TRE	C4-C3-C2	2.67	115.54	110.84
2	B	502	TRE	O2-C2-C1	2.73	115.75	110.03
2	A	501	TRE	O2-C2-C3	2.74	116.31	110.36
2	B	502	TRE	C3P-C4P-C5P	2.76	115.09	110.22
2	A	501	TRE	C4-C3-C2	2.77	115.72	110.84
2	A	501	TRE	C4P-C3P-C2P	2.79	115.75	110.84
2	B	502	TRE	O3-C3-C4	2.81	116.48	110.36
2	C	503	TRE	O3-C3-C2	2.94	116.75	110.36
2	C	503	TRE	O3P-C3P-C4P	3.09	117.08	110.36
2	A	501	TRE	O2P-C2P-C1P	3.09	116.49	110.03
2	C	503	TRE	C3P-C4P-C5P	3.18	115.81	110.22
2	C	503	TRE	O5P-C5P-C4P	3.25	115.65	109.66
2	D	504	TRE	O5-C5-C4	3.27	115.68	109.66
2	B	502	TRE	C1P-C2P-C3P	3.35	116.20	109.98
2	B	502	TRE	O5P-C1P-C2P	3.36	116.77	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	503	TRE	O2P-C2P-C3P	3.37	117.68	110.36
2	C	503	TRE	O2P-C2P-C1P	3.41	117.16	110.03
2	B	502	TRE	O3P-C3P-C2P	3.51	118.00	110.36
2	D	504	TRE	O5P-C1P-C2P	3.55	117.15	110.30
2	A	501	TRE	O5-C1-C2	3.59	117.22	110.30
2	D	504	TRE	O2-C2-C1	3.62	117.59	110.03
2	C	503	TRE	C4P-C3P-C2P	3.71	117.38	110.84
2	C	503	TRE	C4-C3-C2	3.78	117.51	110.84
2	D	504	TRE	C3P-C4P-C5P	3.84	116.99	110.22
2	C	503	TRE	C3-C4-C5	3.89	117.08	110.22
2	C	503	TRE	C1P-C2P-C3P	3.93	117.27	109.98
2	D	504	TRE	C1P-C2P-C3P	3.94	117.30	109.98
2	D	504	TRE	O5P-C5P-C4P	3.95	116.94	109.66
2	C	503	TRE	O3-C3-C4	4.08	119.22	110.36
2	A	501	TRE	C1P-O1-C1	4.13	121.82	114.37
2	A	501	TRE	O5P-C1P-C2P	4.20	118.39	110.30
2	A	501	TRE	O3-C3-C2	4.29	119.69	110.36
2	D	504	TRE	C4P-C3P-C2P	4.29	118.41	110.84
2	C	503	TRE	O2-C2-C1	4.33	119.08	110.03
2	D	504	TRE	C1P-O1-C1	4.38	122.28	114.37
2	A	501	TRE	O5-C5-C4	4.40	117.77	109.66
2	A	501	TRE	O5P-C5P-C4P	4.44	117.83	109.66
2	B	502	TRE	C3-C4-C5	4.45	118.05	110.22
2	B	502	TRE	O5-C5-C4	4.54	118.02	109.66
2	C	503	TRE	C1-C2-C3	4.55	118.44	109.98
2	D	504	TRE	O2P-C2P-C1P	4.60	119.66	110.03
2	A	501	TRE	C1-C2-C3	4.65	118.62	109.98
2	C	503	TRE	O5-C5-C4	4.67	118.26	109.66
2	D	504	TRE	C3-C4-C5	4.77	118.61	110.22
2	A	501	TRE	C3P-C4P-C5P	5.06	119.14	110.22
2	A	501	TRE	C1P-O5P-C5P	5.11	123.33	113.72
2	A	501	TRE	C1P-C2P-C3P	5.17	119.59	109.98
2	B	502	TRE	O5P-C5P-C4P	5.18	119.19	109.66
2	D	504	TRE	C1-C2-C3	5.27	119.78	109.98
2	B	502	TRE	C4P-C3P-C2P	5.38	120.34	110.84
2	A	501	TRE	C3-C4-C5	5.54	119.97	110.22
2	D	504	TRE	C1P-O5P-C5P	5.56	124.18	113.72
2	C	503	TRE	C1-O5-C5	5.71	124.47	113.72
2	B	502	TRE	C1-C2-C3	5.84	120.84	109.98
2	B	502	TRE	C1P-O5P-C5P	5.95	124.92	113.72
2	A	501	TRE	C1-O5-C5	6.35	125.67	113.72
2	D	504	TRE	C1-O5-C5	6.49	125.94	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	TRE	C1-O5-C5	7.22	127.32	113.72
2	C	503	TRE	C1P-O5P-C5P	7.49	127.82	113.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	TRE	5	0
2	B	502	TRE	2	0
2	C	503	TRE	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	239/287 (83%)	0.20	21 (8%)	11	7	20, 54, 93, 97	0
1	B	243/287 (84%)	-0.18	6 (2%)	58	50	19, 40, 76, 89	0
1	C	244/287 (85%)	-0.19	4 (1%)	72	67	12, 35, 62, 81	0
1	D	247/287 (86%)	-0.18	6 (2%)	59	52	17, 34, 58, 70	1 (0%)
All	All	973/1148 (84%)	-0.09	37 (3%)	41	33	12, 38, 79, 97	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	GLY	5.3
1	D	3	ASP	4.7
1	A	265	LEU	4.3
1	B	249	SER	4.2
1	B	171	ASP	4.1
1	A	266	PRO	4.0
1	A	262	ARG	4.0
1	A	211	TYR	3.7
1	A	263	ASP	3.6
1	A	3	ASP	3.4
1	A	261	GLN	3.3
1	A	179	GLY	3.3
1	A	4	HIS	3.1
1	A	64	ARG	3.0
1	D	249	SER	2.9
1	A	175	GLU	2.9
1	A	213	TYR	2.8
1	A	251	GLU	2.8
1	A	158	GLN	2.7
1	B	265	LEU	2.7
1	A	176	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	4	HIS	2.6
1	D	142	HIS	2.6
1	C	239	PRO	2.6
1	A	220	GLU	2.6
1	C	211	TYR	2.5
1	C	205	GLU	2.2
1	C	251	GLU	2.2
1	A	215	TRP	2.2
1	B	172	ALA	2.2
1	D	267	LEU	2.1
1	B	248	ARG	2.1
1	D	214	LEU	2.1
1	A	58	GLU	2.1
1	A	227	GLU	2.1
1	B	213	TYR	2.0
1	A	216	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	TRE	C	503	23/23	0.95	0.18	1.82	24,30,36,38	0
2	TRE	B	502	23/23	0.96	0.18	1.61	23,29,34,49	0
2	TRE	D	504	23/23	0.94	0.20	0.95	24,27,31,37	0
2	TRE	A	501	23/23	0.92	0.14	-0.17	28,33,41,42	0

6.5 Other polymers (i)

There are no such residues in this entry.