Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 09:25 PM EDT

PDB ID	:	1IB1
Title	:	CRYSTAL STRUCTURE OF THE 14-3-3 ZETA:SEROTONIN N-ACETYLTRANSFERASE COMPLEX
Authors	:	Obsil, T.; Ghirlando, R.; Klein, D.C.; Ganguly, S.; Dyda, F.
Deposited on	:	2001-03-26
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

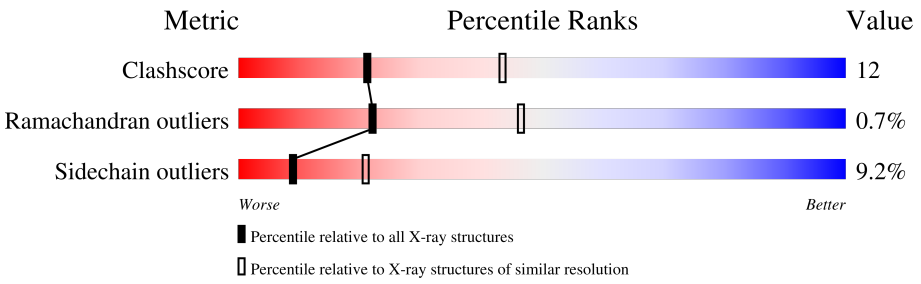
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	245	62% 27% • 7%
1	B	245	67% 24% • 7%
1	C	245	64% 24% • 7%
1	D	245	63% 26% • 7%
2	E	200	64% 22% • 10%
2	F	200	62% 24% • 10%
2	G	200	61% 26% • 10%
2	H	200	65% 22% • 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13407 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 14-3-3 ZETA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	1821	1142	306	364	9	0	0	0
1	B	227	1821	1142	306	364	9	0	0	0
1	C	227	1821	1142	306	364	9	0	0	0
1	D	227	1821	1142	306	364	9	0	0	0

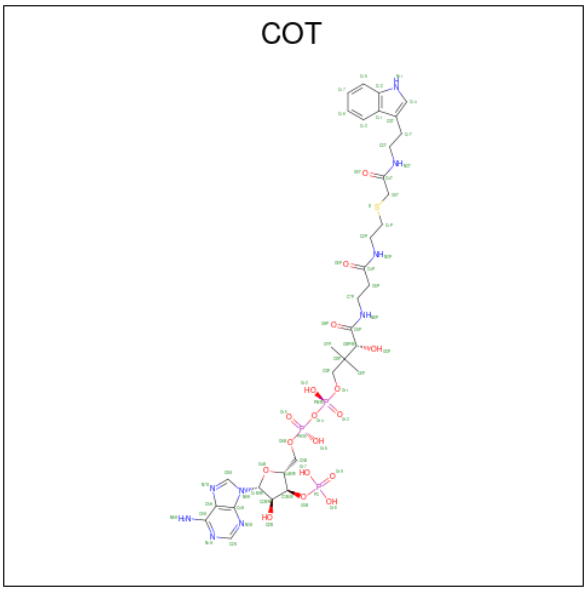
- Molecule 2 is a protein called SEROTONIN N-ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	E	179	1415	897	263	246	1	8	0	0	0
2	F	179	1415	897	263	246	1	8	0	0	0
2	G	179	1415	897	263	246	1	8	0	0	0
2	H	179	1415	897	263	246	1	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	31	TPO	THR	modified residue	UNP Q29495
F	31	TPO	THR	modified residue	UNP Q29495
G	31	TPO	THR	modified residue	UNP Q29495
H	31	TPO	THR	modified residue	UNP Q29495

- Molecule 3 is COA-S-ACETYL TRYPTAMINE (three-letter code: COT) (formula: $C_{33}H_{48}N_9O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	E	1	63	33	9	17	3	1	0	0
3	F	1	63	33	9	17	3	1	0	0
3	G	1	63	33	9	17	3	1	0	0
3	H	1	63	33	9	17	3	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	28	28	28	0	0
4	B	20	20	20	0	0
4	C	42	42	42	0	0
4	D	31	31	31	0	0
4	E	24	24	24	0	0
4	F	21	21	21	0	0
4	G	23	23	23	0	0
4	H	22	22	22	0	0

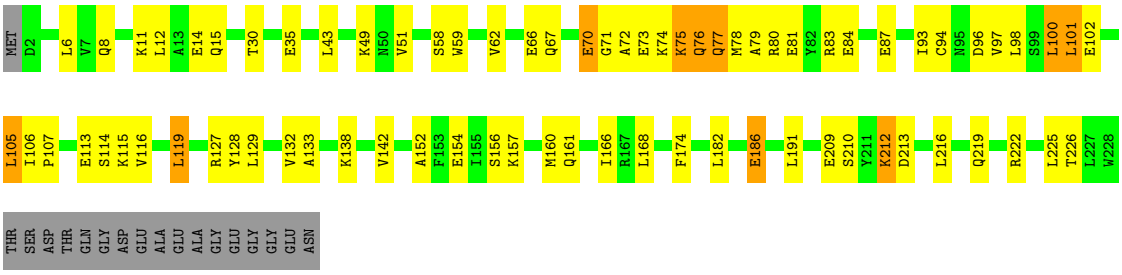
3 Residue-property plots (i)

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. 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. 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: 14-3-3 ZETA ISOFORM

Chain A: 62% 27% • 7%

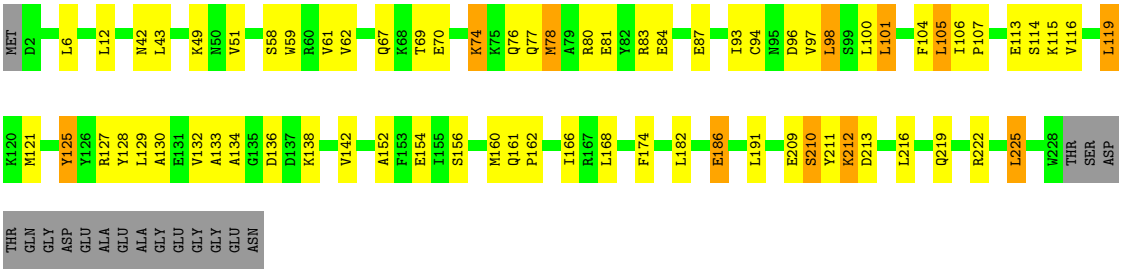


• Molecule 1: 14-3-3 ZETA ISOFORM

Chain B: 67% 24% • 7%

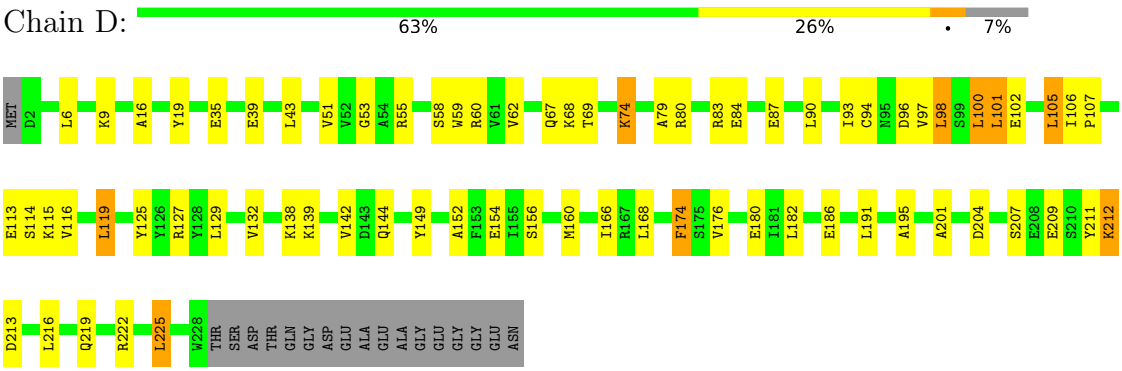
• Molecule 1: 14-3-3 ZETA ISOFORM

Chain C: 64% 24% • 7%



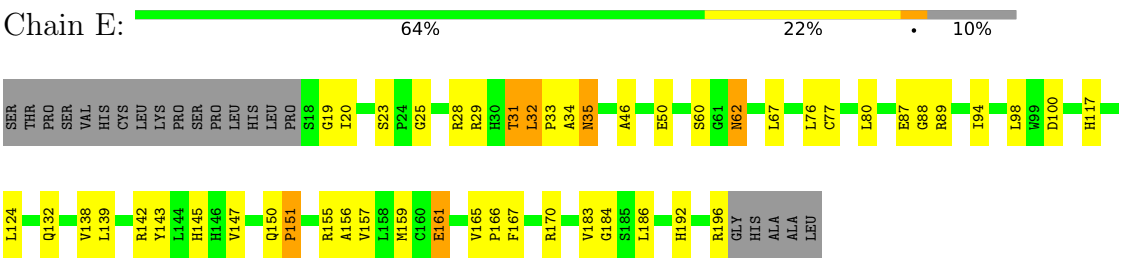
• Molecule 1: 14-3-3 ZETA ISOFORM

Chain D:



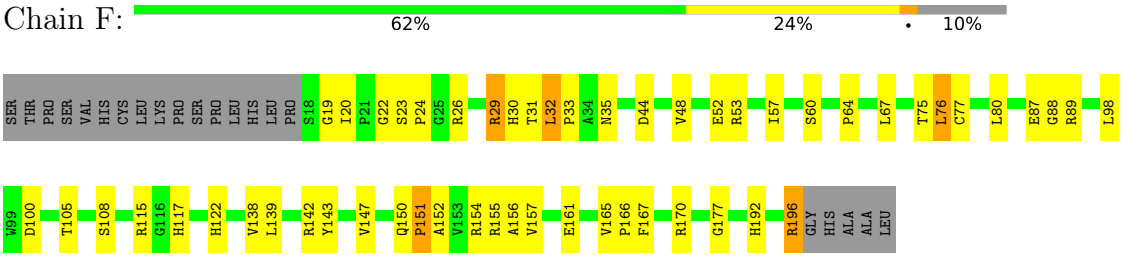
- Molecule 2: SEROTONIN N-ACETYLTRANSFERASE

Chain E:



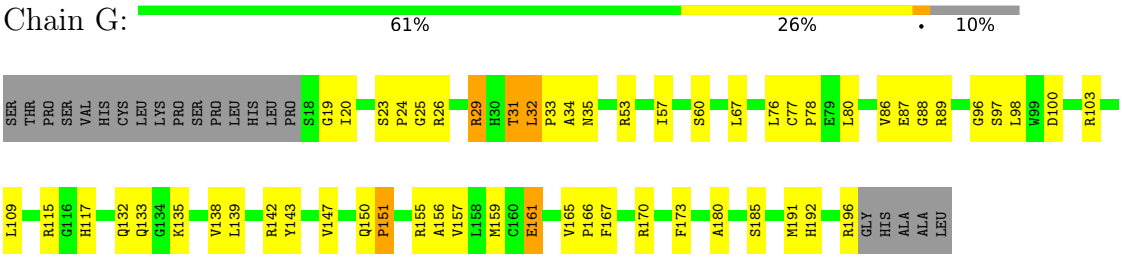
- Molecule 2: SEROTONIN N-ACETYLTRANSFERASE

Chain F:



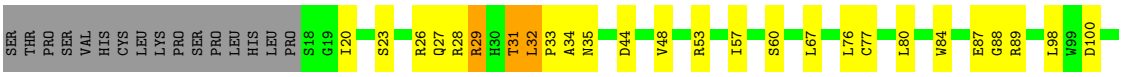
- Molecule 2: SEROTONIN N-ACETYLTRANSFERASE

Chain G:



- Molecule 2: SEROTONIN N-ACETYLTRANSFERASE

Chain H:



T105
Q106
E107
S108
H117
V138
L139
R142
Y143
L144
V147
Q150
P151
R155
A156
V157
L158
M159
C160
E161
V165
P166
F167
R170
H192
R196
GLY
HIS
ALA
ALA
LEU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	74.72Å 75.08Å 101.78Å 90.14° 90.06° 63.04°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	99.3 (20.00-2.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.204 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13407	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

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: TPO, COT

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	0.42	0/1846	0.67	0/2482
1	B	0.42	0/1846	0.62	0/2482
1	C	0.42	0/1846	0.64	0/2482
1	D	0.41	0/1846	0.65	0/2482
2	E	0.44	0/1443	0.69	1/1956 (0.1%)
2	F	0.46	0/1443	0.71	1/1956 (0.1%)
2	G	0.44	0/1443	0.68	1/1956 (0.1%)
2	H	0.45	0/1443	0.68	0/1956
All	All	0.43	0/13156	0.67	3/17752 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	19	GLY	N-CA-C	5.19	126.06	113.10
2	F	19	GLY	N-CA-C	5.18	126.05	113.10
2	E	19	GLY	N-CA-C	5.16	125.99	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	125	TYR	Sidechain
1	C	125	TYR	Sidechain
1	D	125	TYR	Sidechain

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	1821	0	1809	67	0
1	B	1821	0	1809	40	1
1	C	1821	0	1809	48	0
1	D	1821	0	1809	49	0
2	E	1415	0	1382	32	0
2	F	1415	0	1382	43	1
2	G	1415	0	1382	44	0
2	H	1415	0	1382	34	0
3	E	63	0	44	1	0
3	F	63	0	44	1	0
3	G	63	0	44	1	0
3	H	63	0	44	0	0
4	A	28	0	0	19	0
4	B	20	0	0	5	0
4	C	42	0	0	7	1
4	D	31	0	0	13	1
4	E	24	0	0	2	0
4	F	21	0	0	6	0
4	G	23	0	0	10	0
4	H	22	0	0	2	0
All	All	13407	0	12940	317	2

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 12.

All (317) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ARG:HD2	4:D:3635:HOH:O	1.34	1.22
1:D:144:GLN:HG3	4:D:4412:HOH:O	1.37	1.20
1:A:73:GLU:HB2	4:A:2487:HOH:O	1.57	1.03
1:A:75:LYS:HE3	1:B:8:GLN:HG2	1.48	0.94
1:A:226:THR:CB	4:A:3511:HOH:O	2.24	0.86
1:C:74:LYS:HD3	1:C:74:LYS:N	1.90	0.84
1:A:226:THR:HB	4:A:3511:HOH:O	1.77	0.83
1:A:75:LYS:CE	1:B:8:GLN:HG2	2.10	0.81
1:C:129:LEU:HD21	4:C:2870:HOH:O	1.83	0.77
1:A:73:GLU:CB	4:A:2487:HOH:O	2.22	0.77
2:F:117:HIS:HB3	4:F:3100:HOH:O	1.85	0.76
1:C:78:MET:HB3	4:C:3675:HOH:O	1.86	0.75
2:E:159:MET:HE2	4:E:3297:HOH:O	1.85	0.75
2:F:76:LEU:HG	2:G:185:SER:HA	1.69	0.75
2:F:154:ARG:NH1	4:F:3100:HOH:O	2.18	0.74
2:G:115:ARG:HD2	4:G:3362:HOH:O	1.89	0.72
1:C:69:THR:HB	1:C:76:GLN:HG2	1.72	0.72
1:A:73:GLU:CA	4:A:2487:HOH:O	2.36	0.71
2:G:115:ARG:NH1	4:G:3483:HOH:O	2.23	0.70
2:G:115:ARG:CD	4:G:3362:HOH:O	2.40	0.69
1:C:211:TYR:O	1:C:212:LYS:HG2	1.93	0.69
1:A:210:SER:HB2	1:A:212:LYS:NZ	2.09	0.68
1:B:210:SER:O	1:B:212:LYS:HG3	1.93	0.68
1:D:19:TYR:HD2	4:D:3597:HOH:O	1.77	0.68
2:E:159:MET:CE	4:E:3297:HOH:O	2.42	0.67
2:G:96:GLY:O	4:G:2928:HOH:O	2.13	0.67
1:A:66:GLU:O	1:A:76:GLN:NE2	2.27	0.66
1:A:119:LEU:HB3	1:A:152:ALA:HB2	1.77	0.66
1:A:75:LYS:HE3	1:B:8:GLN:CG	2.24	0.65
1:A:51:VAL:HG12	1:A:93:ILE:HD13	1.78	0.65
1:D:139:LYS:HB2	4:D:4357:HOH:O	1.96	0.64
2:F:32:LEU:HD22	2:F:33:PRO:HD2	1.80	0.64
1:C:77:GLN:O	1:C:81:GLU:HG3	1.98	0.64
1:D:60:ARG:NH2	4:D:3777:HOH:O	2.29	0.63
1:C:51:VAL:HG12	1:C:93:ILE:HD13	1.80	0.63
2:G:32:LEU:HD22	2:G:33:PRO:HD2	1.79	0.63
1:A:219:GLN:NE2	1:A:222:ARG:HD3	2.14	0.62
2:H:20:ILE:HD11	4:H:1440:HOH:O	1.98	0.62
1:A:74:LYS:C	1:A:76:GLN:H	2.02	0.62
1:A:226:THR:HG21	4:A:3511:HOH:O	1.99	0.62
1:C:119:LEU:HB3	1:C:152:ALA:HB2	1.80	0.62
1:A:213:ASP:HB3	2:E:89:ARG:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:GLN:NE2	1:D:222:ARG:HD3	2.15	0.62
1:B:119:LEU:HB3	1:B:152:ALA:HB2	1.82	0.61
1:D:100:LEU:HD13	4:D:4194:HOH:O	2.01	0.61
2:E:32:LEU:HD22	2:E:33:PRO:HD2	1.81	0.61
1:A:226:THR:CG2	4:A:3511:HOH:O	2.46	0.61
1:C:136:ASP:HB3	4:C:2713:HOH:O	1.99	0.61
2:H:32:LEU:HD22	2:H:33:PRO:HD2	1.83	0.61
1:B:68:LYS:NZ	2:F:22:GLY:HA2	2.16	0.61
1:B:116:VAL:HG23	1:B:152:ALA:HB1	1.83	0.61
1:D:195:ALA:HA	4:D:4520:HOH:O	2.01	0.61
2:F:152:ALA:N	4:F:3059:HOH:O	2.34	0.60
1:C:104:PHE:HB3	4:C:2676:HOH:O	2.00	0.60
1:B:213:ASP:HB3	2:F:89:ARG:HG3	1.82	0.60
1:C:161:GLN:HE21	1:C:209:GLU:HB3	1.67	0.60
1:B:51:VAL:HG12	1:B:93:ILE:HD13	1.82	0.60
1:B:216:LEU:HD23	2:F:88:GLY:HA2	1.82	0.60
1:C:116:VAL:HG23	1:C:152:ALA:HB1	1.84	0.60
2:H:143:TYR:O	2:H:147:VAL:HG22	2.02	0.60
1:D:211:TYR:O	1:D:212:LYS:HG2	2.01	0.59
1:A:101:LEU:HA	1:A:105:LEU:HB2	1.83	0.59
2:E:143:TYR:O	2:E:147:VAL:HG22	2.02	0.59
1:C:212:LYS:HA	4:C:2423:HOH:O	2.01	0.59
1:D:119:LEU:HB3	1:D:152:ALA:HB2	1.85	0.59
1:A:73:GLU:N	4:A:2487:HOH:O	2.34	0.59
1:C:101:LEU:HA	1:C:105:LEU:HB2	1.84	0.59
2:F:143:TYR:O	2:F:147:VAL:HG22	2.03	0.59
2:G:143:TYR:O	2:G:147:VAL:HG22	2.02	0.59
1:C:12:LEU:HD21	1:D:79:ALA:HA	1.84	0.58
1:D:101:LEU:HA	1:D:105:LEU:HB2	1.84	0.58
1:A:210:SER:HB2	1:A:212:LYS:HZ2	1.68	0.58
1:A:116:VAL:HG23	1:A:152:ALA:HB1	1.85	0.58
1:D:127:ARG:NH2	2:H:31:TPO:O1P	2.37	0.58
1:A:66:GLU:HG2	1:A:76:GLN:NE2	2.18	0.58
1:D:74:LYS:HB3	4:D:3157:HOH:O	2.03	0.58
1:D:51:VAL:HG12	1:D:93:ILE:HD13	1.84	0.58
1:D:213:ASP:HB3	2:H:89:ARG:HG3	1.85	0.58
1:D:116:VAL:HG23	1:D:152:ALA:HB1	1.85	0.57
1:B:101:LEU:HA	1:B:105:LEU:HB2	1.87	0.57
2:F:53:ARG:HA	2:F:57:ILE:HD12	1.86	0.57
1:D:35:GLU:HA	4:D:4441:HOH:O	2.04	0.57
1:C:70:GLU:OE2	2:H:170:ARG:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLN:NE2	1:C:222:ARG:HD3	2.20	0.56
2:F:115:ARG:HE	2:G:103:ARG:NH2	2.03	0.56
1:A:133:ALA:HB3	1:A:138:LYS:HD2	1.87	0.56
2:H:44:ASP:O	2:H:48:VAL:HG23	2.05	0.56
1:D:138:LYS:O	1:D:142:VAL:HG23	2.06	0.55
1:B:219:GLN:NE2	1:B:222:ARG:HD3	2.22	0.55
1:D:53:GLY:CA	4:D:3872:HOH:O	2.54	0.55
2:E:80:LEU:HD11	2:E:98:LEU:HG	1.88	0.55
1:D:74:LYS:HA	1:D:74:LYS:NZ	2.22	0.55
2:G:100:ASP:HA	2:G:117:HIS:CE1	2.42	0.55
1:A:74:LYS:O	1:A:74:LYS:HG3	2.07	0.55
2:E:25:GLY:O	2:F:196:ARG:HB3	2.07	0.55
1:D:219:GLN:HE22	1:D:222:ARG:HD3	1.73	0.54
2:F:157:VAL:HG12	2:F:192:HIS:CD2	2.42	0.54
1:A:138:LYS:O	1:A:142:VAL:HG23	2.08	0.54
1:C:83:ARG:O	1:C:87:GLU:HG3	2.08	0.54
1:D:113:GLU:HG2	1:D:166:ILE:HD12	1.89	0.54
1:A:15:GLN:HG3	4:A:3061:HOH:O	2.07	0.54
2:F:80:LEU:HD11	2:F:98:LEU:HG	1.89	0.54
1:A:58:SER:O	1:A:62:VAL:HG12	2.09	0.53
2:G:80:LEU:HD11	2:G:98:LEU:HG	1.89	0.53
2:E:100:ASP:HA	2:E:117:HIS:CE1	2.43	0.53
1:A:75:LYS:HD3	1:A:78:MET:CG	2.39	0.53
1:A:75:LYS:CD	1:A:78:MET:HG3	2.39	0.53
1:C:58:SER:O	1:C:62:VAL:HG12	2.09	0.53
1:D:39:GLU:HB2	4:D:4270:HOH:O	2.08	0.53
2:H:100:ASP:HA	2:H:117:HIS:CE1	2.43	0.53
1:A:74:LYS:O	1:A:76:GLN:N	2.43	0.52
1:D:116:VAL:HG11	1:D:160:MET:CE	2.39	0.52
2:G:180:ALA:CB	4:G:3032:HOH:O	2.57	0.52
2:H:80:LEU:HD11	2:H:98:LEU:HG	1.92	0.52
1:A:219:GLN:HE22	1:A:222:ARG:HD3	1.74	0.52
1:A:100:LEU:CD1	4:A:3264:HOH:O	2.57	0.52
2:F:100:ASP:HA	2:F:117:HIS:CE1	2.45	0.52
2:F:152:ALA:CB	4:F:3059:HOH:O	2.57	0.52
1:B:116:VAL:HG11	1:B:160:MET:CE	2.40	0.52
1:D:83:ARG:O	1:D:87:GLU:HG3	2.10	0.51
1:C:113:GLU:HB2	4:C:2183:HOH:O	2.09	0.51
1:A:161:GLN:HE21	1:A:209:GLU:HB3	1.76	0.51
1:A:116:VAL:HG11	1:A:160:MET:CE	2.41	0.51
1:C:94:CYS:HB2	1:C:129:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LYS:O	1:C:142:VAL:HG23	2.11	0.51
1:D:58:SER:O	1:D:62:VAL:HG12	2.11	0.51
2:H:77:CYS:HB2	2:H:80:LEU:HD12	1.93	0.50
1:A:113:GLU:HG2	1:A:166:ILE:HD12	1.93	0.50
1:D:212:LYS:HA	4:D:4321:HOH:O	2.09	0.50
2:G:77:CYS:HB2	2:G:80:LEU:HD12	1.94	0.50
2:G:157:VAL:HG12	2:G:192:HIS:CD2	2.46	0.50
2:F:75:THR:HB	2:G:185:SER:HB3	1.94	0.50
2:H:31:TPO:O1P	2:H:31:TPO:HG21	2.12	0.50
1:C:80:ARG:O	1:C:84:GLU:HG3	2.12	0.50
1:B:59:TRP:CE2	1:B:132:VAL:HG12	2.47	0.50
1:C:74:LYS:HD3	1:C:74:LYS:H	1.71	0.49
1:C:78:MET:HE1	1:D:9:LYS:HG3	1.93	0.49
2:G:109:LEU:HD21	2:G:159:MET:HE1	1.94	0.49
1:A:14:GLU:HB3	4:A:3061:HOH:O	2.11	0.49
1:B:58:SER:O	1:B:62:VAL:HG12	2.12	0.49
2:G:25:GLY:O	2:H:196:ARG:HB3	2.12	0.49
1:A:83:ARG:O	1:A:87:GLU:HG3	2.12	0.49
1:B:127:ARG:NH2	2:F:31:TPO:O1P	2.45	0.49
1:D:207:SER:C	1:D:209:GLU:H	2.16	0.49
2:H:157:VAL:HG12	2:H:192:HIS:CD2	2.48	0.49
1:A:70:GLU:OE2	2:F:170:ARG:HD2	2.12	0.49
1:C:213:ASP:HB3	2:G:89:ARG:HG3	1.95	0.49
2:G:115:ARG:HA	4:G:3337:HOH:O	2.11	0.49
1:A:115:LYS:O	1:A:119:LEU:HB2	2.13	0.49
1:C:113:GLU:HG2	1:C:166:ILE:HD12	1.95	0.48
1:D:176:VAL:HG13	2:H:29:ARG:HD2	1.96	0.48
2:F:167:PHE:O	2:F:170:ARG:HG3	2.14	0.48
1:A:77:GLN:O	1:A:81:GLU:HG3	2.14	0.48
1:C:210:SER:HB2	1:C:212:LYS:NZ	2.27	0.48
1:C:219:GLN:HE22	1:C:222:ARG:HD3	1.78	0.48
1:C:161:GLN:NE2	1:C:209:GLU:O	2.47	0.48
1:A:30:THR:HG23	4:A:3467:HOH:O	2.13	0.48
1:B:168:LEU:CD1	4:B:1726:HOH:O	2.61	0.48
1:C:59:TRP:CE2	1:C:132:VAL:HG12	2.48	0.48
2:G:155:ARG:HG2	2:G:156:ALA:N	2.28	0.48
1:D:80:ARG:O	1:D:84:GLU:HG3	2.14	0.48
2:E:157:VAL:HG12	2:E:192:HIS:CD2	2.48	0.48
1:D:59:TRP:CE2	1:D:132:VAL:HG12	2.49	0.48
1:D:115:LYS:O	1:D:119:LEU:HB2	2.14	0.47
2:E:20:ILE:CG2	2:E:23:SER:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:138:VAL:O	2:E:142:ARG:HB2	2.15	0.47
1:A:35:GLU:OE1	4:A:3725:HOH:O	2.19	0.47
1:B:108:ASN:HB2	4:B:1727:HOH:O	2.14	0.47
2:H:167:PHE:O	2:H:170:ARG:HG3	2.14	0.47
1:A:75:LYS:NZ	1:B:5:GLU:HG2	2.30	0.47
1:C:116:VAL:HG11	1:C:160:MET:CE	2.45	0.47
2:F:31:TPO:O1P	2:F:31:TPO:HG21	2.15	0.47
1:A:94:CYS:HB2	1:A:129:LEU:HD13	1.95	0.47
1:B:150:GLN:HB3	4:B:1438:HOH:O	2.15	0.47
1:D:98:LEU:HD12	1:D:98:LEU:HA	1.83	0.47
2:F:157:VAL:HG12	2:F:192:HIS:HD2	1.80	0.47
1:B:94:CYS:HB2	1:B:129:LEU:HD13	1.97	0.46
1:D:94:CYS:HB2	1:D:129:LEU:HD13	1.98	0.46
2:F:77:CYS:HB2	2:F:80:LEU:HD12	1.96	0.46
1:A:127:ARG:NH2	2:E:31:TPO:O1P	2.49	0.46
4:A:3431:HOH:O	2:E:32:LEU:HB3	2.15	0.46
1:B:219:GLN:HE22	1:B:222:ARG:HD3	1.79	0.46
2:F:20:ILE:CG2	2:F:23:SER:HB2	2.44	0.46
1:B:55:ARG:HB3	1:B:90:LEU:HD13	1.98	0.46
1:B:83:ARG:O	1:B:87:GLU:HG3	2.16	0.46
2:E:155:ARG:HG2	2:E:156:ALA:N	2.30	0.46
2:G:20:ILE:CG2	2:G:23:SER:HB2	2.44	0.46
2:G:133:GLN:HB3	2:G:135:LYS:HE2	1.98	0.46
2:H:32:LEU:HD11	2:H:87:GLU:HB3	1.96	0.46
1:A:210:SER:HB2	1:A:212:LYS:HZ3	1.80	0.46
2:E:132:GLN:HE22	3:E:401:COT:HC8	1.81	0.46
2:F:152:ALA:HB2	4:F:3059:HOH:O	2.15	0.46
1:A:70:GLU:CD	2:F:170:ARG:HD2	2.36	0.46
1:D:106:ILE:CG1	1:D:107:PRO:HD3	2.46	0.46
2:E:77:CYS:HB2	2:E:80:LEU:HD12	1.98	0.46
2:H:105:THR:O	2:H:108:SER:OG	2.33	0.46
1:C:162:PRO:HG2	4:C:2035:HOH:O	2.15	0.46
1:D:201:ALA:O	1:D:204:ASP:HB2	2.16	0.46
2:F:155:ARG:HG2	2:F:156:ALA:N	2.31	0.46
1:A:74:LYS:C	1:A:76:GLN:N	2.67	0.46
1:C:94:CYS:CB	1:C:129:LEU:HD13	2.46	0.46
2:F:44:ASP:O	2:F:48:VAL:HG23	2.16	0.46
1:A:49:LYS:HE3	1:A:128:TYR:OH	2.16	0.45
1:B:94:CYS:CB	1:B:129:LEU:HD13	2.45	0.45
1:A:75:LYS:HE3	1:B:8:GLN:CB	2.47	0.45
1:A:75:LYS:HD3	1:A:78:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:115:ARG:NE	2:G:103:ARG:NH2	2.64	0.45
1:A:12:LEU:HD21	1:B:79:ALA:HA	1.98	0.45
1:C:115:LYS:O	1:C:119:LEU:HB2	2.16	0.45
1:A:79:ALA:HA	1:B:12:LEU:HD21	1.97	0.45
1:B:55:ARG:CB	1:B:90:LEU:HD13	2.46	0.45
2:H:138:VAL:O	2:H:142:ARG:HB2	2.16	0.45
2:H:155:ARG:HG2	2:H:156:ALA:N	2.32	0.45
1:B:80:ARG:O	1:B:84:GLU:HG3	2.17	0.45
2:F:138:VAL:O	2:F:142:ARG:HB2	2.17	0.45
2:E:62:ASN:ND2	2:E:184:GLY:HA3	2.32	0.44
2:G:24:PRO:HB3	2:H:144:LEU:C	2.38	0.44
2:G:34:ALA:HA	2:G:87:GLU:HG2	1.98	0.44
2:G:138:VAL:O	2:G:142:ARG:HB2	2.17	0.44
2:G:161:GLU:H	2:G:161:GLU:HG2	1.54	0.44
2:E:161:GLU:H	2:E:161:GLU:HG2	1.56	0.44
1:B:49:LYS:HE3	1:B:128:TYR:OH	2.17	0.44
2:H:150:GLN:HA	2:H:151:PRO:HD3	1.59	0.44
2:H:165:VAL:HB	2:H:166:PRO:HD3	1.99	0.44
2:H:34:ALA:HA	2:H:87:GLU:HG2	2.00	0.44
1:A:59:TRP:CE2	1:A:132:VAL:HG12	2.53	0.44
1:D:149:TYR:HB3	1:D:174:PHE:CE1	2.53	0.44
2:F:23:SER:HB3	2:F:26:ARG:HD3	2.00	0.44
2:G:132:GLN:HE22	3:G:402:COT:HC8	1.83	0.44
2:H:20:ILE:CG2	2:H:23:SER:HB2	2.47	0.44
1:A:212:LYS:HE2	4:A:3846:HOH:O	2.17	0.44
1:D:216:LEU:HD23	2:H:88:GLY:HA2	2.00	0.44
2:F:165:VAL:HB	2:F:166:PRO:HD3	2.00	0.44
1:A:157:LYS:HE2	4:A:4240:HOH:O	2.17	0.44
4:A:3846:HOH:O	2:E:50:GLU:HG3	2.16	0.44
1:C:49:LYS:HE3	1:C:128:TYR:OH	2.17	0.44
2:G:31:TPO:O1P	2:G:31:TPO:HG21	2.17	0.44
2:G:53:ARG:HA	2:G:57:ILE:HD12	1.99	0.44
1:A:73:GLU:C	4:A:2487:HOH:O	2.53	0.44
1:B:168:LEU:HD11	4:B:1726:HOH:O	2.18	0.44
1:B:113:GLU:HG2	1:B:166:ILE:HD12	2.00	0.43
2:G:29:ARG:H	2:G:29:ARG:HG3	1.60	0.43
2:G:180:ALA:HB3	4:G:3032:HOH:O	2.18	0.43
2:E:167:PHE:O	2:E:170:ARG:HG3	2.18	0.43
2:G:150:GLN:HA	2:G:151:PRO:HD3	1.60	0.43
2:G:165:VAL:HB	2:G:166:PRO:HD3	1.99	0.43
1:B:106:ILE:CG1	1:B:107:PRO:HD3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:HD12	1:C:119:LEU:HA	1.86	0.43
2:E:34:ALA:HA	2:E:87:GLU:HG2	1.99	0.43
1:A:106:ILE:CG1	1:A:107:PRO:HD3	2.48	0.43
1:A:80:ARG:O	1:A:84:GLU:HG3	2.17	0.43
1:B:115:LYS:O	1:B:119:LEU:HB2	2.19	0.43
2:E:145:HIS:CE1	2:F:24:PRO:HA	2.54	0.43
1:C:42:ASN:ND2	2:G:86:VAL:HG13	2.34	0.43
2:E:150:GLN:HA	2:E:151:PRO:HD3	1.60	0.43
2:E:183:VAL:O	2:E:186:LEU:HB2	2.19	0.43
2:G:167:PHE:O	2:G:170:ARG:HG3	2.19	0.43
1:D:55:ARG:CB	1:D:90:LEU:HD13	2.49	0.42
2:F:122:HIS:O	3:F:400:COT:H2T1	2.19	0.42
1:D:94:CYS:CB	1:D:129:LEU:HD13	2.49	0.42
2:E:31:TPO:O1P	2:E:31:TPO:HG21	2.18	0.42
2:H:161:GLU:H	2:H:161:GLU:HG2	1.55	0.42
1:C:127:ARG:NH2	2:G:31:TPO:O1P	2.53	0.42
2:E:46:ALA:O	2:E:50:GLU:HG2	2.19	0.42
1:A:94:CYS:CB	1:A:129:LEU:HD13	2.49	0.42
1:A:216:LEU:HD23	2:E:88:GLY:HA2	2.02	0.42
1:D:225:LEU:HD12	1:D:225:LEU:HA	1.96	0.42
1:D:74:LYS:HA	1:D:74:LYS:HZ1	1.84	0.42
2:G:23:SER:HB3	2:G:26:ARG:HD3	2.00	0.41
1:A:72:ALA:H	1:A:74:LYS:HZ2	1.68	0.41
1:D:101:LEU:O	1:D:106:ILE:HG12	2.20	0.41
2:E:34:ALA:O	2:E:35:ASN:HB2	2.20	0.41
2:F:105:THR:O	2:F:108:SER:OG	2.33	0.41
1:A:11:LYS:O	4:A:3061:HOH:O	2.22	0.41
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.87	0.41
1:B:35:GLU:HA	4:B:1794:HOH:O	2.20	0.41
1:B:186:GLU:H	1:B:186:GLU:CD	2.23	0.41
1:C:121:MET:O	1:C:125:TYR:HD1	2.03	0.41
1:C:130:ALA:HA	1:C:133:ALA:HB2	2.03	0.41
2:H:26:ARG:N	2:H:26:ARG:CD	2.84	0.41
1:D:144:GLN:CG	4:D:4412:HOH:O	2.21	0.41
2:F:115:ARG:HE	2:G:103:ARG:HH21	1.69	0.41
2:H:20:ILE:HD11	2:H:28:ARG:HA	2.01	0.41
1:B:149:TYR:HB3	1:B:174:PHE:CE1	2.55	0.41
2:E:20:ILE:HD11	2:E:28:ARG:HA	2.02	0.41
2:E:94:ILE:HG12	2:E:124:LEU:HD13	2.01	0.41
2:G:115:ARG:HD3	4:G:3362:HOH:O	2.16	0.41
1:A:71:GLY:HA3	1:A:74:LYS:HZ2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LEU:HD23	2:G:88:GLY:HA2	2.01	0.41
2:F:26:ARG:N	2:F:26:ARG:CD	2.84	0.41
2:H:53:ARG:HA	2:H:57:ILE:HD12	2.03	0.41
1:A:186:GLU:H	1:A:186:GLU:CD	2.24	0.41
2:G:78:PRO:HB2	4:G:2927:HOH:O	2.21	0.41
1:C:186:GLU:CD	1:C:186:GLU:H	2.23	0.41
1:C:61:VAL:HG11	1:D:16:ALA:HA	2.02	0.41
1:C:225:LEU:HD12	1:C:225:LEU:HA	1.95	0.41
1:D:113:GLU:CG	1:D:166:ILE:HD12	2.51	0.41
2:E:165:VAL:HB	2:E:166:PRO:HD3	2.02	0.41
2:F:150:GLN:HA	2:F:151:PRO:HD3	1.63	0.41
2:G:132:GLN:NE2	4:G:2717:HOH:O	2.49	0.41
2:H:23:SER:HB3	2:H:26:ARG:HD3	2.02	0.41
1:B:119:LEU:HD12	1:B:119:LEU:HA	1.88	0.41
1:D:180:GLU:OE2	2:H:29:ARG:HD3	2.20	0.41
2:F:29:ARG:H	2:F:29:ARG:HG3	1.63	0.41
2:F:32:LEU:HD11	2:F:87:GLU:HB3	2.03	0.41
2:G:173:PHE:HB3	2:G:191:MET:HB3	2.03	0.40
1:C:106:ILE:CG1	1:C:107:PRO:HD3	2.51	0.40
2:H:84:TRP:HZ3	2:H:138:VAL:HB	1.85	0.40
1:A:49:LYS:HG2	2:E:34:ALA:HB2	2.02	0.40
1:C:106:ILE:HG12	1:C:107:PRO:HD3	2.03	0.40
2:H:159:MET:HG2	4:H:1299:HOH:O	2.20	0.40
1:C:98:LEU:HD12	1:C:98:LEU:HA	1.84	0.40
2:F:30:HIS:HA	4:F:2192:HOH:O	2.22	0.40
2:H:29:ARG:H	2:H:29:ARG:HG3	1.59	0.40
1:B:68:LYS:HZ2	2:F:22:GLY:HA2	1.87	0.40
2:F:52:GLU:OE2	2:F:64:PRO:HD2	2.21	0.40
2:G:80:LEU:HD13	2:G:97:SER:HA	2.03	0.40

All (2) 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:F:177:GLY:N	4:C:2713:HOH:O[1_554]	2.05	0.15
1:B:31:GLU:O	4:D:4373:HOH:O[1_464]	2.09	0.11

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	225/245 (92%)	216 (96%)	8 (4%)	1 (0%)	34	60
1	B	225/245 (92%)	215 (96%)	8 (4%)	2 (1%)	17	40
1	C	225/245 (92%)	218 (97%)	6 (3%)	1 (0%)	34	60
1	D	225/245 (92%)	216 (96%)	9 (4%)	0	100	100
2	E	176/200 (88%)	167 (95%)	7 (4%)	2 (1%)	14	34
2	F	176/200 (88%)	169 (96%)	5 (3%)	2 (1%)	14	34
2	G	176/200 (88%)	169 (96%)	5 (3%)	2 (1%)	14	34
2	H	176/200 (88%)	168 (96%)	6 (3%)	2 (1%)	14	34
All	All	1604/1780 (90%)	1538 (96%)	54 (3%)	12 (1%)	22	46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	ALA
1	C	134	ALA
1	A	75	LYS
2	E	151	PRO
2	F	151	PRO
2	G	151	PRO
2	H	151	PRO
1	B	211	TYR
2	H	35	ASN
2	E	35	ASN
2	F	35	ASN
2	G	35	ASN

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	197/209 (94%)	172 (87%)	25 (13%)	4 10
1	B	197/209 (94%)	177 (90%)	20 (10%)	7 17
1	C	197/209 (94%)	174 (88%)	23 (12%)	5 12
1	D	197/209 (94%)	173 (88%)	24 (12%)	5 11
2	E	148/166 (89%)	139 (94%)	9 (6%)	18 41
2	F	148/166 (89%)	140 (95%)	8 (5%)	22 47
2	G	148/166 (89%)	140 (95%)	8 (5%)	22 47
2	H	148/166 (89%)	138 (93%)	10 (7%)	16 36
All	All	1380/1500 (92%)	1253 (91%)	127 (9%)	9 21

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	8	GLN
1	A	43	LEU
1	A	67	GLN
1	A	70	GLU
1	A	76	GLN
1	A	77	GLN
1	A	96	ASP
1	A	97	VAL
1	A	98	LEU
1	A	100	LEU
1	A	101	LEU
1	A	102	GLU
1	A	105	LEU
1	A	114	SER
1	A	119	LEU
1	A	154	GLU
1	A	156	SER
1	A	168	LEU
1	A	174	PHE
1	A	182	LEU
1	A	186	GLU
1	A	191	LEU

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Mol	Chain	Res	Type
1	A	212	LYS
1	A	225	LEU
1	B	6	LEU
1	B	43	LEU
1	B	96	ASP
1	B	97	VAL
1	B	98	LEU
1	B	100	LEU
1	B	101	LEU
1	B	102	GLU
1	B	105	LEU
1	B	114	SER
1	B	119	LEU
1	B	136	ASP
1	B	154	GLU
1	B	156	SER
1	B	168	LEU
1	B	174	PHE
1	B	182	LEU
1	B	186	GLU
1	B	191	LEU
1	B	225	LEU
1	C	6	LEU
1	C	43	LEU
1	C	67	GLN
1	C	74	LYS
1	C	78	MET
1	C	96	ASP
1	C	97	VAL
1	C	98	LEU
1	C	100	LEU
1	C	101	LEU
1	C	105	LEU
1	C	114	SER
1	C	119	LEU
1	C	154	GLU
1	C	156	SER
1	C	168	LEU
1	C	174	PHE
1	C	182	LEU
1	C	186	GLU
1	C	191	LEU

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Mol	Chain	Res	Type
1	C	210	SER
1	C	212	LYS
1	C	225	LEU
1	D	6	LEU
1	D	43	LEU
1	D	67	GLN
1	D	68	LYS
1	D	69	THR
1	D	74	LYS
1	D	96	ASP
1	D	97	VAL
1	D	98	LEU
1	D	100	LEU
1	D	101	LEU
1	D	102	GLU
1	D	105	LEU
1	D	114	SER
1	D	119	LEU
1	D	154	GLU
1	D	156	SER
1	D	168	LEU
1	D	174	PHE
1	D	182	LEU
1	D	186	GLU
1	D	191	LEU
1	D	212	LYS
1	D	225	LEU
2	E	29	ARG
2	E	32	LEU
2	E	60	SER
2	E	62	ASN
2	E	67	LEU
2	E	76	LEU
2	E	139	LEU
2	E	161	GLU
2	E	196	ARG
2	F	29	ARG
2	F	32	LEU
2	F	60	SER
2	F	67	LEU
2	F	76	LEU
2	F	139	LEU

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Mol	Chain	Res	Type
2	F	161	GLU
2	F	196	ARG
2	G	29	ARG
2	G	32	LEU
2	G	60	SER
2	G	67	LEU
2	G	76	LEU
2	G	139	LEU
2	G	161	GLU
2	G	196	ARG
2	H	27	GLN
2	H	29	ARG
2	H	32	LEU
2	H	60	SER
2	H	67	LEU
2	H	76	LEU
2	H	107	GLU
2	H	139	LEU
2	H	161	GLU
2	H	196	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	111	GLN
1	A	161	GLN
1	A	219	GLN
1	B	77	GLN
1	B	108	ASN
1	B	219	GLN
1	C	76	GLN
1	C	77	GLN
1	C	108	ASN
1	C	146	GLN
1	C	161	GLN
1	C	219	GLN
1	D	108	ASN
1	D	219	GLN
2	E	62	ASN
2	E	117	HIS
2	E	132	GLN

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Mol	Chain	Res	Type
2	F	62	ASN
2	F	117	HIS
2	F	174	HIS
2	G	62	ASN
2	G	117	HIS
2	G	132	GLN
2	H	62	ASN
2	H	117	HIS
2	H	132	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TPO	G	31	2	8,10,11	1.29	2 (25%)	10,14,16	1.21	0
2	TPO	F	31	2	8,10,11	1.13	0	10,14,16	1.13	0
2	TPO	H	31	2	8,10,11	1.44	2 (25%)	10,14,16	1.15	0
2	TPO	E	31	2	8,10,11	1.39	2 (25%)	10,14,16	1.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	G	31	2	-	1/9/11/13	-
2	TPO	F	31	2	-	1/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	H	31	2	-	1/9/11/13	-
2	TPO	E	31	2	-	1/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	31	TPO	P-O2P	-2.40	1.45	1.54
2	E	31	TPO	P-O3P	-2.32	1.45	1.54
2	G	31	TPO	P-O2P	-2.32	1.45	1.54
2	E	31	TPO	P-O2P	-2.17	1.46	1.54
2	G	31	TPO	P-O3P	-2.04	1.47	1.54
2	H	31	TPO	P-OG1	-2.04	1.55	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	31	TPO	O-C-CA-CB
2	F	31	TPO	O-C-CA-CB
2	G	31	TPO	O-C-CA-CB
2	H	31	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	31	TPO	2	0
2	F	31	TPO	2	0
2	H	31	TPO	2	0
2	E	31	TPO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
3	COT	E	401	-	58,67,67	0.84	1 (1%)	69,98,98	0.99	4 (5%)
3	COT	G	402	-	58,67,67	0.84	1 (1%)	69,98,98	0.98	3 (4%)
3	COT	F	400	-	58,67,67	0.87	1 (1%)	69,98,98	0.96	2 (2%)
3	COT	H	403	-	58,67,67	0.83	1 (1%)	69,98,98	0.97	3 (4%)

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
3	COT	E	401	-	-	10/54/74/74	0/5/5/5
3	COT	G	402	-	-	10/54/74/74	0/5/5/5
3	COT	F	400	-	-	10/54/74/74	0/5/5/5
3	COT	H	403	-	-	10/54/74/74	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	COT	O4B-C1B	2.52	1.44	1.41
3	G	402	COT	O4B-C1B	2.40	1.44	1.41
3	H	403	COT	O4B-C1B	2.38	1.44	1.41
3	F	400	COT	O4B-C1B	2.34	1.44	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	403	COT	N3A-C2A-N1A	-3.42	123.34	128.68
3	F	400	COT	N3A-C2A-N1A	-3.37	123.41	128.68
3	E	401	COT	N3A-C2A-N1A	-3.30	123.52	128.68
3	G	402	COT	N3A-C2A-N1A	-3.17	123.72	128.68
3	G	402	COT	C16-C13-C11	-2.42	117.54	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	401	COT	C5A-C6A-N6A	2.30	123.85	120.35
3	E	401	COT	C17-C15-C12	-2.18	116.95	120.08
3	H	403	COT	C5A-C6A-N6A	2.15	123.63	120.35
3	F	400	COT	C17-C15-C12	-2.15	116.99	120.08
3	E	401	COT	C16-C13-C11	-2.14	117.92	120.89
3	G	402	COT	C17-C15-C12	-2.10	117.06	120.08
3	H	403	COT	C17-C15-C12	-2.05	117.14	120.08

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	401	COT	CGT-C1T-C2T-N3T
3	E	401	COT	C3B-O3B-PC-O19
3	F	400	COT	CGT-C1T-C2T-N3T
3	F	400	COT	C3B-O3B-PC-O19
3	G	402	COT	CGT-C1T-C2T-N3T
3	G	402	COT	C3B-O3B-PC-O19
3	H	403	COT	CGT-C1T-C2T-N3T
3	H	403	COT	C3B-O3B-PC-O19
3	G	402	COT	C3B-C4B-C5B-O5B
3	E	401	COT	C3B-C4B-C5B-O5B
3	F	400	COT	C3B-C4B-C5B-O5B
3	H	403	COT	C3B-C4B-C5B-O5B
3	G	402	COT	N8P-C9P-CBP-OCP
3	E	401	COT	C3B-O3B-PC-O17
3	F	400	COT	C3B-O3B-PC-O17
3	G	402	COT	C3B-O3B-PC-O17
3	H	403	COT	C3B-O3B-PC-O17
3	G	402	COT	O4B-C4B-C5B-O5B
3	F	400	COT	C6P-C7P-N8P-C9P
3	F	400	COT	O4B-C4B-C5B-O5B
3	G	402	COT	C6P-C7P-N8P-C9P
3	E	401	COT	O4B-C4B-C5B-O5B
3	H	403	COT	O4B-C4B-C5B-O5B
3	E	401	COT	C6P-C7P-N8P-C9P
3	H	403	COT	C6P-C7P-N8P-C9P
3	G	402	COT	PA-O14-PB-O12
3	E	401	COT	OAP-C9P-CBP-OCP
3	F	400	COT	OAP-C9P-CBP-OCP
3	G	402	COT	OAP-C9P-CBP-OCP
3	H	403	COT	OAP-C9P-CBP-OCP

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Mol	Chain	Res	Type	Atoms
3	E	401	COT	N8P-C9P-CBP-OCP
3	F	400	COT	N8P-C9P-CBP-OCP
3	H	403	COT	N8P-C9P-CBP-OCP
3	E	401	COT	PA-O14-PB-O12
3	E	401	COT	PA-O14-PB-O13
3	F	400	COT	PA-O14-PB-O12
3	F	400	COT	PA-O14-PB-O13
3	G	402	COT	PA-O14-PB-O13
3	H	403	COT	PA-O14-PB-O12
3	H	403	COT	PA-O14-PB-O13

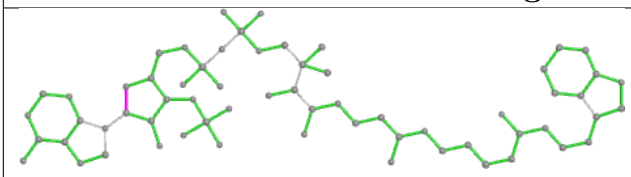
There are no ring outliers.

3 monomers are involved in 3 short contacts:

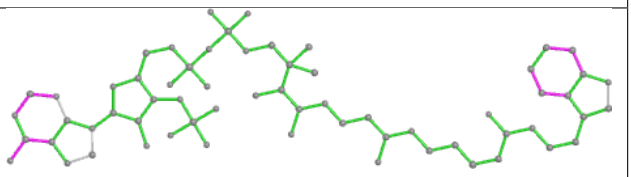
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	401	COT	1	0
3	G	402	COT	1	0
3	F	400	COT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

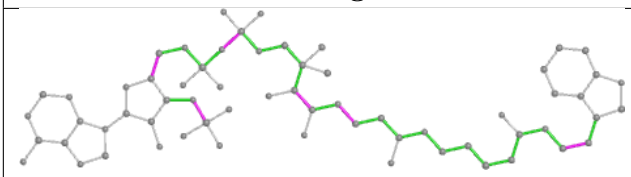
Ligand COT E 401



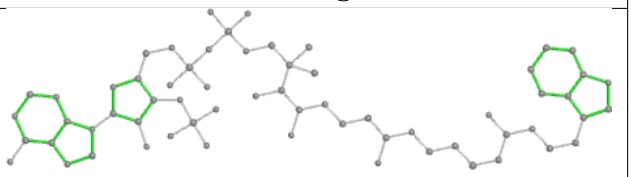
Bond lengths



Bond angles

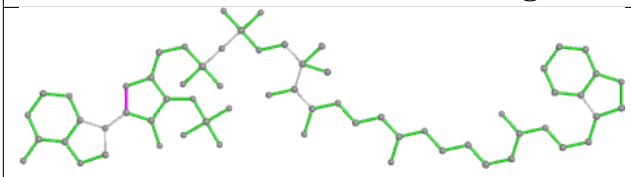


Torsions

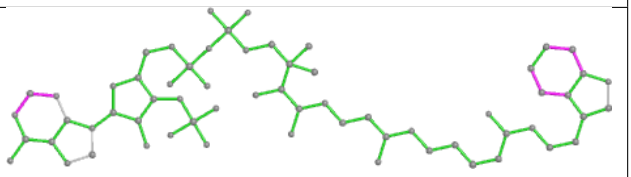


Rings

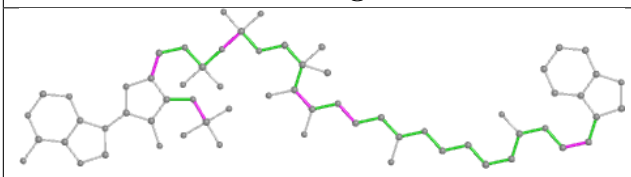
Ligand COT G 402



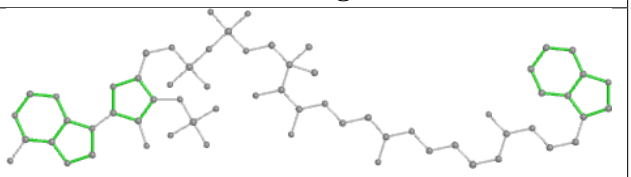
Bond lengths



Bond angles

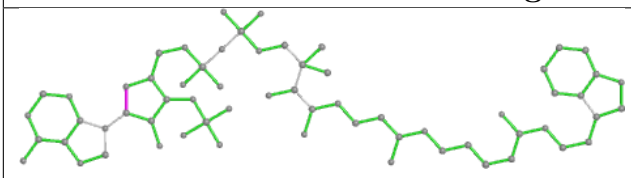


Torsions

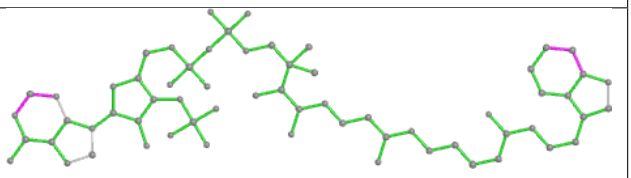


Rings

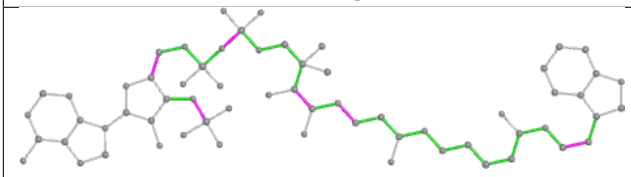
Ligand COT F 400



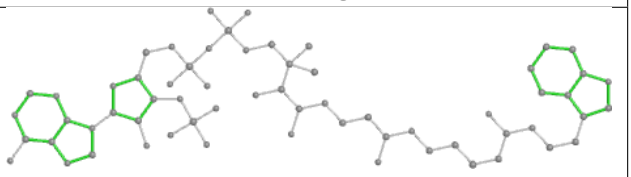
Bond lengths



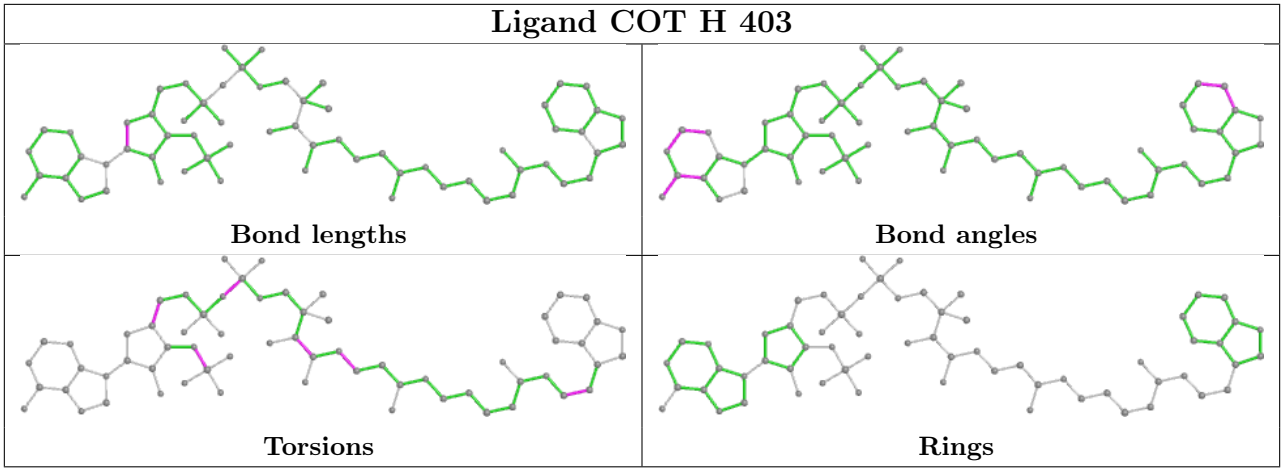
Bond angles



Torsions



Rings



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.