Full wwPDB X-ray Structure Validation Report (i)

Apr 20, 2024 – 12:42 pm BST

PDB ID	:	5MBM
Title	:	Cathepsin B in complex with DARPin 8h6
Authors	:	Turk, D.; Kramer, L.; Renko, M.; Turk, B.
Deposited on	:	2016-11-08
Resolution	:	2.76 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:

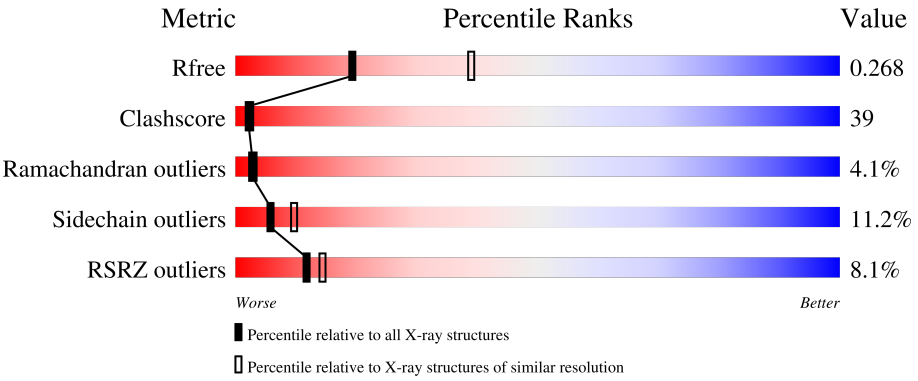
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	256	4% 40% 52% 8%
1	B	256	12% 42% 46% 10% •
2	C	171	12% 39% 48% 8% • 5%
2	D	171	4% 49% 36% 9% • 5%

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
1	SCH	A	29	-	-	X	-
1	SCH	B	29	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6499 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 Cathepsin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	14	0	0
			1971	1235	337	380	19			
1	B	255	Total	C	N	O	S	15	0	0
			1963	1229	336	379	19			

- Molecule 2 is a protein called DARPin 8h6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	163	Total	C	N	O	0	0	0
			1211	751	217	243			
2	D	163	Total	C	N	O	29	0	0
			1211	751	217	243			

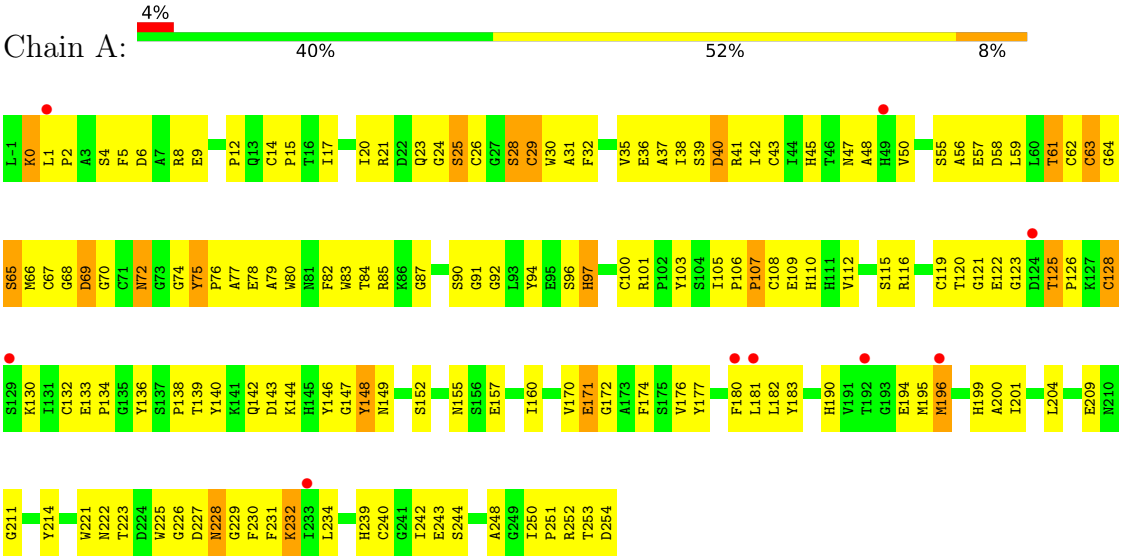
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	51	Total	O	0	0
			51	51		
3	C	22	Total	O	0	0
			22	22		
3	D	23	Total	O	0	0
			23	23		

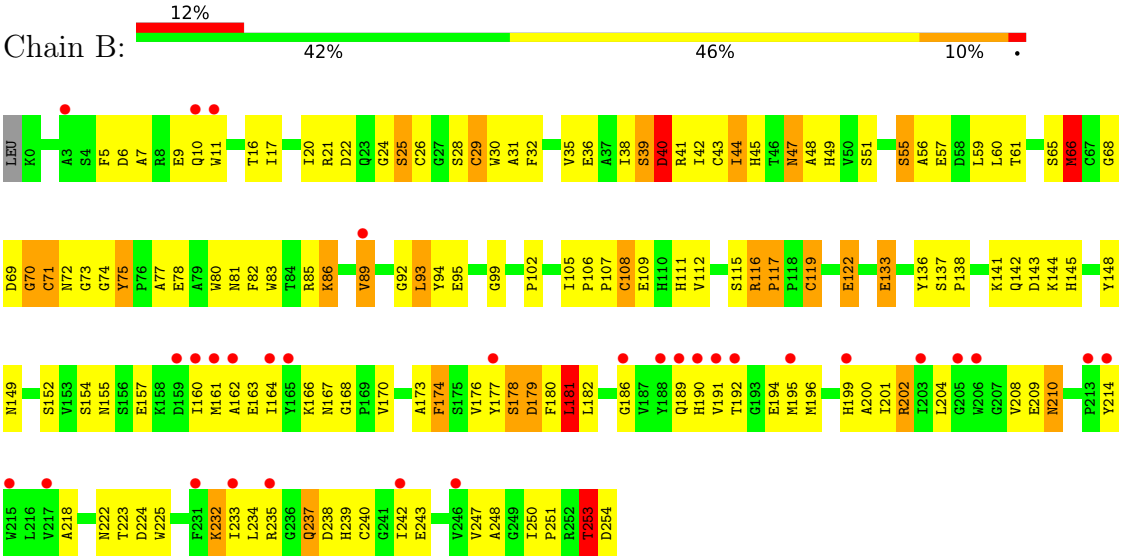
3 Residue-property plots (i)

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: Cathepsin B

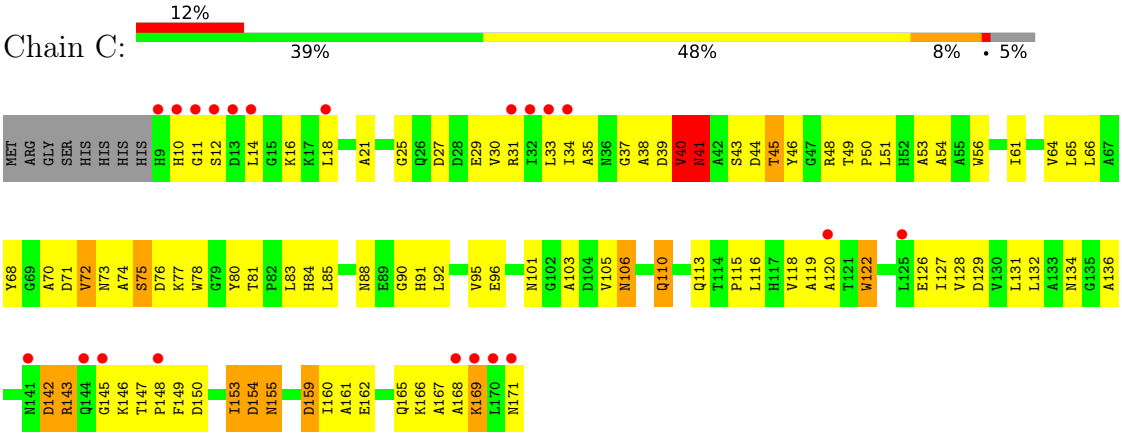


• Molecule 1: Cathepsin B



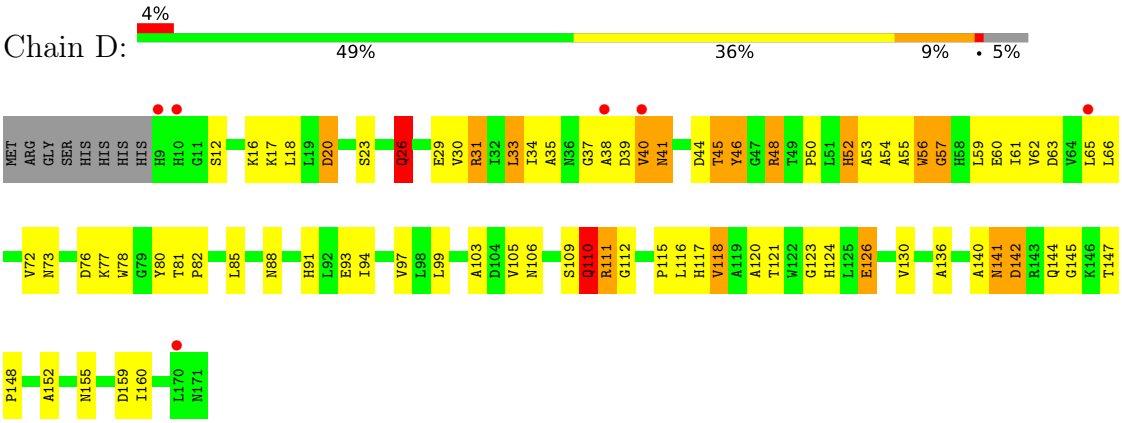
• Molecule 2: DARPin 8h6

Chain C:



• Molecule 2: DARPin 8h6

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.45Å 201.52Å 46.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 2.76 46.86 – 2.76	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.70-2.76) 98.6 (46.86-2.76)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.77Å)	Xtriage
Refinement program	MAIN 2016	Depositor
R, R_{free}	0.256 , 0.281 0.258 , 0.268	Depositor DCC
R_{free} test set	1257 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	56.3	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 72.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6499	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: SCH

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	1.11	3/2021 (0.1%)	1.19	5/2744 (0.2%)
1	B	0.96	0/2013	1.24	12/2733 (0.4%)
2	C	1.03	0/1232	1.15	4/1682 (0.2%)
2	D	1.11	2/1232 (0.2%)	1.23	4/1682 (0.2%)
All	All	1.05	5/6498 (0.1%)	1.21	25/8841 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	GLU	CD-OE2	-6.84	1.18	1.25
1	A	148	TYR	CA-C	6.04	1.68	1.52
2	D	56	TRP	CB-CG	5.52	1.60	1.50
1	A	107	PRO	CA-C	-5.46	1.42	1.52
2	D	82	PRO	CA-C	-5.17	1.42	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	55	SER	C-N-CA	-7.00	104.20	121.70
1	B	86	LYS	CA-C-N	6.11	128.42	116.20
1	B	253	THR	N-CA-C	-6.01	94.77	111.00
1	B	66	MET	N-CA-C	-6.00	94.81	111.00
1	B	253	THR	N-CA-CB	5.96	121.63	110.30
1	B	116	ARG	CB-CA-C	5.96	122.33	110.40
1	B	145	HIS	C-N-CA	-5.89	106.98	121.70
2	D	142	ASP	CB-CA-C	-5.76	98.87	110.40
2	C	41	ASN	N-CA-C	-5.70	95.60	111.00
1	A	97	HIS	N-CA-CB	-5.68	100.37	110.60
1	A	123	GLY	N-CA-C	5.67	127.28	113.10
1	A	196	MET	N-CA-CB	-5.54	100.62	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	62	CYS	C-N-CA	-5.53	107.87	121.70
1	B	122	GLU	CB-CA-C	5.46	121.32	110.40
2	C	122	TRP	N-CA-CB	5.38	120.29	110.60
1	B	66	MET	N-CA-CB	5.38	120.28	110.60
2	D	26	GLN	N-CA-CB	-5.37	100.93	110.60
1	B	71	CYS	C-N-CA	5.29	134.92	121.70
2	C	41	ASN	CB-CA-C	-5.26	99.87	110.40
2	D	91	HIS	CA-CB-CG	-5.25	104.68	113.60
2	D	52	HIS	C-N-CA	-5.20	108.69	121.70
2	C	41	ASN	N-CA-CB	5.18	119.93	110.60
1	B	40	ASP	CB-CA-C	-5.15	100.10	110.40
1	A	97	HIS	CB-CA-C	5.10	120.60	110.40
1	B	70	GLY	C-N-CA	-5.06	109.05	121.70

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	1971	0	1823	163	0
1	B	1963	0	1812	153	1
2	C	1211	0	1164	125	2
2	D	1211	0	1164	73	2
3	A	47	0	0	3	0
3	B	51	0	0	3	0
3	C	22	0	0	3	0
3	D	23	0	0	1	0
All	All	6499	0	5963	480	3

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 39.

All (480) 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:A:66:MET:HE1	2:C:56:TRP:HB2	1.46	0.95
1:B:108:CYS:SG	1:B:109:GLU:N	2.41	0.94
2:C:168:ALA:O	2:C:171:ASN:HB2	1.72	0.89
1:A:29:SCH:HA	1:A:199:HIS:CE1	2.09	0.88
2:C:110:GLN:HE21	2:C:110:GLN:HA	1.39	0.86
1:A:177:TYR:CD2	1:A:190:HIS:CE1	2.65	0.84
2:C:110:GLN:HA	2:C:110:GLN:NE2	1.93	0.81
1:A:85:ARG:HD3	2:C:56:TRP:CH2	2.17	0.80
1:A:242:ILE:HG23	1:A:243:GLU:HG3	1.65	0.79
1:A:65:SER:H	2:C:88:ASN:ND2	1.81	0.79
1:A:29:SCH:HB2	1:A:200:ALA:H	1.46	0.78
1:B:29:SCH:SG	1:B:30:TRP:CE3	2.75	0.78
1:A:0:LYS:H	1:A:0:LYS:HD3	1.51	0.75
1:A:85:ARG:HD2	2:C:56:TRP:CZ2	2.20	0.75
1:B:75:TYR:CZ	2:D:48:ARG:HG3	2.21	0.75
1:A:177:TYR:CG	1:A:190:HIS:CE1	2.75	0.75
2:C:66:LEU:HD13	2:C:101:ASN:ND2	2.03	0.74
2:D:50:PRO:HB2	2:D:65:LEU:HD21	1.69	0.73
1:A:23:GLN:NE2	1:A:26:CYS:O	2.21	0.73
2:D:33:LEU:O	2:D:38:ALA:HB2	1.88	0.73
2:C:72:VAL:HG12	3:C:205:HOH:O	1.90	0.72
1:A:66:MET:CE	2:C:56:TRP:HB2	2.20	0.72
1:A:21:ARG:NH1	1:A:35:VAL:HG23	2.06	0.70
1:B:29:SCH:SG	1:B:30:TRP:HE3	2.14	0.70
2:D:93:GLU:CD	2:D:93:GLU:H	1.94	0.69
1:A:69:ASP:HB2	2:C:78:TRP:CD1	2.27	0.69
1:A:24:GLY:HA2	1:A:108:CYS:SG	2.33	0.69
1:A:17:ILE:HG12	1:A:40:ASP:HB3	1.75	0.69
2:D:59:LEU:O	2:D:62:VAL:N	2.26	0.69
2:D:110:GLN:NE2	2:D:110:GLN:HA	2.08	0.68
1:A:66:MET:HE1	2:C:56:TRP:CB	2.22	0.68
1:B:116:ARG:HG3	1:B:117:PRO:HD2	1.76	0.68
2:C:165:GLN:HE21	2:C:169:LYS:H	1.39	0.68
1:B:30:TRP:CG	1:B:31:ALA:N	2.63	0.67
1:A:37:ALA:HB3	1:A:80:TRP:CH2	2.30	0.67
1:A:94:TYR:CD2	1:A:106:PRO:HA	2.30	0.67
2:D:120:ALA:HB1	2:D:152:ALA:HB2	1.78	0.66
1:A:38:ILE:HG23	1:A:83:TRP:CZ2	2.30	0.66
2:D:57:GLY:HA3	3:D:209:HOH:O	1.96	0.66
2:D:109:SER:O	2:D:111:ARG:N	2.29	0.66
1:A:85:ARG:CD	2:C:56:TRP:CH2	2.78	0.66
2:C:72:VAL:HG22	2:C:72:VAL:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:TRP:CE3	1:B:74:GLY:N	2.64	0.65
1:B:38:ILE:HG12	1:B:80:TRP:CZ3	2.31	0.65
1:A:130:LYS:O	1:A:140:TYR:CG	2.50	0.65
2:D:56:TRP:CE3	2:D:57:GLY:N	2.65	0.65
1:B:30:TRP:CZ2	1:B:70:GLY:O	2.49	0.65
1:A:30:TRP:CE3	1:A:79:ALA:HB2	2.31	0.64
1:A:146:TYR:HB2	1:A:252:ARG:HE	1.63	0.64
2:C:106:ASN:N	2:C:106:ASN:HD22	1.96	0.64
1:B:85:ARG:HB3	2:D:56:TRP:CZ2	2.33	0.64
1:A:17:ILE:HA	1:A:40:ASP:OD1	1.98	0.64
1:B:26:CYS:SG	1:B:60:LEU:HD21	2.38	0.64
1:B:35:VAL:HG21	1:B:56:ALA:HB2	1.80	0.64
1:B:99:GLY:O	1:B:133:GLU:HG2	1.97	0.64
1:A:65:SER:H	2:C:88:ASN:HD22	1.43	0.64
1:A:2:PRO:HG2	1:A:5:PHE:HB2	1.79	0.63
2:C:40:VAL:O	2:C:40:VAL:CG1	2.46	0.63
2:C:128:VAL:O	2:C:132:LEU:HD13	1.98	0.63
1:A:23:GLN:NE2	1:A:28:SER:H	1.97	0.63
1:A:65:SER:HB2	2:C:85:LEU:HD23	1.79	0.63
1:B:85:ARG:HG3	2:D:56:TRP:CE2	2.33	0.63
1:A:26:CYS:HB2	1:A:105:ILE:HD13	1.81	0.62
1:B:41:ARG:NH2	1:B:248:ALA:HB1	2.15	0.62
1:B:173:ALA:O	1:B:174:PHE:HB3	1.99	0.62
2:C:149:PHE:HE1	2:C:161:ALA:O	1.81	0.62
1:B:26:CYS:SG	1:B:105:ILE:CD1	2.88	0.62
1:B:25:SER:O	1:B:122:GLU:O	2.16	0.62
2:C:30:VAL:HG21	2:C:61:ILE:CD1	2.28	0.62
1:B:30:TRP:CZ3	1:B:74:GLY:N	2.68	0.61
1:B:6:ASP:HB3	1:B:9:GLU:CB	2.30	0.61
2:D:141:ASN:N	2:D:141:ASN:HD22	1.98	0.61
1:A:38:ILE:HG21	1:A:83:TRP:CE2	2.35	0.61
1:A:43:CYS:HA	1:A:50:VAL:O	2.00	0.61
1:B:234:LEU:HB3	1:B:239:HIS:CB	2.31	0.61
1:A:177:TYR:CE2	1:A:195:MET:HB2	2.36	0.60
1:A:85:ARG:HD2	2:C:56:TRP:CE2	2.35	0.60
1:A:214:TYR:CE1	1:A:232:LYS:HG2	2.36	0.60
1:A:38:ILE:O	1:A:42:ILE:HG13	2.01	0.60
2:C:29:GLU:HG3	2:C:33:LEU:HD23	1.83	0.60
1:B:136:TYR:CE1	1:B:138:PRO:HG2	2.36	0.60
2:C:106:ASN:N	2:C:106:ASN:ND2	2.50	0.60
1:B:234:LEU:HB3	1:B:239:HIS:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:HIS:CD2	1:A:240:CYS:HG	2.19	0.60
1:B:239:HIS:O	1:B:240:CYS:HB2	2.00	0.60
1:A:30:TRP:CG	1:A:31:ALA:N	2.69	0.59
1:A:85:ARG:CD	2:C:56:TRP:CZ2	2.85	0.59
1:A:94:TYR:CD2	1:A:107:PRO:HD3	2.37	0.59
1:B:65:SER:O	2:D:85:LEU:HD22	2.02	0.59
1:B:30:TRP:CZ3	1:B:73:GLY:CA	2.85	0.59
2:C:45:THR:O	2:C:46:TYR:HB2	2.02	0.59
1:B:89:VAL:HG13	1:B:144:LYS:NZ	2.17	0.59
2:D:54:ALA:HB1	2:D:62:VAL:HG23	1.85	0.59
2:D:33:LEU:O	2:D:38:ALA:CB	2.51	0.59
1:B:157:GLU:O	1:B:161:MET:SD	2.61	0.59
1:A:183:TYR:CE2	1:A:231:PHE:CB	2.86	0.58
1:B:82:PHE:CE1	1:B:86:LYS:HD2	2.38	0.58
1:A:87:GLY:O	1:A:144:LYS:HE3	2.03	0.58
2:C:142:ASP:HB3	2:C:146:LYS:O	2.03	0.58
1:B:66:MET:O	2:D:48:ARG:NH2	2.36	0.58
1:A:29:SCH:HA	1:A:199:HIS:ND1	2.18	0.58
1:B:85:ARG:CB	2:D:56:TRP:CZ2	2.88	0.57
2:C:34:ILE:HD11	2:C:64:VAL:HG11	1.86	0.57
1:A:136:TYR:CE2	1:A:138:PRO:HG2	2.40	0.57
1:A:109:GLU:O	1:A:119:CYS:SG	2.63	0.57
1:B:78:GLU:HA	1:B:81:ASN:HB2	1.87	0.57
1:B:38:ILE:HG23	1:B:83:TRP:CZ2	2.39	0.57
1:B:80:TRP:CD1	1:B:247:VAL:HG21	2.40	0.57
2:D:147:THR:HB	2:D:148:PRO:HD2	1.86	0.57
1:A:8:ARG:HG2	1:A:17:ILE:HG22	1.87	0.57
1:A:103:TYR:CE2	1:A:105:ILE:HB	2.40	0.57
1:A:0:LYS:H	1:A:0:LYS:CD	2.17	0.56
2:C:54:ALA:C	2:C:56:TRP:H	2.08	0.56
1:A:75:TYR:CE1	2:C:48:ARG:NH1	2.74	0.56
1:B:65:SER:OG	2:D:88:ASN:ND2	2.38	0.56
1:B:29:SCH:SG	1:B:30:TRP:CZ3	2.98	0.56
2:C:21:ALA:O	2:C:25:GLY:N	2.37	0.56
1:B:73:GLY:O	2:D:78:TRP:NE1	2.38	0.56
1:B:77:ALA:HB2	3:B:328:HOH:O	2.06	0.56
1:A:75:TYR:HE1	2:C:48:ARG:NH1	2.03	0.56
2:C:34:ILE:CD1	2:C:64:VAL:CG1	2.83	0.56
1:A:29:SCH:C	1:A:200:ALA:HB3	2.36	0.56
1:A:63:CYS:SG	1:A:82:PHE:CD1	2.99	0.56
2:D:117:HIS:HE1	2:D:140:ALA:HB3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:168:ALA:O	2:C:171:ASN:N	2.34	0.55
1:B:6:ASP:HB3	1:B:9:GLU:H	1.70	0.55
2:D:109:SER:O	2:D:112:GLY:N	2.37	0.55
1:A:171:GLU:HG2	1:A:172:GLY:N	2.20	0.55
1:B:30:TRP:HZ2	1:B:70:GLY:O	1.88	0.55
1:B:69:ASP:HB3	1:B:72:ASN:HB2	1.87	0.55
1:A:177:TYR:CD2	1:A:190:HIS:HE1	2.22	0.55
1:A:183:TYR:CE2	1:A:231:PHE:HB2	2.42	0.55
1:B:195:MET:O	1:B:195:MET:HG2	2.06	0.55
1:B:176:VAL:HG21	1:B:199:HIS:ND1	2.22	0.55
1:B:204:LEU:HD23	1:B:204:LEU:H	1.72	0.55
2:C:149:PHE:CE1	2:C:161:ALA:O	2.60	0.55
1:B:30:TRP:CD1	1:B:31:ALA:N	2.76	0.55
1:B:41:ARG:NH2	1:B:170:VAL:HG12	2.22	0.55
1:B:89:VAL:HG12	1:B:143:ASP:HB3	1.89	0.55
1:B:38:ILE:O	1:B:42:ILE:HG13	2.07	0.54
1:B:234:LEU:HD22	1:B:239:HIS:HB2	1.89	0.54
1:A:38:ILE:CG2	1:A:83:TRP:CE2	2.91	0.54
1:A:47:ASN:O	1:A:48:ALA:HB3	2.08	0.54
1:A:70:GLY:HA3	1:A:125:THR:HG23	1.89	0.54
1:B:30:TRP:CZ3	1:B:73:GLY:HA2	2.42	0.54
1:A:20:ILE:HD11	1:A:230:PHE:CE2	2.42	0.54
1:A:29:SCH:CB	1:A:199:HIS:ND1	2.70	0.54
2:C:40:VAL:O	2:C:41:ASN:CB	2.55	0.54
2:C:143:ARG:HD3	2:C:143:ARG:O	2.08	0.54
1:B:38:ILE:CG1	1:B:80:TRP:CZ3	2.90	0.54
1:A:29:SCH:CB	1:A:199:HIS:HD1	2.20	0.53
1:B:47:ASN:HD21	1:B:49:HIS:CE1	2.27	0.53
1:B:234:LEU:CD2	1:B:237:GLN:HB2	2.38	0.53
2:D:18:LEU:HD22	2:D:50:PRO:HB3	1.90	0.53
1:B:180:PHE:O	1:B:182:LEU:N	2.40	0.53
1:B:202:ARG:HG2	1:B:218:ALA:HB3	1.89	0.53
2:C:127:ILE:O	2:C:131:LEU:HD13	2.08	0.53
2:D:73:ASN:OD1	2:D:103:ALA:HA	2.08	0.53
2:D:44:ASP:O	2:D:46:TYR:N	2.42	0.53
1:B:44:ILE:O	1:B:47:ASN:N	2.34	0.53
2:C:34:ILE:HG13	2:C:35:ALA:N	2.23	0.53
1:B:181:LEU:HD11	1:B:196:MET:SD	2.48	0.53
2:D:116:LEU:O	2:D:116:LEU:HD23	2.09	0.53
1:A:29:SCH:HB2	1:A:200:ALA:N	2.20	0.53
2:C:66:LEU:HD13	2:C:101:ASN:HD22	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:109:SER:C	2:D:111:ARG:H	2.11	0.53
2:C:30:VAL:HG21	2:C:61:ILE:HG12	1.91	0.53
2:C:51:LEU:HB2	3:C:209:HOH:O	2.09	0.53
2:C:143:ARG:O	2:C:145:GLY:N	2.42	0.52
1:A:17:ILE:HG12	1:A:40:ASP:OD1	2.09	0.52
1:A:30:TRP:HE3	1:A:79:ALA:HB2	1.74	0.52
2:C:70:ALA:HB1	3:C:209:HOH:O	2.08	0.52
2:C:143:ARG:C	2:C:145:GLY:N	2.63	0.52
1:B:24:GLY:O	1:B:119:CYS:SG	2.68	0.52
2:C:34:ILE:O	2:C:37:GLY:N	2.42	0.52
1:A:58:ASP:HA	1:A:101:ARG:NH1	2.25	0.52
1:A:253:THR:O	1:A:254:ASP:CB	2.57	0.52
1:B:89:VAL:HG13	1:B:144:LYS:HZ3	1.75	0.52
2:C:40:VAL:O	2:C:40:VAL:HG13	2.10	0.52
1:A:221:TRP:O	1:A:222:ASN:HB3	2.10	0.51
2:D:93:GLU:CD	2:D:93:GLU:N	2.63	0.51
1:A:107:PRO:HB2	1:A:116:ARG:CD	2.40	0.51
1:B:44:ILE:HG22	1:B:45:HIS:N	2.25	0.51
1:B:6:ASP:HB3	1:B:9:GLU:HB2	1.92	0.51
2:C:40:VAL:O	2:C:41:ASN:CG	2.48	0.51
1:A:17:ILE:CG1	1:A:40:ASP:HB3	2.39	0.51
1:B:35:VAL:O	1:B:39:SER:OG	2.29	0.51
2:C:105:VAL:O	2:C:115:PRO:HD2	2.11	0.51
2:C:153:ILE:O	2:C:155:ASN:O	2.28	0.51
1:A:120:THR:HG22	1:A:120:THR:O	2.11	0.51
2:C:153:ILE:HG22	2:C:154:ASP:N	2.26	0.51
1:A:23:GLN:NE2	1:A:28:SER:N	2.57	0.51
1:B:68:GLY:HA3	1:B:74:GLY:HA2	1.91	0.51
1:B:71:CYS:O	1:B:122:GLU:HB3	2.11	0.51
1:B:38:ILE:HG23	1:B:83:TRP:CH2	2.45	0.51
1:B:164:ILE:HG12	1:B:170:VAL:HG13	1.93	0.51
1:A:24:GLY:O	1:A:25:SER:CB	2.59	0.50
1:A:109:GLU:N	1:A:119:CYS:SG	2.84	0.50
2:C:18:LEU:HD12	2:C:38:ALA:HB3	1.92	0.50
2:D:123:GLY:O	2:D:124:HIS:CD2	2.63	0.50
1:A:65:SER:HB2	2:C:85:LEU:CD2	2.42	0.50
2:C:14:LEU:CD1	2:C:33:LEU:CD1	2.90	0.50
2:C:61:ILE:O	2:C:65:LEU:HD13	2.11	0.50
1:B:41:ARG:HH21	1:B:170:VAL:HG12	1.75	0.50
1:A:80:TRP:CZ3	1:A:248:ALA:HA	2.47	0.50
2:D:59:LEU:O	2:D:60:GLU:C	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:110:GLN:HE21	2:C:110:GLN:CA	2.19	0.50
2:C:116:LEU:HD22	2:C:148:PRO:CB	2.42	0.50
1:A:148:TYR:N	1:A:250:ILE:O	2.42	0.50
1:B:47:ASN:C	1:B:49:HIS:H	2.14	0.50
2:C:41:ASN:OD1	2:C:70:ALA:HA	2.11	0.50
1:B:57:GLU:OE2	1:B:61:THR:HG21	2.12	0.50
2:D:39:ASP:O	2:D:40:VAL:HG12	2.11	0.49
2:D:141:ASN:N	2:D:141:ASN:ND2	2.60	0.49
1:B:233:ILE:HG12	1:B:234:LEU:N	2.27	0.49
1:B:253:THR:O	1:B:254:ASP:O	2.31	0.49
2:D:126:GLU:O	2:D:130:VAL:HG23	2.12	0.49
1:A:20:ILE:HD11	1:A:230:PHE:CZ	2.47	0.49
1:B:5:PHE:HE1	1:B:10:GLN:OE1	1.95	0.49
2:C:83:LEU:CD1	2:C:95:VAL:HG23	2.42	0.49
1:B:214:TYR:CD1	1:B:214:TYR:C	2.85	0.49
2:D:39:ASP:O	2:D:41:ASN:N	2.46	0.49
1:A:0:LYS:O	1:A:1:LEU:HD23	2.13	0.49
1:A:209:GLU:HB2	1:A:214:TYR:CE2	2.48	0.49
1:A:221:TRP:O	1:A:222:ASN:CB	2.61	0.49
1:A:227:ASP:C	1:A:228:ASN:HD22	2.16	0.49
1:B:41:ARG:HH12	1:B:167:ASN:HB2	1.77	0.49
1:A:38:ILE:CG2	1:A:83:TRP:CZ2	2.96	0.49
2:C:16:LYS:HZ1	2:C:44:ASP:HB3	1.78	0.49
1:B:31:ALA:O	1:B:35:VAL:HG22	2.13	0.49
2:C:30:VAL:HG11	2:C:61:ILE:HG23	1.95	0.49
1:A:223:THR:O	1:A:228:ASN:HA	2.13	0.49
2:D:26:GLN:HB3	2:D:29:GLU:HB3	1.94	0.49
1:A:21:ARG:NH1	1:A:35:VAL:CG2	2.75	0.48
1:A:37:ALA:HB3	1:A:80:TRP:HH2	1.78	0.48
1:A:234:LEU:HB3	1:A:239:HIS:HB2	1.95	0.48
1:B:78:GLU:HA	1:B:81:ASN:CB	2.43	0.48
2:C:34:ILE:HD12	2:C:64:VAL:HG12	1.95	0.48
1:B:48:ALA:O	1:B:49:HIS:C	2.52	0.48
1:B:80:TRP:CD1	1:B:247:VAL:CG2	2.96	0.48
1:B:237:GLN:O	1:B:238:ASP:HB3	2.12	0.48
2:D:76:ASP:OD2	2:D:80:TYR:HB2	2.14	0.48
1:B:40:ASP:O	1:B:43:CYS:HB3	2.13	0.48
1:A:209:GLU:HB2	1:A:214:TYR:HE2	1.78	0.48
1:A:225:TRP:CD2	1:A:226:GLY:N	2.81	0.48
1:B:38:ILE:CG2	1:B:83:TRP:CZ2	2.96	0.48
2:C:168:ALA:O	2:C:171:ASN:CB	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:HIS:CD2	1:A:240:CYS:SG	3.06	0.48
2:D:116:LEU:HD12	2:D:136:ALA:HB1	1.96	0.48
1:B:30:TRP:HZ3	1:B:73:GLY:HA2	1.79	0.48
1:B:60:LEU:HD11	1:B:70:GLY:O	2.13	0.48
2:C:29:GLU:O	2:C:33:LEU:HD23	2.14	0.48
2:D:60:GLU:O	2:D:63:ASP:HB2	2.13	0.48
2:C:143:ARG:C	2:C:145:GLY:H	2.17	0.48
1:B:38:ILE:HG21	1:B:83:TRP:CE2	2.49	0.48
2:C:150:ASP:O	2:C:154:ASP:N	2.47	0.48
1:A:41:ARG:HH21	1:A:170:VAL:HG12	1.78	0.48
1:A:225:TRP:CE3	1:A:226:GLY:N	2.82	0.48
1:B:75:TYR:CE1	2:D:46:TYR:HB2	2.48	0.47
2:C:14:LEU:HD11	2:C:33:LEU:CD1	2.44	0.47
2:C:34:ILE:CD1	2:C:64:VAL:HG12	2.44	0.47
2:D:121:THR:HG23	2:D:155:ASN:ND2	2.29	0.47
1:B:164:ILE:HA	1:B:168:GLY:O	2.14	0.47
2:C:54:ALA:C	2:C:56:TRP:N	2.67	0.47
1:A:176:VAL:O	1:A:195:MET:HA	2.14	0.47
1:B:112:VAL:HG11	1:B:225:TRP:HA	1.96	0.47
2:C:45:THR:O	2:C:46:TYR:CB	2.62	0.47
2:C:76:ASP:O	2:C:77:LYS:C	2.53	0.47
1:A:90:SER:HB2	1:A:100:CYS:H	1.79	0.47
1:A:100:CYS:HB2	1:A:143:ASP:OD2	2.14	0.47
1:B:5:PHE:CE1	1:B:10:GLN:OE1	2.68	0.47
2:C:83:LEU:HD12	2:C:95:VAL:HG23	1.97	0.47
1:A:214:TYR:CD1	1:A:232:LYS:HG2	2.50	0.47
2:C:75:SER:HA	2:C:80:TYR:O	2.15	0.47
1:A:45:HIS:CG	1:A:251:PRO:HG2	2.50	0.46
1:A:57:GLU:O	1:A:61:THR:HG23	2.14	0.46
1:A:140:TYR:OH	1:A:144:LYS:NZ	2.48	0.46
1:B:92:GLY:O	1:B:93:LEU:O	2.33	0.46
2:C:153:ILE:O	2:C:154:ASP:C	2.53	0.46
2:C:14:LEU:CD1	2:C:33:LEU:HD12	2.46	0.46
1:A:78:GLU:O	1:A:82:PHE:N	2.46	0.46
2:C:167:ALA:O	2:C:168:ALA:C	2.52	0.46
1:A:133:GLU:HA	1:A:134:PRO:HD2	1.77	0.46
1:B:29:SCH:HB3	1:B:200:ALA:H	1.80	0.46
1:A:9:GLU:O	1:A:12:PRO:HD3	2.16	0.46
2:D:123:GLY:HA2	2:D:160:ILE:HD12	1.98	0.46
1:A:43:CYS:O	1:A:48:ALA:N	2.46	0.46
1:A:174:PHE:HA	3:A:316:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:VAL:HG21	2:C:61:ILE:CG1	2.45	0.46
2:C:54:ALA:O	2:C:56:TRP:N	2.48	0.46
1:A:234:LEU:HB3	1:A:239:HIS:CB	2.46	0.46
1:B:30:TRP:CH2	1:B:70:GLY:O	2.69	0.46
2:C:30:VAL:HG21	2:C:61:ILE:HD13	1.97	0.46
2:D:110:GLN:NE2	2:D:110:GLN:CA	2.78	0.46
1:A:35:VAL:HG13	1:A:59:LEU:HD23	1.98	0.46
1:A:38:ILE:HD13	1:A:83:TRP:CD2	2.51	0.46
2:C:105:VAL:HG21	2:C:134:ASN:O	2.16	0.46
1:A:64:GLY:HA3	2:C:88:ASN:HD21	1.81	0.46
1:B:222:ASN:CG	1:B:223:THR:N	2.69	0.46
1:B:214:TYR:HA	1:B:235:ARG:H	1.81	0.45
3:B:306:HOH:O	2:D:53:ALA:HB1	2.15	0.45
2:C:127:ILE:N	2:C:127:ILE:HD12	2.31	0.45
1:B:55:SER:OG	1:B:57:GLU:HB3	2.17	0.45
1:A:29:SCH:SG	1:A:199:HIS:ND1	2.79	0.45
1:B:20:ILE:HG22	1:B:21:ARG:N	2.31	0.45
2:C:30:VAL:O	2:C:34:ILE:HG12	2.17	0.45
1:B:20:ILE:CG2	1:B:21:ARG:N	2.80	0.45
1:B:26:CYS:HB2	1:B:105:ILE:HD13	1.99	0.45
2:C:116:LEU:HD12	2:C:136:ALA:HB1	1.99	0.45
1:B:160:ILE:O	1:B:163:GLU:HB3	2.16	0.45
1:B:43:CYS:SG	1:B:48:ALA:HA	2.57	0.45
1:B:75:TYR:OH	2:D:48:ARG:HB2	2.16	0.45
1:B:75:TYR:CE2	2:D:48:ARG:HG3	2.51	0.45
1:B:190:HIS:H	1:B:239:HIS:CE1	2.34	0.45
1:B:239:HIS:O	1:B:240:CYS:CB	2.64	0.45
2:C:147:THR:HB	2:C:148:PRO:HD2	1.98	0.45
2:D:44:ASP:O	2:D:45:THR:C	2.54	0.45
1:B:162:ALA:O	1:B:166:LYS:N	2.45	0.45
2:D:61:ILE:O	2:D:65:LEU:HD13	2.16	0.45
2:D:110:GLN:HA	2:D:110:GLN:HE21	1.82	0.45
1:A:63:CYS:HB3	1:A:67:CYS:HB2	1.78	0.45
1:A:171:GLU:HG3	1:A:201:ILE:O	2.17	0.45
1:A:181:LEU:O	1:A:182:LEU:CB	2.64	0.45
2:C:66:LEU:HB3	2:C:101:ASN:HD22	1.81	0.45
2:D:34:ILE:HA	2:D:38:ALA:HB3	1.98	0.45
1:A:30:TRP:CZ3	1:A:79:ALA:HB2	2.52	0.44
1:A:39:SER:O	1:A:40:ASP:C	2.54	0.44
1:B:177:TYR:O	1:B:180:PHE:HB3	2.17	0.44
1:A:6:ASP:HB3	1:A:9:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:HB2	1:A:103:TYR:HA	1.99	0.44
1:A:107:PRO:HB2	1:A:116:ARG:HD2	1.97	0.44
2:D:59:LEU:HD13	2:D:94:ILE:CG1	2.47	0.44
1:A:35:VAL:HG21	1:A:56:ALA:CA	2.48	0.44
1:B:142:GLN:O	1:B:142:GLN:HG2	2.17	0.44
2:C:116:LEU:N	2:C:131:LEU:HD23	2.33	0.44
1:A:134:PRO:HB2	2:D:35:ALA:HB1	1.98	0.44
1:A:136:TYR:HE2	1:A:138:PRO:HG2	1.83	0.44
1:A:181:LEU:O	1:A:182:LEU:HG	2.18	0.44
1:A:225:TRP:CE3	1:A:226:GLY:HA3	2.52	0.44
1:A:69:ASP:O	1:A:70:GLY:C	2.55	0.44
1:B:94:TYR:O	1:B:95:GLU:C	2.56	0.44
2:C:50:PRO:O	2:C:53:ALA:N	2.51	0.44
1:B:17:ILE:HG12	1:B:40:ASP:OD2	2.18	0.44
2:C:128:VAL:HG12	2:C:132:LEU:HD13	1.99	0.44
2:C:131:LEU:O	2:C:136:ALA:HB2	2.18	0.44
2:D:18:LEU:HD12	2:D:38:ALA:HB1	1.99	0.44
2:D:33:LEU:HD23	2:D:33:LEU:N	2.31	0.44
1:A:147:GLY:HA2	1:A:251:PRO:HA	2.00	0.44
1:B:186:GLY:O	1:B:232:LYS:HB2	2.18	0.44
2:C:39:ASP:OD2	2:C:41:ASN:O	2.36	0.44
2:C:92:LEU:HG	2:C:96:GLU:OE2	2.17	0.44
2:C:168:ALA:O	2:C:169:LYS:C	2.55	0.44
1:B:232:LYS:HD2	1:B:232:LYS:N	2.33	0.43
1:B:75:TYR:HE1	2:D:46:TYR:HB2	1.83	0.43
1:B:214:TYR:CA	1:B:235:ARG:HB3	2.47	0.43
2:C:39:ASP:O	2:C:40:VAL:O	2.35	0.43
2:D:56:TRP:HE3	2:D:57:GLY:N	2.11	0.43
1:A:14:CYS:HA	1:A:15:PRO:HD2	1.88	0.43
1:A:139:THR:O	1:A:143:ASP:N	2.48	0.43
1:B:35:VAL:HG13	1:B:59:LEU:HD23	1.99	0.43
1:B:222:ASN:CG	1:B:223:THR:H	2.22	0.43
2:C:105:VAL:HB	2:C:106:ASN:ND2	2.32	0.43
2:C:116:LEU:HD11	2:C:132:LEU:HD11	2.00	0.43
2:D:142:ASP:HB2	2:D:145:GLY:H	1.83	0.43
1:A:103:TYR:OH	1:A:105:ILE:HD12	2.17	0.43
1:B:80:TRP:NE1	1:B:247:VAL:HG23	2.32	0.43
1:B:238:ASP:HB2	1:B:243:GLU:OE1	2.18	0.43
2:C:34:ILE:HG13	2:C:35:ALA:H	1.83	0.43
1:B:224:ASP:O	1:B:225:TRP:C	2.55	0.43
2:C:120:ALA:CB	2:C:160:ILE:HG21	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:VAL:O	2:C:105:VAL:HG12	2.18	0.43
2:D:142:ASP:HB3	2:D:144:GLN:H	1.83	0.43
1:A:29:SCH:CA	1:A:199:HIS:ND1	2.82	0.43
2:D:105:VAL:HB	2:D:106:ASN:ND2	2.33	0.43
1:A:26:CYS:HB2	1:A:105:ILE:CD1	2.49	0.43
1:B:40:ASP:O	1:B:43:CYS:N	2.52	0.43
1:B:41:ARG:NH1	1:B:167:ASN:CB	2.81	0.43
1:B:164:ILE:CG1	1:B:170:VAL:HG13	2.49	0.43
1:A:21:ARG:HH11	1:A:35:VAL:HG23	1.83	0.43
2:D:52:HIS:HE1	2:D:81:THR:CA	2.32	0.43
1:A:61:THR:O	1:A:128:CYS:HB2	2.18	0.42
2:C:44:ASP:C	2:C:45:THR:O	2.56	0.42
2:D:16:LYS:O	2:D:20:ASP:N	2.48	0.42
2:D:40:VAL:CG1	2:D:41:ASN:H	2.32	0.42
2:D:115:PRO:O	2:D:118:VAL:HG13	2.19	0.42
1:A:96:SER:O	1:A:97:HIS:HB2	2.19	0.42
1:A:107:PRO:HB2	1:A:116:ARG:HD3	2.01	0.42
1:B:26:CYS:SG	1:B:105:ILE:HD12	2.57	0.42
2:D:120:ALA:HA	2:D:160:ILE:HG21	2.01	0.42
1:B:6:ASP:CB	1:B:9:GLU:HB2	2.50	0.42
1:B:41:ARG:NH2	1:B:248:ALA:CB	2.81	0.42
1:B:157:GLU:HG2	1:B:161:MET:SD	2.59	0.42
2:D:111:ARG:HH11	2:D:111:ARG:CG	2.32	0.42
1:A:140:TYR:CZ	1:A:144:LYS:NZ	2.88	0.42
1:B:148:TYR:CD2	1:B:149:ASN:HB3	2.55	0.42
1:A:23:GLN:HE21	1:A:28:SER:H	1.64	0.42
1:A:180:PHE:O	1:A:181:LEU:C	2.56	0.42
1:B:148:TYR:HD2	1:B:149:ASN:HB3	1.84	0.42
1:B:242:ILE:HG13	1:B:242:ILE:O	2.20	0.42
1:A:94:TYR:CE2	1:A:106:PRO:HA	2.54	0.42
1:B:208:VAL:HG12	1:B:209:GLU:N	2.34	0.42
2:C:66:LEU:CB	2:C:101:ASN:HD22	2.32	0.42
2:C:110:GLN:NE2	2:C:110:GLN:CA	2.75	0.42
2:C:118:VAL:HG23	2:C:119:ALA:N	2.35	0.42
1:A:20:ILE:HG21	1:A:229:GLY:HA3	2.02	0.42
1:A:157:GLU:O	1:A:160:ILE:N	2.53	0.42
1:A:234:LEU:HD11	3:A:327:HOH:O	2.18	0.42
1:A:32:PHE:HB3	1:A:36:GLU:OE2	2.19	0.42
1:A:61:THR:HG22	1:A:126:PRO:HG2	2.01	0.42
1:A:84:THR:HG21	1:A:149:ASN:C	2.40	0.42
1:A:227:ASP:OD1	1:A:228:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:PHE:HA	1:B:35:VAL:HG22	2.02	0.42
1:B:179:ASP:HB3	1:B:192:THR:O	2.19	0.42
2:C:29:GLU:HG3	2:C:29:GLU:O	2.20	0.42
2:C:49:THR:HB	2:C:50:PRO:CD	2.50	0.42
2:C:146:LYS:HA	2:C:150:ASP:OD2	2.20	0.42
2:C:34:ILE:CD1	2:C:64:VAL:HG11	2.48	0.42
2:C:70:ALA:O	2:C:71:ASP:C	2.57	0.42
2:C:149:PHE:CE1	2:C:165:GLN:HB2	2.55	0.42
1:A:227:ASP:HB3	1:A:230:PHE:O	2.20	0.42
1:B:89:VAL:N	1:B:144:LYS:HZ3	2.17	0.42
2:C:80:TYR:HD2	2:C:84:HIS:CD2	2.38	0.41
1:A:100:CYS:O	1:A:132:CYS:HB3	2.20	0.41
2:C:73:ASN:HD21	2:C:103:ALA:HA	1.84	0.41
2:C:159:ASP:O	2:C:162:GLU:N	2.49	0.41
1:A:35:VAL:HG13	1:A:59:LEU:CD2	2.51	0.41
1:A:69:ASP:HB3	1:A:72:ASN:HB2	2.01	0.41
1:B:65:SER:O	2:D:85:LEU:CD2	2.66	0.41
2:C:70:ALA:O	2:C:72:VAL:N	2.52	0.41
2:C:74:ALA:O	2:C:81:THR:HA	2.21	0.41
2:C:90:GLY:O	2:C:91:HIS:HB2	2.20	0.41
1:A:65:SER:N	2:C:88:ASN:ND2	2.61	0.41
1:A:171:GLU:HG2	1:A:172:GLY:H	1.84	0.41
1:A:242:ILE:HG13	1:A:242:ILE:O	2.20	0.41
1:B:41:ARG:NH1	1:B:167:ASN:HB2	2.35	0.41
1:B:85:ARG:CB	2:D:56:TRP:HZ2	2.31	0.41
1:B:178:SER:C	1:B:180:PHE:H	2.23	0.41
2:D:142:ASP:CB	2:D:144:GLN:H	2.33	0.41
1:A:130:LYS:HD2	3:A:333:HOH:O	2.19	0.41
1:B:174:PHE:HE2	1:B:201:ILE:HG12	1.86	0.41
1:B:250:ILE:HG22	1:B:251:PRO:N	2.35	0.41
2:C:39:ASP:O	2:C:40:VAL:HG12	2.20	0.41
2:C:165:GLN:NE2	2:C:169:LYS:H	2.13	0.41
1:A:177:TYR:O	1:A:180:PHE:HB3	2.21	0.41
1:A:209:GLU:C	1:A:211:GLY:N	2.73	0.41
1:B:177:TYR:HA	1:B:194:GLU:O	2.21	0.41
1:B:189:GLN:O	1:B:191:VAL:HG23	2.21	0.41
2:D:40:VAL:HG13	2:D:41:ASN:N	2.36	0.41
1:B:173:ALA:O	1:B:174:PHE:CB	2.69	0.41
2:C:83:LEU:HD22	2:C:103:ALA:HB1	2.02	0.41
1:A:109:GLU:OE2	1:A:116:ARG:HB2	2.21	0.41
1:A:110:HIS:O	1:A:112:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLU:CG	1:A:201:ILE:O	2.68	0.41
1:B:28:SER:O	1:B:29:SCH:C	2.69	0.41
1:B:178:SER:OG	1:B:194:GLU:N	2.54	0.41
2:C:10:HIS:O	2:C:14:LEU:HB2	2.21	0.41
2:C:18:LEU:HD23	2:C:18:LEU:O	2.21	0.41
2:D:55:ALA:C	2:D:56:TRP:O	2.57	0.41
2:D:66:LEU:CD1	2:D:97:VAL:HG12	2.51	0.41
1:B:47:ASN:O	1:B:47:ASN:ND2	2.54	0.41
1:B:180:PHE:C	1:B:182:LEU:N	2.74	0.41
1:A:55:SER:HB2	1:A:91:GLY:HA3	2.02	0.40
1:A:57:GLU:O	1:A:58:ASP:C	2.59	0.40
1:A:76:PRO:O	1:A:77:ALA:C	2.60	0.40
1:B:6:ASP:O	1:B:7:ALA:C	2.57	0.40
1:B:85:ARG:HB3	2:D:56:TRP:HZ2	1.79	0.40
2:C:34:ILE:HG21	2:C:34:ILE:HD13	1.82	0.40
1:A:64:GLY:HA2	2:C:122:TRP:CZ2	2.56	0.40
1:A:79:ALA:O	1:A:82:PHE:HB3	2.22	0.40
1:B:38:ILE:CG2	1:B:83:TRP:CE2	3.04	0.40
1:B:10:GLN:HB3	1:B:11:TRP:CE3	2.56	0.40
1:A:68:GLY:HA3	1:A:74:GLY:HA2	2.03	0.40
1:A:80:TRP:O	1:A:83:TRP:HB3	2.22	0.40
1:B:21:ARG:HB2	1:B:36:GLU:OE1	2.21	0.40
1:B:44:ILE:HG21	1:B:167:ASN:O	2.21	0.40
1:B:209:GLU:O	1:B:210:ASN:HB2	2.21	0.40
1:B:25:SER:HB2	3:B:312:HOH:O	2.21	0.40
1:B:106:PRO:HA	1:B:107:PRO:HD3	2.00	0.40
2:C:14:LEU:HD12	2:C:33:LEU:CD1	2.51	0.40
2:D:66:LEU:HD21	2:D:72:VAL:HG23	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:68:TYR:CD2	2:D:31:ARG:NH1[4_558]	1.52	0.68
1:B:111:HIS:CD2	1:B:141:LYS:NZ[1_554]	2.15	0.05
2:C:68:TYR:CG	2:D:31:ARG:NH1[4_558]	2.15	0.05

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	253/256 (99%)	210 (83%)	39 (15%)	4 (2%)	9 16
1	B	252/256 (98%)	195 (77%)	48 (19%)	9 (4%)	3 5
2	C	161/171 (94%)	117 (73%)	34 (21%)	10 (6%)	1 1
2	D	161/171 (94%)	136 (84%)	14 (9%)	11 (7%)	1 1
All	All	827/854 (97%)	658 (80%)	135 (16%)	34 (4%)	3 3

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLU
1	B	93	LEU
1	B	253	THR
2	C	41	ASN
2	C	154	ASP
2	D	26	GLN
2	D	45	THR
2	D	57	GLY
2	D	110	GLN
1	B	117	PRO
1	B	181	LEU
2	D	41	ASN
1	B	174	PHE
2	C	155	ASN
2	C	169	LYS
2	D	31	ARG
2	D	37	GLY
1	A	25	SER
2	C	40	VAL
2	C	153	ILE
2	D	77	LYS
1	A	121	GLY

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Mol	Chain	Res	Type
2	C	126	GLU
2	C	27	ASP
2	D	46	TYR
1	B	137	SER
2	C	11	GLY
2	C	72	VAL
2	D	30	VAL
2	D	40	VAL
1	A	92	GLY
1	B	89	VAL
1	B	44	ILE
1	B	102	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	210/210 (100%)	188 (90%)	22 (10%)	7 11
1	B	209/210 (100%)	185 (88%)	24 (12%)	5 9
2	C	122/129 (95%)	108 (88%)	14 (12%)	5 9
2	D	122/129 (95%)	108 (88%)	14 (12%)	5 9
All	All	663/678 (98%)	589 (89%)	74 (11%)	6 10

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	LYS
1	A	4	SER
1	A	28	SER
1	A	40	ASP
1	A	61	THR
1	A	63	CYS
1	A	65	SER
1	A	69	ASP
1	A	72	ASN

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Mol	Chain	Res	Type
1	A	75	TYR
1	A	115	SER
1	A	125	THR
1	A	128	CYS
1	A	142	GLN
1	A	152	SER
1	A	155	ASN
1	A	194	GLU
1	A	196	MET
1	A	204	LEU
1	A	228	ASN
1	A	232	LYS
1	A	244	SER
1	B	16	THR
1	B	22	ASP
1	B	25	SER
1	B	39	SER
1	B	40	ASP
1	B	47	ASN
1	B	51	SER
1	B	66	MET
1	B	75	TYR
1	B	108	CYS
1	B	115	SER
1	B	119	CYS
1	B	133	GLU
1	B	152	SER
1	B	154	SER
1	B	155	ASN
1	B	178	SER
1	B	179	ASP
1	B	181	LEU
1	B	202	ARG
1	B	210	ASN
1	B	232	LYS
1	B	237	GLN
1	B	253	THR
2	C	12	SER
2	C	31	ARG
2	C	40	VAL
2	C	43	SER
2	C	45	THR

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Mol	Chain	Res	Type
2	C	75	SER
2	C	106	ASN
2	C	110	GLN
2	C	113	GLN
2	C	129	ASP
2	C	142	ASP
2	C	143	ARG
2	C	159	ASP
2	C	166	LYS
2	D	12	SER
2	D	17	LYS
2	D	20	ASP
2	D	23	SER
2	D	26	GLN
2	D	33	LEU
2	D	48	ARG
2	D	99	LEU
2	D	110	GLN
2	D	111	ARG
2	D	118	VAL
2	D	126	GLU
2	D	141	ASN
2	D	159	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	190	HIS
1	A	228	ASN
1	B	47	ASN
1	B	72	ASN
1	B	142	GLN
1	B	155	ASN
1	B	189	GLN
1	B	210	ASN
1	B	228	ASN
1	B	237	GLN
2	C	36	ASN
2	C	73	ASN
2	C	88	ASN
2	C	106	ASN

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Mol	Chain	Res	Type
2	C	110	GLN
2	C	113	GLN
2	C	165	GLN
2	D	88	ASN
2	D	110	GLN
2	D	124	HIS
2	D	141	ASN
2	D	155	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	SCH	B	29	1	6,7,8	0.46	0	3,7,9	1.84	1 (33%)
1	SCH	A	29	1	6,7,8	0.56	0	3,7,9	1.51	1 (33%)

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	SCH	B	29	1	-	0/2/6/8	-
1	SCH	A	29	1	-	1/2/6/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	29	SCH	CB-SG-SD	2.76	110.98	103.82
1	A	29	SCH	CE-SD-SG	2.43	110.98	102.58

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	29	SCH	CA-CB-SG-SD

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	29	SCH	5	0
1	A	29	SCH	9	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	254/256 (99%)	0.09	9 (3%) 44 52	13, 49, 92, 99	2 (0%)
1	B	254/256 (99%)	0.60	31 (12%) 4 4	20, 78, 99, 99	5 (1%)
2	C	163/171 (95%)	0.58	21 (12%) 3 4	28, 71, 99, 99	0
2	D	161/171 (94%)	0.26	6 (3%) 41 49	21, 55, 89, 99	3 (1%)
All	All	832/854 (97%)	0.37	67 (8%) 12 14	13, 61, 98, 99	10 (1%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	170	LEU	9.3
1	B	206	TRP	6.2
1	B	192	THR	6.0
1	A	192	THR	5.9
2	C	13	ASP	5.5
2	C	12	SER	5.5
2	D	9	HIS	5.0
1	B	165	TYR	5.0
2	C	169	LYS	5.0
2	C	11	GLY	4.8
1	B	160	ILE	4.4
1	B	231	PHE	4.1
1	B	10	GLN	4.0
1	B	191	VAL	4.0
1	B	217	VAL	3.8
1	B	215	TRP	3.8
1	A	180	PHE	3.5
1	B	213	PRO	3.4
1	A	196	MET	3.4
2	C	14	LEU	3.4
1	B	177	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	205	GLY	3.3
2	C	144	GLN	3.3
1	B	164	ILE	3.1
1	B	161	MET	3.0
1	B	188	TYR	3.0
2	D	38	ALA	3.0
2	C	141	ASN	2.9
1	A	124	ASP	2.9
2	C	168	ALA	2.9
2	C	10	HIS	2.9
1	A	181	LEU	2.8
2	C	32	ILE	2.7
1	B	195	MET	2.7
1	A	1	LEU	2.7
1	B	186	GLY	2.6
1	B	89	VAL	2.6
1	B	3	ALA	2.6
2	C	31	ARG	2.6
2	C	33	LEU	2.6
1	B	235	ARG	2.6
1	B	246	VAL	2.6
1	B	203	ILE	2.4
1	A	129	SER	2.4
1	B	189	GLN	2.4
2	C	34	ILE	2.4
1	B	162	ALA	2.4
2	C	145	GLY	2.4
2	C	9	HIS	2.4
1	B	159	ASP	2.3
1	B	11	TRP	2.3
1	B	190	HIS	2.3
1	B	214	TYR	2.3
2	C	148	PRO	2.3
2	C	125	LEU	2.3
1	B	233	ILE	2.3
1	B	242	ILE	2.2
2	D	10	HIS	2.2
2	C	170	LEU	2.1
2	D	65	LEU	2.1
1	B	199	HIS	2.1
2	C	18	LEU	2.1
2	C	120	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	171	ASN	2.0
1	A	49	HIS	2.0
1	A	233	ILE	2.0
2	D	40	VAL	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	SCH	A	29	8/9	0.80	0.23	54,65,70,84	0
1	SCH	B	29	8/9	0.91	0.19	56,66,70,71	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.