Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:30 PM GMT

PDB ID	:	1KK4
Title	:	Crystal Structure of Vat(D) in Complex with Acetyl-CoA
Authors	:	Sugantino, M.; Roderick, S.L.
Deposited on	:	2001-12-06
Resolution	:	2.70 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 (i) symbol.

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

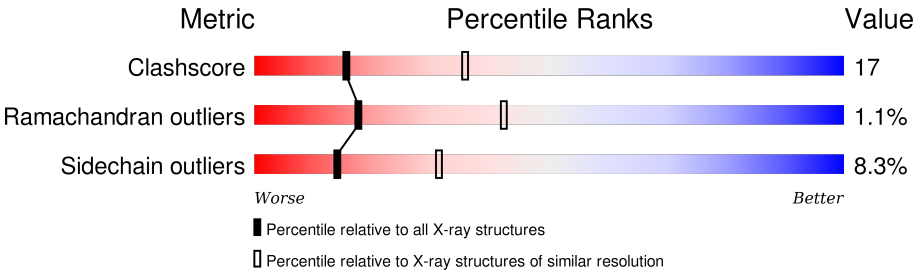
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	209	59% 34% 5% •
1	B	209	67% 27% • •
1	C	209	63% 33% • •
1	D	209	64% 31% • •
1	E	209	67% 29% • •
1	F	209	65% 30% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10155 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 STREPTOGRAMIN A ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1621	1044	267	301	9			
1	B	205	Total	C	N	O	S	0	0	0
			1614	1040	266	299	9			
1	C	205	Total	C	N	O	S	0	0	0
			1617	1041	266	301	9			
1	D	206	Total	C	N	O	S	0	0	0
			1625	1047	267	302	9			
1	E	206	Total	C	N	O	S	0	0	0
			1613	1037	265	302	9			
1	F	206	Total	C	N	O	S	0	0	0
			1624	1045	268	302	9			

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	25	Total	O	0	0
			25	25		
3	C	21	Total	O	0	0
			21	21		
3	D	24	Total	O	0	0
			24	24		
3	E	21	Total	O	0	0
			21	21		
3	F	24	Total	O	0	0
			24	24		

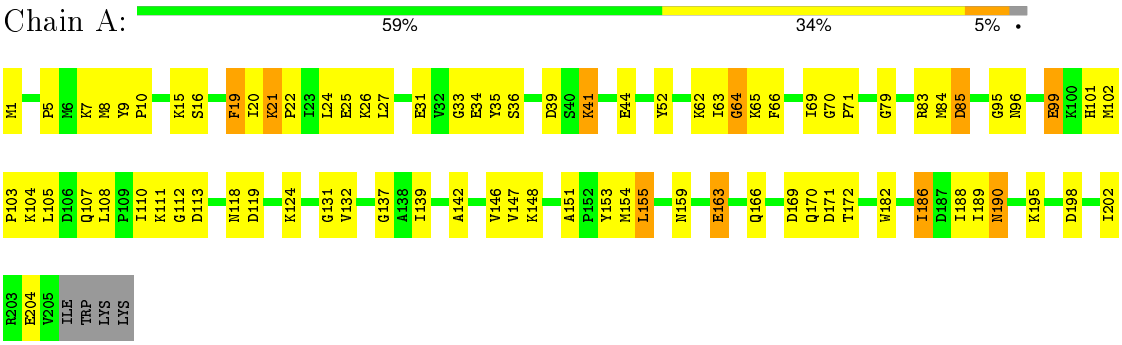
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

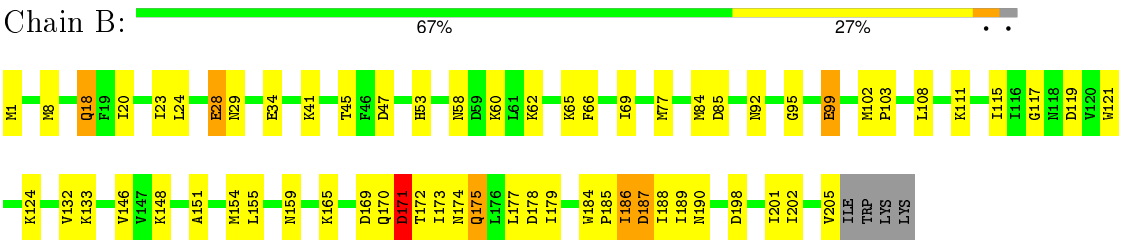
• Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain A:



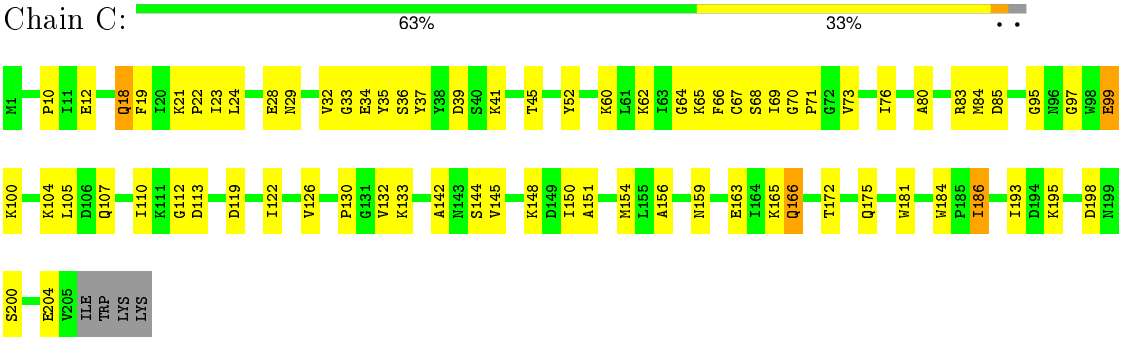
• Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain B:



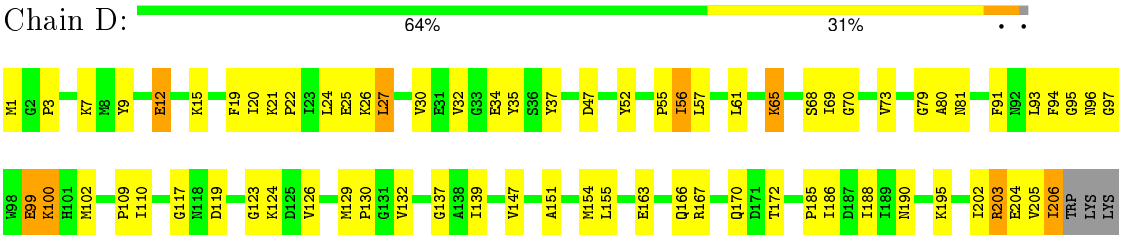
• Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain C:



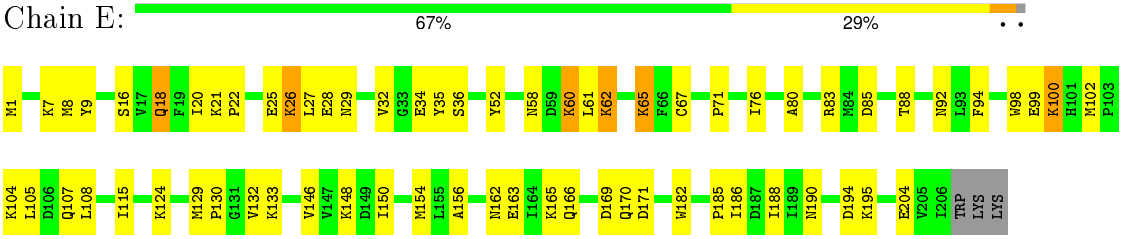
• Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain D:



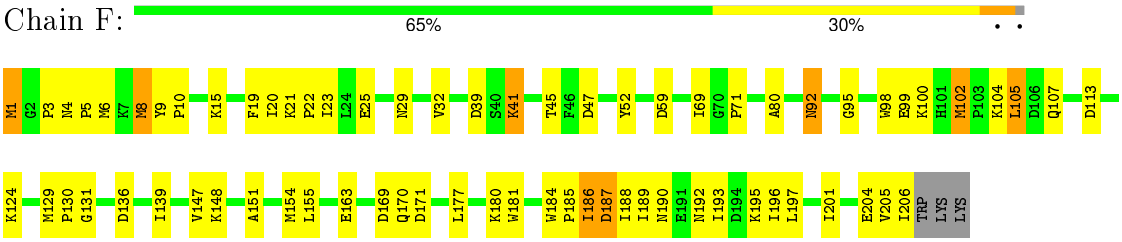
• Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain E:



• Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE

Chain F:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	186.30Å 186.30Å 186.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.70	Depositor
% Data completeness (in resolution range)	94.0 (99.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.188 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10155	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.47	0/1660	0.70	0/2251
1	B	0.47	1/1653 (0.1%)	0.74	3/2243 (0.1%)
1	C	0.41	0/1656	0.66	0/2247
1	D	0.43	0/1664	0.68	1/2258 (0.0%)
1	E	0.43	0/1652	0.67	0/2245
1	F	0.44	0/1663	0.66	0/2255
All	All	0.44	1/9948 (0.0%)	0.69	4/13499 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	VAL	CA-CB	-5.95	1.42	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	205	VAL	N-CA-C	10.39	139.05	111.00
1	D	206	ILE	N-CA-C	6.96	129.80	111.00
1	B	205	VAL	CB-CA-C	-6.26	99.50	111.40
1	B	205	VAL	CA-C-O	5.67	132.00	120.10

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	1621	0	1611	75	0
1	B	1614	0	1601	50	0
1	C	1617	0	1600	44	0
1	D	1625	0	1614	67	0
1	E	1613	0	1575	53	0
1	F	1624	0	1609	64	0
2	A	51	0	27	5	0
2	B	51	0	27	3	0
2	C	51	0	27	6	0
2	D	51	0	27	1	0
2	E	51	0	27	0	0
2	F	51	0	27	1	0
3	A	20	0	0	2	0
3	B	25	0	0	3	0
3	C	21	0	0	0	0
3	D	24	0	0	8	0
3	E	21	0	0	9	0
3	F	24	0	0	4	0
All	All	10155	0	9772	340	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 (340) 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:E:26:LYS:O	1:E:27:LEU:HD23	1.53	1.05
1:B:60:LYS:HE3	3:B:3512:HOH:O	1.58	1.01
1:F:195:LYS:NZ	1:F:204:GLU:HG3	1.77	0.99
1:B:186:ILE:HG23	1:B:187:ASP:H	1.30	0.93
1:A:195:LYS:HZ1	1:A:204:GLU:CD	1.70	0.93
1:D:95:GLY:HA2	1:D:99:GLU:HG3	1.52	0.92
1:F:195:LYS:HZ2	1:F:204:GLU:HG3	1.33	0.89
1:A:195:LYS:NZ	1:A:204:GLU:CD	2.30	0.84
1:B:184:TRP:CH2	1:B:201:ILE:HD11	2.12	0.84
1:D:24:LEU:O	1:D:27:LEU:HB2	1.78	0.83
1:F:95:GLY:HA2	1:F:99:GLU:HG3	1.62	0.81
1:C:151:ALA:HB3	1:C:154:MET:HG3	1.62	0.81
1:E:62:LYS:HD2	1:E:115:ILE:HG12	1.62	0.80
1:F:196:ILE:HG12	1:F:201:ILE:HD12	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:LYS:O	1:E:27:LEU:CD2	2.30	0.79
1:B:187:ASP:HA	1:B:190:ASN:HD22	1.48	0.79
1:D:204:GLU:OE1	1:D:204:GLU:HA	1.84	0.78
1:F:184:TRP:CZ3	1:F:201:ILE:HD11	2.19	0.77
1:B:155:LEU:HD11	2:B:302:ACO:H131	1.67	0.77
1:D:205:VAL:O	1:D:206:ILE:CB	2.33	0.77
1:A:21:LYS:HB3	1:A:22:PRO:HD3	1.68	0.76
1:C:95:GLY:HA2	1:C:99:GLU:HG3	1.68	0.75
1:B:169:ASP:OD1	1:B:171:ASP:HB2	1.87	0.74
1:B:173:ILE:HG22	1:B:177:LEU:HD12	1.69	0.73
1:B:23:ILE:HG22	1:B:24:LEU:HD23	1.70	0.73
1:B:186:ILE:HG23	1:B:187:ASP:N	2.03	0.73
1:F:1:MET:N	3:F:3634:HOH:O	2.22	0.73
1:D:203:ARG:HD2	3:D:3582:HOH:O	1.87	0.73
1:A:169:ASP:OD1	1:A:171:ASP:HB3	1.89	0.72
1:D:20:ILE:HG22	1:D:32:VAL:HG11	1.72	0.71
1:D:34:GLU:HG2	1:D:65:LYS:HD2	1.72	0.71
1:D:130:PRO:HG3	3:D:3543:HOH:O	1.91	0.71
1:B:186:ILE:O	1:B:189:ILE:N	2.24	0.71
1:A:10:PRO:HG3	1:A:19:PHE:CD1	2.26	0.71
1:D:172:THR:HG23	1:D:202:ILE:HD11	1.73	0.71
1:A:35:TYR:OH	1:A:186:ILE:HD13	1.91	0.70
1:F:147:VAL:HB	3:F:3557:HOH:O	1.91	0.70
1:D:130:PRO:CG	3:D:3543:HOH:O	2.39	0.69
1:D:151:ALA:HB3	1:D:154:MET:HG3	1.72	0.69
1:E:25:GLU:HG3	3:E:3517:HOH:O	1.92	0.69
1:A:186:ILE:O	1:A:190:ASN:HB2	1.91	0.69
1:D:52:TYR:CD1	1:D:80:ALA:HB2	2.28	0.69
1:D:195:LYS:NZ	1:D:204:GLU:HG3	2.08	0.68
1:E:148:LYS:HE3	3:E:3644:HOH:O	1.92	0.68
1:A:31:GLU:OE2	1:A:62:LYS:HE2	1.94	0.67
1:F:204:GLU:OE1	1:F:204:GLU:HA	1.94	0.67
1:F:41:LYS:HB2	1:F:71:PRO:HB2	1.77	0.67
1:A:70:GLY:HA2	2:A:301:ACO:CH3	2.25	0.67
1:B:184:TRP:CZ3	1:B:201:ILE:HD11	2.29	0.67
1:A:113:ASP:O	1:A:131:GLY:HA2	1.94	0.67
1:D:57:LEU:HD22	1:D:110:ILE:HD11	1.76	0.66
1:C:23:ILE:HG22	1:C:24:LEU:HD23	1.76	0.66
1:E:102:MET:HE3	3:E:3553:HOH:O	1.96	0.66
1:D:94:PHE:HB3	1:F:3:PRO:HG3	1.76	0.66
1:F:139:ILE:HB	1:F:155:LEU:HD12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ILE:O	1:B:188:ILE:N	2.28	0.66
1:D:185:PRO:HD2	1:D:188:ILE:HD12	1.79	0.65
1:C:69:ILE:HG12	1:C:122:ILE:HD12	1.79	0.65
1:F:184:TRP:CH2	1:F:201:ILE:HD11	2.31	0.65
1:E:8:MET:HE1	1:E:9:TYR:CE1	2.32	0.65
1:D:25:GLU:C	1:D:27:LEU:H	1.98	0.64
1:D:21:LYS:HE3	1:D:25:GLU:OE2	1.97	0.64
1:F:195:LYS:HZ3	1:F:204:GLU:HG3	1.61	0.64
1:A:41:LYS:O	1:A:41:LYS:HG3	1.97	0.64
1:A:70:GLY:HA2	2:A:301:ACO:HH32	1.79	0.63
1:A:41:LYS:HB2	1:A:71:PRO:HB2	1.80	0.63
1:C:37:TYR:CE2	1:C:68:SER:HA	2.33	0.63
1:A:154:MET:CE	1:A:163:GLU:HG2	2.28	0.63
1:A:35:TYR:CZ	1:A:186:ILE:HD13	2.34	0.63
1:A:26:LYS:O	1:A:26:LYS:HG3	1.98	0.62
1:F:151:ALA:HB3	1:F:154:MET:HG3	1.80	0.62
1:B:95:GLY:HA2	1:B:99:GLU:HG3	1.82	0.62
1:A:9:TYR:CD2	1:A:15:LYS:HA	2.35	0.61
1:E:71:PRO:HG2	1:E:124:LYS:HB2	1.83	0.61
1:C:165:LYS:HG2	1:C:166:GLN:N	2.15	0.60
1:D:19:PHE:O	1:D:22:PRO:HD2	2.01	0.60
1:B:169:ASP:OD1	1:B:171:ASP:CB	2.49	0.60
1:F:151:ALA:O	1:F:154:MET:HB2	2.02	0.60
1:A:83:ARG:HG2	3:A:3613:HOH:O	2.02	0.60
1:F:186:ILE:HG23	1:F:187:ASP:H	1.65	0.60
1:A:8:MET:O	1:A:10:PRO:HD3	2.02	0.60
1:B:20:ILE:CD1	1:B:69:ILE:HD12	2.31	0.59
1:C:195:LYS:HG2	1:C:200:SER:OG	2.03	0.59
1:A:65:LYS:O	1:A:66:PHE:HB2	2.02	0.59
1:D:91:PHE:HD1	1:F:197:LEU:HD21	1.67	0.59
1:A:172:THR:HG23	1:A:202:ILE:CD1	2.33	0.59
1:F:139:ILE:HB	1:F:155:LEU:CD1	2.33	0.58
1:B:186:ILE:CG2	1:B:187:ASP:H	2.10	0.58
1:A:36:SER:OG	1:A:65:LYS:HA	2.04	0.58
1:D:25:GLU:HG3	3:D:3628:HOH:O	2.02	0.58
1:D:154:MET:HE2	1:D:163:GLU:HG2	1.85	0.58
1:E:21:LYS:HB2	3:E:3529:HOH:O	2.03	0.58
1:E:1:MET:HE2	1:E:190:ASN:HB3	1.85	0.58
1:B:173:ILE:HG22	1:B:177:LEU:CD1	2.33	0.58
1:F:169:ASP:OD1	1:F:171:ASP:HB3	2.02	0.58
1:D:20:ILE:CG2	1:D:32:VAL:HG11	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:ARG:HG2	3:E:3519:HOH:O	2.04	0.57
1:A:26:LYS:O	1:A:27:LEU:HD23	2.05	0.56
1:B:172:THR:HG23	1:B:202:ILE:HD11	1.86	0.56
3:B:3505:HOH:O	1:C:83:ARG:HG2	2.05	0.56
1:F:205:VAL:O	1:F:206:ILE:C	2.44	0.56
1:D:172:THR:HG23	1:D:202:ILE:CD1	2.35	0.56
1:C:70:GLY:O	1:C:73:VAL:HG23	2.05	0.56
1:F:154:MET:CE	1:F:163:GLU:HB3	2.36	0.56
1:E:20:ILE:HG22	1:E:32:VAL:HG11	1.87	0.56
1:F:21:LYS:HB3	1:F:22:PRO:HD3	1.88	0.56
1:C:28:GLU:O	1:C:29:ASN:HB2	2.06	0.56
1:E:20:ILE:CG2	1:E:32:VAL:HG11	2.36	0.55
1:F:20:ILE:HG22	1:F:32:VAL:HG11	1.88	0.55
1:B:184:TRP:CH2	1:B:201:ILE:CD1	2.89	0.54
1:D:91:PHE:CD1	1:F:197:LEU:HD21	2.41	0.54
1:C:66:PHE:O	1:C:119:ASP:HA	2.06	0.54
1:B:186:ILE:HG12	1:B:190:ASN:HD21	1.70	0.54
1:A:1:MET:CE	1:A:190:ASN:OD1	2.55	0.54
1:C:24:LEU:HD12	1:C:32:VAL:HG21	1.88	0.54
1:B:174:ASN:O	1:B:178:ASP:HB2	2.08	0.54
1:B:66:PHE:O	1:B:119:ASP:HA	2.08	0.54
1:C:19:PHE:O	1:C:22:PRO:HD2	2.08	0.54
1:F:10:PRO:HB3	1:F:19:PHE:CE1	2.42	0.54
1:E:76:ILE:O	1:E:130:PRO:HG3	2.07	0.54
1:D:35:TYR:OH	1:D:186:ILE:HD13	2.08	0.53
1:F:29:ASN:ND2	3:F:3545:HOH:O	2.42	0.53
1:D:97:GLY:N	1:D:99:GLU:OE2	2.39	0.53
1:E:52:TYR:CD1	1:E:80:ALA:HB2	2.43	0.53
1:A:66:PHE:O	1:A:119:ASP:HA	2.08	0.53
1:A:21:LYS:HB3	1:A:22:PRO:CD	2.38	0.53
1:F:185:PRO:HD2	1:F:188:ILE:HD12	1.90	0.53
1:D:195:LYS:HZ3	1:D:204:GLU:HG3	1.73	0.53
1:E:92:ASN:HB2	3:E:3553:HOH:O	2.08	0.53
1:E:34:GLU:HG2	1:E:65:LYS:HD2	1.91	0.53
1:B:20:ILE:HD11	1:B:69:ILE:HD12	1.90	0.53
1:E:65:LYS:HE3	1:E:182:TRP:O	2.09	0.52
1:A:195:LYS:NZ	1:A:204:GLU:CG	2.72	0.52
1:E:21:LYS:HB3	1:E:22:PRO:HD3	1.92	0.52
1:B:102:MET:HG3	1:B:103:PRO:HD2	1.91	0.52
1:D:123:GLY:O	1:D:126:VAL:HG23	2.10	0.52
1:D:20:ILE:CD1	1:D:69:ILE:HD12	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:MET:HE2	1:D:163:GLU:HB3	1.90	0.52
1:C:21:LYS:HB3	1:C:22:PRO:HD3	1.92	0.52
1:C:126:VAL:HG22	1:C:144:SER:H	1.75	0.52
1:A:69:ILE:C	2:A:301:ACO:HH31	2.31	0.52
1:D:195:LYS:HZ2	1:D:204:GLU:HG3	1.74	0.52
1:A:96:ASN:HD22	1:A:96:ASN:N	2.08	0.52
1:F:9:TYR:CD2	1:F:15:LYS:HA	2.45	0.52
1:A:195:LYS:HE3	1:A:204:GLU:OE2	2.10	0.51
1:F:39:ASP:O	1:F:71:PRO:HB3	2.10	0.51
1:B:159:ASN:HB2	1:C:159:ASN:HD22	1.76	0.51
1:B:28:GLU:O	1:B:29:ASN:HB2	2.10	0.51
1:D:9:TYR:CE2	1:D:15:LYS:HA	2.46	0.51
1:C:104:LYS:HB2	1:C:107:GLN:OE1	2.10	0.51
1:A:142:ALA:HB2	2:A:301:ACO:O5P	2.10	0.51
1:B:18:GLN:OE1	1:B:45:THR:HA	2.11	0.51
1:D:56:ILE:O	1:D:56:ILE:CG1	2.59	0.51
1:D:37:TYR:HE2	1:D:68:SER:HG	1.56	0.51
1:B:187:ASP:HA	1:B:190:ASN:ND2	2.23	0.51
1:A:111:LYS:HE2	2:C:303:ACO:O4A	2.10	0.51
1:A:188:ILE:O	1:A:189:ILE:C	2.50	0.50
1:A:154:MET:HE2	1:A:163:GLU:HG2	1.93	0.50
1:E:132:VAL:HG11	1:E:146:VAL:HG12	1.93	0.50
1:D:93:LEU:O	1:D:93:LEU:HG	2.11	0.50
1:E:100:LYS:C	1:E:102:MET:H	2.14	0.50
1:C:69:ILE:C	2:C:303:ACO:HH31	2.31	0.50
1:A:111:LYS:NZ	2:C:303:ACO:CBP	2.74	0.50
1:B:132:VAL:HG11	1:B:146:VAL:HG12	1.93	0.50
1:B:198:ASP:HA	1:C:85:ASP:OD1	2.11	0.50
1:C:60:LYS:O	1:C:113:ASP:HB3	2.11	0.50
1:A:195:LYS:HZ2	1:A:204:GLU:CG	2.25	0.50
1:D:186:ILE:HD11	1:E:98:TRP:HZ2	1.77	0.50
1:A:44:GLU:N	1:A:44:GLU:OE1	2.43	0.50
1:E:186:ILE:HD11	1:F:98:TRP:HZ2	1.76	0.50
1:A:101:HIS:CD2	1:C:193:ILE:HG21	2.47	0.49
1:A:1:MET:HE3	1:A:190:ASN:OD1	2.12	0.49
1:F:177:LEU:O	1:F:180:LYS:HG3	2.12	0.49
1:D:81:ASN:HB3	1:D:109:PRO:HG2	1.94	0.49
1:A:1:MET:HB2	1:A:190:ASN:OD1	2.13	0.49
1:B:175:GLN:OE1	1:B:202:ILE:CG2	2.61	0.49
1:F:129:MET:HB3	1:F:130:PRO:HD2	1.95	0.49
1:E:169:ASP:O	1:E:171:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:ILE:O	1:E:133:LYS:HA	2.13	0.49
1:F:169:ASP:HA	3:F:3560:HOH:O	2.13	0.49
1:F:184:TRP:HZ3	1:F:201:ILE:HD11	1.76	0.49
1:B:151:ALA:HB3	1:B:154:MET:HG3	1.93	0.49
1:A:172:THR:HG23	1:A:202:ILE:HD11	1.95	0.49
1:E:102:MET:HB2	3:E:3553:HOH:O	2.13	0.48
1:C:10:PRO:HB3	1:C:19:PHE:CE1	2.48	0.48
1:F:69:ILE:C	2:F:306:ACO:HH31	2.33	0.48
1:F:104:LYS:N	1:F:107:GLN:OE1	2.43	0.48
1:D:95:GLY:O	1:D:96:ASN:HB2	2.13	0.48
1:D:37:TYR:OH	2:D:304:ACO:HH33	2.13	0.48
1:C:39:ASP:O	1:C:71:PRO:HB3	2.13	0.48
1:D:20:ILE:HG23	1:D:24:LEU:HG	1.94	0.48
1:D:186:ILE:HD11	1:E:98:TRP:CZ2	2.49	0.48
1:F:154:MET:HE3	1:F:163:GLU:HB3	1.96	0.48
1:F:20:ILE:CG2	1:F:32:VAL:HG11	2.43	0.48
1:C:172:THR:O	1:C:175:GLN:HB2	2.13	0.48
1:B:58:ASN:ND2	3:B:3512:HOH:O	2.47	0.48
1:E:154:MET:HE3	1:E:163:GLU:HB3	1.95	0.48
1:F:47:ASP:OD1	1:F:47:ASP:N	2.45	0.48
1:A:154:MET:HE3	1:A:163:GLU:HG2	1.95	0.48
1:C:154:MET:HE3	1:C:165:LYS:O	2.13	0.48
1:E:29:ASN:O	1:E:60:LYS:HA	2.13	0.48
1:A:95:GLY:HA2	1:A:99:GLU:HG2	1.95	0.48
1:D:12:GLU:CG	3:D:3532:HOH:O	2.62	0.47
1:F:8:MET:HG2	1:F:23:ILE:HG12	1.96	0.47
1:E:36:SER:HB3	1:E:67:CYS:HB2	1.97	0.47
1:D:119:ASP:O	1:D:137:GLY:HA2	2.15	0.47
1:F:92:ASN:HD22	1:F:92:ASN:H	1.63	0.47
1:C:18:GLN:OE1	1:C:45:THR:HA	2.14	0.47
1:D:129:MET:HB3	1:D:130:PRO:CD	2.45	0.47
1:E:21:LYS:HB3	1:E:22:PRO:CD	2.45	0.47
1:D:25:GLU:C	1:D:27:LEU:N	2.65	0.47
1:D:52:TYR:HB3	1:D:79:GLY:HA3	1.96	0.47
1:E:71:PRO:HG2	1:E:124:LYS:CB	2.44	0.47
1:D:56:ILE:O	1:D:56:ILE:HG12	2.15	0.47
1:E:104:LYS:O	1:E:107:GLN:N	2.38	0.47
1:F:113:ASP:O	1:F:131:GLY:HA2	2.15	0.46
1:D:3:PRO:HG3	1:E:94:PHE:HB3	1.97	0.46
1:F:186:ILE:O	1:F:189:ILE:N	2.48	0.46
1:A:39:ASP:O	1:A:71:PRO:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:MET:CE	1:E:163:GLU:HB3	2.45	0.46
1:F:196:ILE:CG1	1:F:201:ILE:HD12	2.41	0.46
1:B:175:GLN:OE1	1:B:202:ILE:HG23	2.15	0.46
1:E:35:TYR:CZ	1:E:186:ILE:HD12	2.51	0.46
1:F:59:ASP:OD1	1:F:59:ASP:N	2.47	0.46
1:F:99:GLU:H	1:F:99:GLU:CD	2.19	0.46
1:D:130:PRO:HG2	3:D:3543:HOH:O	2.11	0.46
1:D:129:MET:HB3	1:D:130:PRO:HD2	1.98	0.46
1:C:97:GLY:N	1:C:99:GLU:OE2	2.41	0.46
1:A:34:GLU:HG2	1:A:65:LYS:HD2	1.98	0.46
1:A:151:ALA:O	1:A:154:MET:HB2	2.16	0.45
1:E:62:LYS:CD	1:E:115:ILE:HG12	2.38	0.45
1:D:94:PHE:CB	1:F:3:PRO:HG3	2.44	0.45
1:A:33:GLY:HA3	1:A:65:LYS:HB3	1.98	0.45
1:E:129:MET:O	1:E:132:VAL:HG23	2.17	0.45
1:E:156:ALA:HB1	1:E:162:ASN:O	2.15	0.45
1:F:21:LYS:HG3	1:F:32:VAL:O	2.17	0.45
1:F:185:PRO:O	1:F:186:ILE:C	2.55	0.45
1:C:142:ALA:HB2	2:C:303:ACO:O5P	2.17	0.45
1:B:115:ILE:HD12	1:B:133:LYS:HE2	1.98	0.45
1:E:108:LEU:HA	1:E:108:LEU:HD23	1.86	0.45
1:A:52:TYR:HB3	1:A:79:GLY:HA3	1.99	0.45
1:D:97:GLY:O	1:D:100:LYS:HG2	2.17	0.45
1:A:25:GLU:C	1:A:27:LEU:H	2.18	0.45
1:E:190:ASN:ND2	3:E:3631:HOH:O	2.49	0.45
1:C:36:SER:HB3	1:C:67:CYS:HB2	1.98	0.45
1:D:12:GLU:HG2	3:D:3532:HOH:O	2.16	0.45
1:B:175:GLN:O	1:B:179:ILE:HG13	2.16	0.45
1:D:139:ILE:HD12	1:D:167:ARG:HD2	1.99	0.45
1:D:30:VAL:HG22	1:D:61:LEU:HB3	1.99	0.45
1:B:62:LYS:HD2	1:B:115:ILE:HG12	1.99	0.44
1:F:52:TYR:CD1	1:F:80:ALA:HB2	2.52	0.44
1:E:25:GLU:HG2	3:E:3565:HOH:O	2.18	0.44
1:F:92:ASN:OD1	1:F:102:MET:HE3	2.18	0.44
1:A:63:ILE:O	1:A:64:GLY:O	2.36	0.44
1:B:8:MET:HG2	1:B:23:ILE:HG13	2.00	0.44
1:A:188:ILE:C	1:A:190:ASN:N	2.70	0.44
1:C:181:TRP:HA	1:C:184:TRP:CE2	2.52	0.44
1:A:36:SER:HG	1:A:65:LYS:HA	1.83	0.44
1:A:65:LYS:HE3	1:A:182:TRP:O	2.18	0.43
1:E:8:MET:HE2	1:E:8:MET:HB3	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:MET:HE2	1:D:163:GLU:CG	2.49	0.43
1:D:186:ILE:O	1:D:190:ASN:HB2	2.18	0.43
1:E:104:LYS:O	1:E:105:LEU:C	2.56	0.43
1:C:145:VAL:HB	1:C:159:ASN:OD1	2.17	0.43
1:A:101:HIS:O	1:A:102:MET:C	2.55	0.43
1:A:99:GLU:HG3	1:A:99:GLU:H	1.29	0.43
1:F:184:TRP:O	1:F:185:PRO:C	2.57	0.43
1:A:147:VAL:HG11	2:C:303:ACO:N7A	2.33	0.43
1:B:132:VAL:HG11	1:B:146:VAL:CG1	2.48	0.43
1:A:137:GLY:O	1:A:153:TYR:HA	2.19	0.43
1:A:111:LYS:HZ1	2:C:303:ACO:CBP	2.32	0.43
1:C:154:MET:HE2	1:C:163:GLU:HG2	2.01	0.43
1:A:198:ASP:C	1:A:198:ASP:OD1	2.57	0.43
1:B:121:TRP:NE1	2:B:302:ACO:O	2.45	0.43
1:F:154:MET:HE2	1:F:163:GLU:HB3	2.00	0.43
1:B:132:VAL:HG12	1:B:133:LYS:N	2.33	0.43
1:B:108:LEU:HD23	1:B:108:LEU:HA	1.81	0.43
1:F:105:LEU:HA	1:F:105:LEU:HD23	1.78	0.43
1:A:132:VAL:HG11	1:A:146:VAL:HG12	1.99	0.43
1:F:129:MET:HB3	1:F:130:PRO:CD	2.49	0.42
1:D:9:TYR:CD2	1:D:15:LYS:HA	2.54	0.42
1:A:9:TYR:CE2	1:A:15:LYS:HA	2.54	0.42
1:D:21:LYS:HB3	1:D:22:PRO:HD3	2.01	0.42
1:B:121:TRP:CZ2	2:B:302:ACO:H61	2.54	0.42
1:A:1:MET:HB2	1:A:190:ASN:HD21	1.84	0.42
1:D:55:PRO:O	1:D:57:LEU:N	2.53	0.42
1:A:151:ALA:HB3	1:A:154:MET:HG3	2.00	0.42
1:F:186:ILE:O	1:F:187:ASP:C	2.57	0.42
1:B:92:ASN:ND2	1:B:103:PRO:HD3	2.35	0.42
1:C:198:ASP:OD1	1:C:198:ASP:C	2.57	0.42
1:E:169:ASP:C	1:E:171:ASP:N	2.72	0.42
1:A:103:PRO:CG	1:A:108:LEU:HD21	2.49	0.42
1:E:195:LYS:HD2	1:E:204:GLU:HG3	2.02	0.42
1:D:70:GLY:O	1:D:73:VAL:HG23	2.20	0.42
1:F:195:LYS:NZ	1:F:204:GLU:CG	2.66	0.42
1:A:70:GLY:N	2:A:301:ACO:HH31	2.35	0.42
1:E:169:ASP:C	1:E:171:ASP:H	2.22	0.42
1:F:192:ASN:O	1:F:195:LYS:N	2.52	0.42
1:D:27:LEU:HA	1:D:27:LEU:HD23	1.86	0.42
1:A:104:LYS:O	1:A:105:LEU:C	2.57	0.41
1:C:34:GLU:HG2	1:C:65:LYS:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:PRO:O	1:B:186:ILE:C	2.59	0.41
1:D:25:GLU:CG	3:D:3628:HOH:O	2.66	0.41
1:A:95:GLY:HA2	1:A:99:GLU:CG	2.50	0.41
1:F:181:TRP:CE3	1:F:196:ILE:HD13	2.55	0.41
1:A:83:ARG:HG3	1:A:85:ASP:OD1	2.20	0.41
1:E:185:PRO:HD2	1:E:188:ILE:HD12	2.02	0.41
1:C:165:LYS:HG2	1:C:166:GLN:O	2.21	0.41
1:A:1:MET:HE2	1:A:190:ASN:OD1	2.20	0.41
1:A:20:ILE:CG2	1:A:24:LEU:HG	2.49	0.41
1:F:4:ASN:HA	1:F:5:PRO:HD2	1.89	0.41
1:F:1:MET:HE3	1:F:190:ASN:CG	2.40	0.41
1:E:58:ASN:ND2	1:E:60:LYS:HE3	2.36	0.41
1:C:35:TYR:OH	1:C:186:ILE:HD13	2.20	0.41
1:A:34:GLU:H	1:A:65:LYS:HB3	1.86	0.41
1:E:18:GLN:HE21	1:E:18:GLN:HB3	1.70	0.41
1:D:95:GLY:HA2	1:D:99:GLU:CG	2.36	0.41
1:A:159:ASN:HD22	1:C:159:ASN:HB2	1.86	0.41
1:C:33:GLY:HA3	1:C:64:GLY:C	2.42	0.41
1:C:150:ILE:HD12	1:C:156:ALA:CB	2.51	0.41
1:F:192:ASN:O	1:F:193:ILE:C	2.59	0.41
1:B:159:ASN:CB	1:C:159:ASN:HD22	2.34	0.41
1:C:110:ILE:HG22	1:C:112:GLY:H	1.86	0.41
1:B:53:HIS:CG	1:B:77:MET:HG3	2.55	0.41
1:D:139:ILE:HB	1:D:155:LEU:HD13	2.03	0.41
1:C:52:TYR:CD2	1:C:80:ALA:HB2	2.56	0.41
1:B:186:ILE:O	1:B:187:ASP:C	2.58	0.40
1:C:33:GLY:HA3	1:C:64:GLY:O	2.21	0.40
1:D:129:MET:HG3	1:D:147:VAL:HG12	2.03	0.40
1:B:45:THR:OG1	1:B:47:ASP:OD1	2.35	0.40
1:F:45:THR:HB	1:F:47:ASP:OD1	2.20	0.40
1:C:76:ILE:O	1:C:130:PRO:HG3	2.21	0.40
1:E:25:GLU:O	1:E:27:LEU:N	2.47	0.40
1:E:28:GLU:O	1:E:29:ASN:HB2	2.22	0.40
1:A:110:ILE:HG22	1:A:112:GLY:H	1.87	0.40
1:B:170:GLN:O	1:B:171:ASP:C	2.59	0.40
1:E:154:MET:SD	1:E:166:GLN:HG3	2.61	0.40
1:F:195:LYS:HZ3	1:F:204:GLU:CG	2.31	0.40
1:A:107:GLN:OE1	3:A:3615:HOH:O	2.22	0.40
1:A:139:ILE:HB	1:A:155:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	203/209 (97%)	185 (91%)	16 (8%)	2 (1%)	19 45
1	B	203/209 (97%)	187 (92%)	12 (6%)	4 (2%)	9 24
1	C	203/209 (97%)	188 (93%)	15 (7%)	0	100 100
1	D	204/209 (98%)	186 (91%)	15 (7%)	3 (2%)	13 32
1	E	204/209 (98%)	187 (92%)	15 (7%)	2 (1%)	19 45
1	F	204/209 (98%)	188 (92%)	14 (7%)	2 (1%)	19 45
All	All	1221/1254 (97%)	1121 (92%)	87 (7%)	13 (1%)	17 42

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	ILE
1	B	187	ASP
1	A	64	GLY
1	D	56	ILE
1	E	170	GLN
1	B	171	ASP
1	F	187	ASP
1	D	26	LYS
1	D	117	GLY
1	A	5	PRO
1	E	26	LYS
1	F	186	ILE
1	B	117	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	176/183 (96%)	159 (90%)	17 (10%)	10	23
1	B	175/183 (96%)	160 (91%)	15 (9%)	13	29
1	C	175/183 (96%)	161 (92%)	14 (8%)	15	33
1	D	177/183 (97%)	163 (92%)	14 (8%)	15	34
1	E	172/183 (94%)	158 (92%)	14 (8%)	15	33
1	F	176/183 (96%)	163 (93%)	13 (7%)	17	39
All	All	1051/1098 (96%)	964 (92%)	87 (8%)	14	31

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	16	SER
1	A	19	PHE
1	A	21	LYS
1	A	41	LYS
1	A	84	MET
1	A	85	ASP
1	A	99	GLU
1	A	118	ASN
1	A	124	LYS
1	A	148	LYS
1	A	155	LEU
1	A	163	GLU
1	A	166	GLN
1	A	170	GLN
1	A	186	ILE
1	A	190	ASN
1	B	1	MET
1	B	18	GLN
1	B	28	GLU
1	B	34	GLU
1	B	41	LYS
1	B	65	LYS
1	B	84	MET
1	B	85	ASP
1	B	99	GLU
1	B	111	LYS

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Mol	Chain	Res	Type
1	B	124	LYS
1	B	148	LYS
1	B	165	LYS
1	B	171	ASP
1	B	175	GLN
1	C	12	GLU
1	C	18	GLN
1	C	41	LYS
1	C	62	LYS
1	C	84	MET
1	C	99	GLU
1	C	100	LYS
1	C	105	LEU
1	C	132	VAL
1	C	133	LYS
1	C	148	LYS
1	C	166	GLN
1	C	186	ILE
1	C	204	GLU
1	D	1	MET
1	D	7	LYS
1	D	12	GLU
1	D	27	LEU
1	D	47	ASP
1	D	65	LYS
1	D	99	GLU
1	D	100	LYS
1	D	102	MET
1	D	124	LYS
1	D	132	VAL
1	D	166	GLN
1	D	170	GLN
1	D	203	ARG
1	E	7	LYS
1	E	16	SER
1	E	18	GLN
1	E	60	LYS
1	E	61	LEU
1	E	62	LYS
1	E	65	LYS
1	E	85	ASP
1	E	88	THR

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Mol	Chain	Res	Type
1	E	99	GLU
1	E	100	LYS
1	E	150	ILE
1	E	165	LYS
1	E	194	ASP
1	F	1	MET
1	F	6	MET
1	F	8	MET
1	F	25	GLU
1	F	41	LYS
1	F	92	ASN
1	F	100	LYS
1	F	102	MET
1	F	105	LEU
1	F	124	LYS
1	F	136	ASP
1	F	148	LYS
1	F	170	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	166	GLN
1	A	174	ASN
1	B	58	ASN
1	B	143	ASN
1	B	166	GLN
1	B	174	ASN
1	B	190	ASN
1	C	92	ASN
1	C	96	ASN
1	C	166	GLN
1	E	58	ASN
1	E	92	ASN
1	E	166	GLN
1	E	170	GLN
1	E	174	ASN
1	F	29	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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	ACO	A	301	-	43,53,53	11.51	15 (34%)	55,79,79	14.46	20 (36%)
2	ACO	B	302	-	43,53,53	11.49	17 (39%)	55,79,79	14.46	21 (38%)
2	ACO	C	303	-	43,53,53	11.45	16 (37%)	55,79,79	14.44	21 (38%)
2	ACO	D	304	-	43,53,53	11.46	17 (39%)	55,79,79	14.45	21 (38%)
2	ACO	E	305	-	43,53,53	11.49	15 (34%)	55,79,79	14.46	21 (38%)
2	ACO	F	306	-	43,53,53	11.51	15 (34%)	55,79,79	14.44	20 (36%)

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	ACO	A	301	-	-	0/47/67/67	0/3/3/3
2	ACO	B	302	-	-	0/47/67/67	0/3/3/3
2	ACO	C	303	-	-	0/47/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACO	D	304	-	-	0/47/67/67	0/3/3/3
2	ACO	E	305	-	-	0/47/67/67	0/3/3/3
2	ACO	F	306	-	-	0/47/67/67	0/3/3/3

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	304	ACO	P3B-O9A	-2.91	1.44	1.54
2	F	306	ACO	P3B-O9A	-2.69	1.45	1.54
2	B	302	ACO	P3B-O9A	-2.54	1.45	1.54
2	E	305	ACO	P3B-O9A	-2.46	1.45	1.54
2	F	306	ACO	P2A-O5A	-2.45	1.44	1.54
2	A	301	ACO	P3B-O9A	-2.44	1.45	1.54
2	D	304	ACO	P2A-O5A	-2.43	1.44	1.54
2	C	303	ACO	P2A-O5A	-2.38	1.44	1.54
2	A	301	ACO	P2A-O5A	-2.35	1.44	1.54
2	C	303	ACO	P3B-O9A	-2.34	1.46	1.54
2	B	302	ACO	P2A-O5A	-2.28	1.45	1.54
2	E	305	ACO	P2A-O5A	-2.24	1.45	1.54
2	E	305	ACO	P1A-O2A	-2.18	1.45	1.54
2	A	301	ACO	P2A-O4A	-2.13	1.43	1.51
2	D	304	ACO	P1A-O2A	-2.11	1.45	1.54
2	A	301	ACO	P1A-O2A	-2.07	1.46	1.54
2	F	306	ACO	P1A-O2A	-2.07	1.46	1.54
2	C	303	ACO	P1A-O2A	-2.03	1.46	1.54
2	B	302	ACO	P1A-O2A	-2.03	1.46	1.54
2	E	305	ACO	O-C	2.00	1.31	1.21
2	E	305	ACO	C5P-N4P	2.00	1.38	1.33
2	D	304	ACO	C2P-C3P	2.00	1.59	1.51
2	C	303	ACO	C5P-N4P	2.02	1.38	1.33
2	B	302	ACO	O-C	2.04	1.31	1.21
2	D	304	ACO	O-C	2.04	1.31	1.21
2	C	303	ACO	C2P-C3P	2.04	1.59	1.51
2	B	302	ACO	C2P-C3P	2.06	1.59	1.51
2	F	306	ACO	C2P-C3P	2.08	1.59	1.51
2	B	302	ACO	C5P-N4P	2.09	1.38	1.33
2	D	304	ACO	C5P-N4P	2.15	1.38	1.33
2	A	301	ACO	OAP-CAP	2.18	1.46	1.42
2	C	303	ACO	OAP-CAP	2.23	1.46	1.42
2	F	306	ACO	O5P-C5P	2.42	1.28	1.23
2	B	302	ACO	P2A-O6A	2.47	1.70	1.59
2	F	306	ACO	P2A-O6A	2.55	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	303	ACO	P2A-O6A	2.57	1.70	1.59
2	D	304	ACO	P2A-O6A	2.59	1.70	1.59
2	A	301	ACO	P2A-O6A	2.60	1.70	1.59
2	D	304	ACO	O5P-C5P	2.60	1.28	1.23
2	A	301	ACO	O5P-C5P	2.61	1.28	1.23
2	D	304	ACO	C2A-N1A	2.64	1.38	1.33
2	E	305	ACO	P2A-O6A	2.64	1.71	1.59
2	E	305	ACO	C2A-N1A	2.67	1.39	1.33
2	C	303	ACO	C2A-N1A	2.68	1.39	1.33
2	B	302	ACO	O5P-C5P	2.76	1.29	1.23
2	E	305	ACO	O5P-C5P	2.76	1.29	1.23
2	F	306	ACO	C2A-N1A	2.81	1.39	1.33
2	C	303	ACO	O5P-C5P	2.85	1.29	1.23
2	F	306	ACO	OAP-CAP	2.91	1.48	1.42
2	B	302	ACO	C2A-N1A	2.92	1.39	1.33
2	D	304	ACO	OAP-CAP	2.92	1.48	1.42
2	C	303	ACO	C2P-S1P	2.97	1.95	1.81
2	F	306	ACO	C2P-S1P	3.01	1.95	1.81
2	E	305	ACO	C2P-S1P	3.03	1.95	1.81
2	A	301	ACO	C2A-N1A	3.04	1.39	1.33
2	B	302	ACO	OAP-CAP	3.04	1.48	1.42
2	D	304	ACO	C2P-S1P	3.13	1.95	1.81
2	A	301	ACO	C2P-S1P	3.14	1.95	1.81
2	B	302	ACO	C2P-S1P	3.19	1.96	1.81
2	D	304	ACO	C3P-N4P	3.65	1.54	1.46
2	E	305	ACO	C3P-N4P	3.69	1.54	1.46
2	B	302	ACO	C3P-N4P	3.73	1.54	1.46
2	F	306	ACO	C3P-N4P	3.77	1.55	1.46
2	C	303	ACO	C3P-N4P	3.81	1.55	1.46
2	A	301	ACO	C3P-N4P	3.83	1.55	1.46
2	B	302	ACO	C7P-N8P	4.24	1.56	1.46
2	F	306	ACO	C7P-N8P	4.26	1.56	1.46
2	C	303	ACO	C7P-N8P	4.37	1.56	1.46
2	C	303	ACO	C6P-C5P	4.39	1.59	1.51
2	E	305	ACO	C7P-N8P	4.40	1.56	1.46
2	A	301	ACO	C6P-C5P	4.40	1.59	1.51
2	D	304	ACO	C7P-N8P	4.42	1.56	1.46
2	A	301	ACO	C7P-N8P	4.46	1.56	1.46
2	B	302	ACO	C6P-C5P	4.53	1.60	1.51
2	F	306	ACO	C6P-C5P	4.53	1.60	1.51
2	D	304	ACO	C6P-C5P	4.63	1.60	1.51
2	E	305	ACO	C6P-C5P	4.74	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	304	ACO	O6A-CCP	31.60	2.55	1.43
2	A	301	ACO	O6A-CCP	31.72	2.55	1.43
2	E	305	ACO	O6A-CCP	31.75	2.55	1.43
2	B	302	ACO	O6A-CCP	31.75	2.55	1.43
2	C	303	ACO	O6A-CCP	31.77	2.55	1.43
2	F	306	ACO	O6A-CCP	31.85	2.55	1.43
2	C	303	ACO	CDP-CBP	46.79	2.53	1.53
2	B	302	ACO	CDP-CBP	47.00	2.54	1.53
2	D	304	ACO	CDP-CBP	47.04	2.54	1.53
2	E	305	ACO	CDP-CBP	47.11	2.54	1.53
2	F	306	ACO	CDP-CBP	47.19	2.54	1.53
2	A	301	ACO	CDP-CBP	47.29	2.54	1.53
2	D	304	ACO	CEP-CBP	47.84	2.55	1.53
2	C	303	ACO	CEP-CBP	47.95	2.56	1.53
2	A	301	ACO	CEP-CBP	48.03	2.56	1.53
2	E	305	ACO	CEP-CBP	48.08	2.56	1.53
2	F	306	ACO	CEP-CBP	48.12	2.56	1.53
2	B	302	ACO	CEP-CBP	48.15	2.56	1.53

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	ACO	CDP-CBP-CCP	-58.35	32.86	108.50
2	B	302	ACO	CDP-CBP-CCP	-58.32	32.90	108.50
2	F	306	ACO	CDP-CBP-CCP	-58.26	32.97	108.50
2	E	305	ACO	CDP-CBP-CCP	-58.24	33.00	108.50
2	D	304	ACO	CDP-CBP-CCP	-58.22	33.04	108.50
2	C	303	ACO	CDP-CBP-CCP	-58.07	33.23	108.50
2	E	305	ACO	CEP-CBP-CCP	-57.31	34.22	108.50
2	A	301	ACO	CEP-CBP-CCP	-57.30	34.22	108.50
2	F	306	ACO	CEP-CBP-CCP	-57.28	34.25	108.50
2	B	302	ACO	CEP-CBP-CCP	-57.26	34.27	108.50
2	C	303	ACO	CEP-CBP-CCP	-57.26	34.27	108.50
2	D	304	ACO	CEP-CBP-CCP	-57.24	34.30	108.50
2	C	303	ACO	O6A-CCP-CBP	-48.62	32.37	110.55
2	B	302	ACO	O6A-CCP-CBP	-48.59	32.42	110.55
2	D	304	ACO	O6A-CCP-CBP	-48.53	32.51	110.55
2	E	305	ACO	O6A-CCP-CBP	-48.52	32.53	110.55
2	A	301	ACO	O6A-CCP-CBP	-48.46	32.63	110.55
2	F	306	ACO	O6A-CCP-CBP	-48.44	32.67	110.55
2	B	302	ACO	CDP-CBP-CAP	-26.75	60.52	109.34
2	E	305	ACO	CDP-CBP-CAP	-26.71	60.58	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	ACO	CDP-CBP-CAP	-26.70	60.60	109.34
2	F	306	ACO	CDP-CBP-CAP	-26.63	60.72	109.34
2	D	304	ACO	CDP-CBP-CAP	-26.63	60.73	109.34
2	C	303	ACO	CDP-CBP-CAP	-26.59	60.81	109.34
2	A	301	ACO	CEP-CBP-CDP	-26.48	56.11	109.28
2	E	305	ACO	CEP-CBP-CAP	-26.48	61.00	109.34
2	F	306	ACO	CEP-CBP-CDP	-26.43	56.21	109.28
2	B	302	ACO	CEP-CBP-CDP	-26.41	56.26	109.28
2	E	305	ACO	CEP-CBP-CDP	-26.40	56.27	109.28
2	A	301	ACO	CEP-CBP-CAP	-26.38	61.18	109.34
2	D	304	ACO	CEP-CBP-CDP	-26.37	56.33	109.28
2	C	303	ACO	CEP-CBP-CAP	-26.35	61.24	109.34
2	C	303	ACO	CEP-CBP-CDP	-26.34	56.40	109.28
2	D	304	ACO	CEP-CBP-CAP	-26.34	61.26	109.34
2	F	306	ACO	CEP-CBP-CAP	-26.31	61.31	109.34
2	B	302	ACO	CEP-CBP-CAP	-26.30	61.33	109.34
2	B	302	ACO	C1B-N9A-C4A	-6.87	116.58	126.94
2	D	304	ACO	C1B-N9A-C4A	-6.84	116.62	126.94
2	C	303	ACO	C1B-N9A-C4A	-6.83	116.64	126.94
2	F	306	ACO	C1B-N9A-C4A	-6.81	116.67	126.94
2	E	305	ACO	C1B-N9A-C4A	-6.80	116.69	126.94
2	A	301	ACO	C1B-N9A-C4A	-6.79	116.70	126.94
2	E	305	ACO	C6P-C5P-N4P	-6.58	105.02	116.46
2	A	301	ACO	C6P-C5P-N4P	-6.57	105.05	116.46
2	C	303	ACO	C6P-C5P-N4P	-6.56	105.06	116.46
2	D	304	ACO	C6P-C5P-N4P	-6.55	105.08	116.46
2	F	306	ACO	C6P-C5P-N4P	-6.53	105.12	116.46
2	B	302	ACO	C6P-C5P-N4P	-6.52	105.12	116.46
2	B	302	ACO	C7P-N8P-C9P	-6.08	110.50	122.53
2	E	305	ACO	C7P-N8P-C9P	-6.00	110.65	122.53
2	D	304	ACO	C7P-N8P-C9P	-5.98	110.69	122.53
2	A	301	ACO	C7P-N8P-C9P	-5.92	110.81	122.53
2	F	306	ACO	C7P-N8P-C9P	-5.90	110.85	122.53
2	C	303	ACO	C7P-N8P-C9P	-5.88	110.89	122.53
2	B	302	ACO	C2P-C3P-N4P	-3.91	104.54	112.36
2	C	303	ACO	C2P-C3P-N4P	-3.87	104.62	112.36
2	A	301	ACO	C2P-C3P-N4P	-3.87	104.62	112.36
2	F	306	ACO	C2P-C3P-N4P	-3.81	104.73	112.36
2	D	304	ACO	C2P-C3P-N4P	-3.81	104.75	112.36
2	E	305	ACO	C2P-C3P-N4P	-3.76	104.84	112.36
2	A	301	ACO	O5A-P2A-O4A	-3.21	95.11	112.53
2	B	302	ACO	O5A-P2A-O4A	-3.15	95.45	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	304	ACO	O5A-P2A-O4A	-3.11	95.65	112.53
2	C	303	ACO	O5A-P2A-O4A	-3.07	95.88	112.53
2	E	305	ACO	OAP-CAP-C9P	-3.07	103.34	110.38
2	E	305	ACO	O5A-P2A-O4A	-3.05	95.99	112.53
2	A	301	ACO	OAP-CAP-C9P	-3.01	103.48	110.38
2	D	304	ACO	OAP-CAP-C9P	-2.99	103.53	110.38
2	F	306	ACO	O5A-P2A-O4A	-2.99	96.34	112.53
2	C	303	ACO	OAP-CAP-C9P	-2.97	103.56	110.38
2	F	306	ACO	OAP-CAP-C9P	-2.94	103.63	110.38
2	B	302	ACO	OAP-CAP-C9P	-2.92	103.69	110.38
2	A	301	ACO	N3A-C2A-N1A	-2.14	127.25	128.89
2	E	305	ACO	O3A-P2A-O6A	-2.10	97.36	102.94
2	B	302	ACO	O3A-P2A-O6A	-2.07	97.45	102.94
2	C	303	ACO	O3A-P2A-O6A	-2.03	97.54	102.94
2	F	306	ACO	O3A-P2A-O6A	-2.02	97.57	102.94
2	D	304	ACO	O3A-P2A-O6A	-2.00	97.63	102.94
2	C	303	ACO	O6A-P2A-O4A	2.16	118.02	109.62
2	E	305	ACO	O6A-P2A-O4A	2.19	118.13	109.62
2	D	304	ACO	O6A-P2A-O4A	2.21	118.19	109.62
2	C	303	ACO	O5A-P2A-O6A	2.23	119.69	108.46
2	B	302	ACO	O6A-P2A-O4A	2.23	118.26	109.62
2	E	305	ACO	O5A-P2A-O6A	2.27	119.93	108.46
2	B	302	ACO	O5A-P2A-O6A	2.28	119.96	108.46
2	F	306	ACO	O5A-P2A-O6A	2.29	119.99	108.46
2	D	304	ACO	O5A-P2A-O6A	2.29	119.99	108.46
2	A	301	ACO	O5A-P2A-O6A	2.35	120.30	108.46
2	C	303	ACO	CAP-C9P-N8P	2.78	122.64	116.47
2	D	304	ACO	CAP-C9P-N8P	2.83	122.73	116.47
2	A	301	ACO	CAP-C9P-N8P	2.83	122.74	116.47
2	E	305	ACO	CAP-C9P-N8P	2.83	122.75	116.47
2	B	302	ACO	CAP-C9P-N8P	2.87	122.82	116.47
2	F	306	ACO	C7P-C6P-C5P	2.88	117.05	112.31
2	D	304	ACO	C7P-C6P-C5P	2.88	117.06	112.31
2	C	303	ACO	C7P-C6P-C5P	2.88	117.06	112.31
2	F	306	ACO	CAP-C9P-N8P	2.89	122.88	116.47
2	E	305	ACO	C7P-C6P-C5P	2.91	117.11	112.31
2	A	301	ACO	C7P-C6P-C5P	2.92	117.12	112.31
2	B	302	ACO	C7P-C6P-C5P	3.05	117.34	112.31
2	A	301	ACO	O5P-C5P-N4P	3.82	130.51	122.94
2	F	306	ACO	O5P-C5P-N4P	3.86	130.60	122.94
2	D	304	ACO	O5P-C5P-N4P	3.87	130.62	122.94
2	C	303	ACO	O5P-C5P-N4P	3.89	130.66	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	302	ACO	O5P-C5P-N4P	3.90	130.67	122.94
2	E	305	ACO	O5P-C5P-N4P	3.94	130.75	122.94
2	E	305	ACO	C3P-C2P-S1P	4.77	124.13	111.36
2	F	306	ACO	C3P-C2P-S1P	4.87	124.40	111.36
2	A	301	ACO	C3P-C2P-S1P	4.88	124.43	111.36
2	C	303	ACO	C3P-C2P-S1P	4.88	124.44	111.36
2	D	304	ACO	C3P-C2P-S1P	4.90	124.48	111.36
2	B	302	ACO	C3P-C2P-S1P	4.94	124.58	111.36
2	E	305	ACO	C6P-C7P-N8P	5.77	124.54	111.88
2	B	302	ACO	C6P-C7P-N8P	5.80	124.61	111.88
2	A	301	ACO	C6P-C7P-N8P	5.83	124.67	111.88
2	D	304	ACO	C6P-C7P-N8P	5.87	124.76	111.88
2	F	306	ACO	C6P-C7P-N8P	5.87	124.76	111.88
2	C	303	ACO	C6P-C7P-N8P	5.90	124.82	111.88
2	B	302	ACO	C3P-N4P-C5P	7.81	138.15	122.79
2	C	303	ACO	C3P-N4P-C5P	7.87	138.28	122.79
2	E	305	ACO	C3P-N4P-C5P	7.91	138.34	122.79
2	A	301	ACO	C3P-N4P-C5P	7.91	138.35	122.79
2	F	306	ACO	C3P-N4P-C5P	7.94	138.41	122.79
2	D	304	ACO	C3P-N4P-C5P	7.99	138.50	122.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ACO	5	0
2	B	302	ACO	3	0
2	C	303	ACO	6	0
2	D	304	ACO	1	0
2	F	306	ACO	1	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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.