Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:04 PM GMT

PDB ID	:	1DUB
Title	:	2-ENOYL-COA HYDRATASE, DATA COLLECTED AT 100 K, PH 6.5
Authors	:	Wierenga, R.K.; Engel, C.K.
Deposited on	:	1996-06-10
Resolution	:	2.50 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 (1)) were used in the production of this report:

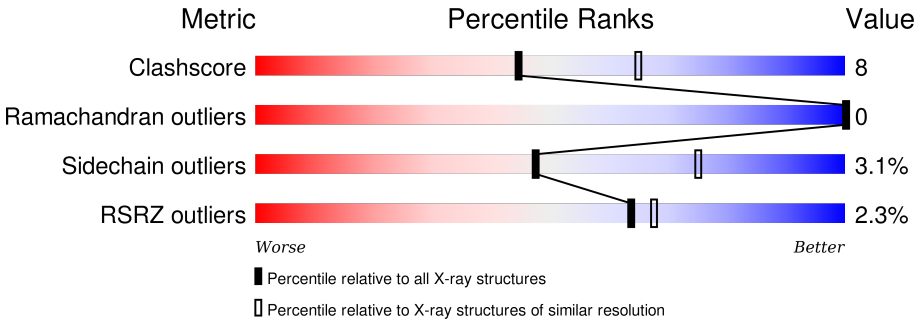
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	261	2% 84% 15%
1	B	261	% 84% 13%
1	C	261	3% 80% 18%
1	D	261	2% 83% 15%
1	E	261	4% 83% 15%
1	F	261	% 88% 10%

2 Entry composition

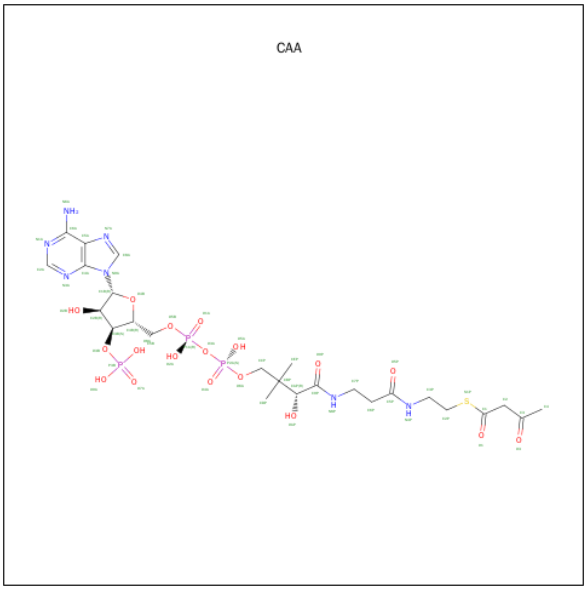
There are 3 unique types of molecules in this entry. The entry contains 12706 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-ENOYL-COA HYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1975	1245	339	378	13			
1	B	259	Total	C	N	O	S	0	0	0
			1970	1242	338	377	13			
1	C	259	Total	C	N	O	S	0	0	0
			1970	1242	338	377	13			
1	D	260	Total	C	N	O	S	0	0	0
			1978	1246	340	379	13			
1	E	260	Total	C	N	O	S	0	0	0
			1978	1246	340	379	13			
1	F	259	Total	C	N	O	S	0	0	0
			1970	1242	338	377	13			

- Molecule 2 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula: $C_{25}H_{40}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

- Molecule 3 is water.

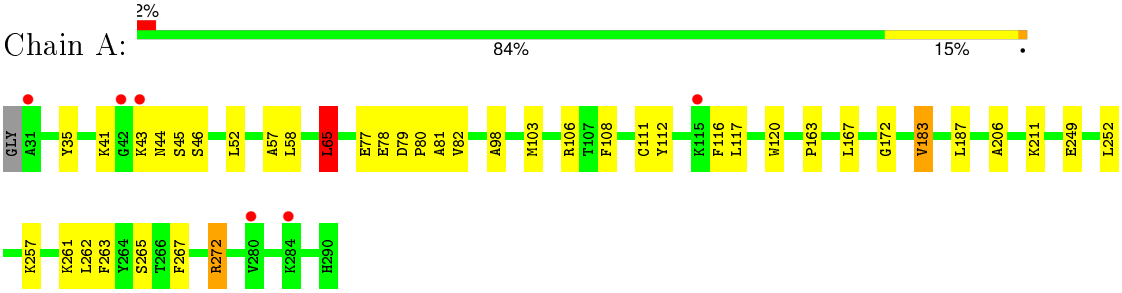
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total	O	0	0
			112	112		
3	B	101	Total	O	0	0
			101	101		
3	C	79	Total	O	0	0
			79	79		
3	D	101	Total	O	0	0
			101	101		
3	E	110	Total	O	0	0
			110	110		
3	F	92	Total	O	0	0
			92	92		

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.

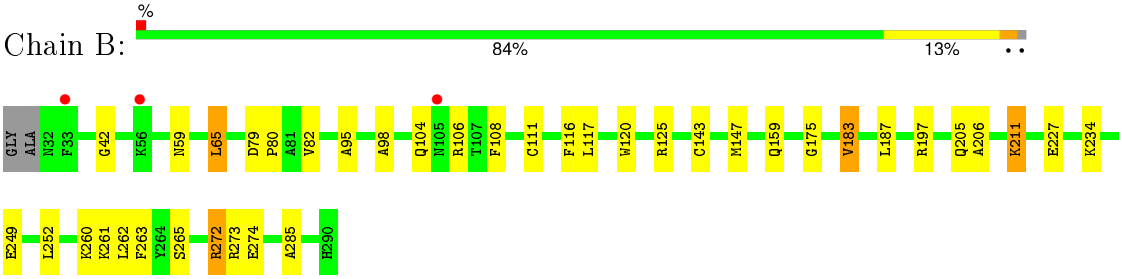
- Molecule 1: 2-ENOYL-COA HYDRATASE

Chain A:



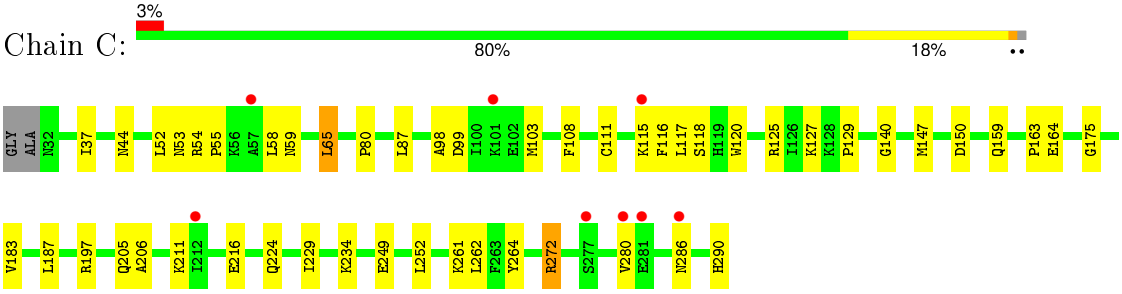
- Molecule 1: 2-ENOYL-COA HYDRATASE

Chain B:



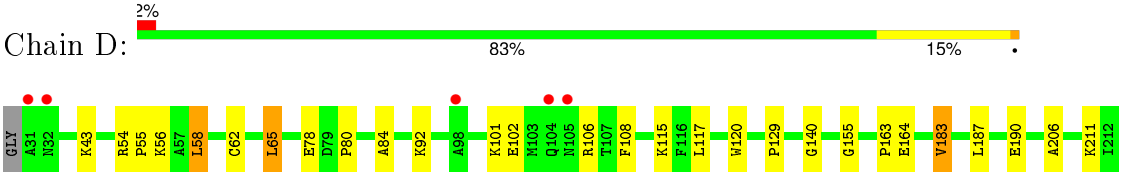
- Molecule 1: 2-ENOYL-COA HYDRATASE

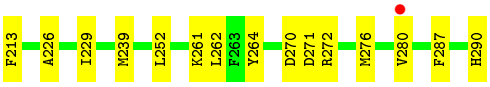
Chain C:



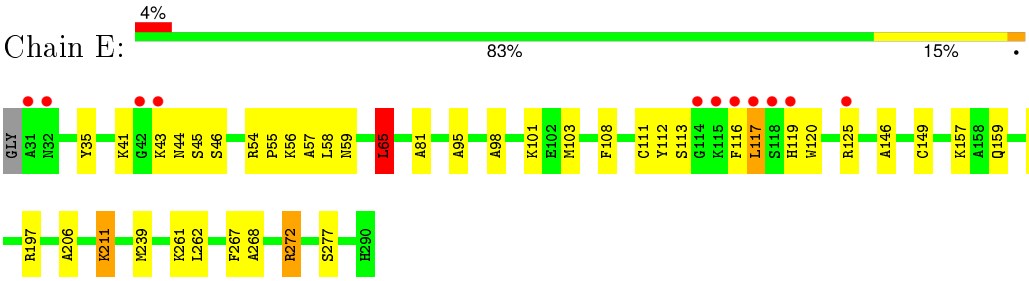
- Molecule 1: 2-ENOYL-COA HYDRATASE

Chain D:

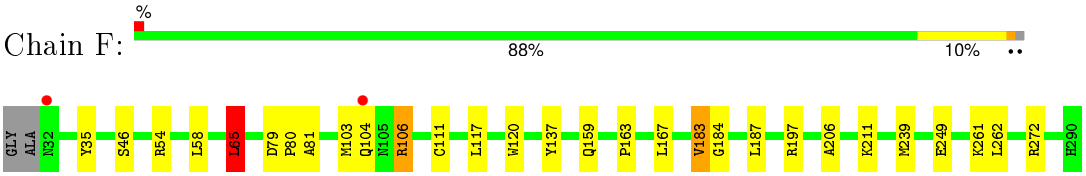




• Molecule 1: 2-ENOYL-COA HYDRATASE



• Molecule 1: 2-ENOYL-COA HYDRATASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.97Å 93.64Å 246.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 28.62 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.9 (8.00-2.50) 95.6 (28.62-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.22 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.209 , 0.265 0.190 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 65.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 59084 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12706	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.73	2/2002 (0.1%)	0.82	2/2689 (0.1%)
1	B	0.65	0/1997	0.77	2/2682 (0.1%)
1	C	0.67	0/1997	0.80	2/2682 (0.1%)
1	D	0.67	0/2005	0.80	1/2693 (0.0%)
1	E	0.68	0/2005	0.79	1/2693 (0.0%)
1	F	0.65	0/1997	0.78	1/2682 (0.0%)
All	All	0.67	2/12003 (0.0%)	0.79	9/16121 (0.1%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	GLU	CD-OE2	-8.03	1.16	1.25
1	A	77	GLU	CD-OE1	-7.17	1.17	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	GLU	OE1-CD-OE2	-11.02	110.08	123.30
1	C	125	ARG	NE-CZ-NH2	7.11	123.86	120.30
1	A	65	LEU	CA-CB-CG	6.82	130.98	115.30
1	B	65	LEU	CA-CB-CG	6.54	130.35	115.30
1	F	65	LEU	CA-CB-CG	6.28	129.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	65	LEU	CA-CB-CG	6.25	129.67	115.30
1	D	65	LEU	CA-CB-CG	6.17	129.49	115.30
1	B	272	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	65	LEU	CA-CB-CG	5.37	127.64	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	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	1975	0	1998	37	0
1	B	1970	0	1993	33	0
1	C	1970	0	1993	40	0
1	D	1978	0	2002	33	1
1	E	1978	0	2002	37	0
1	F	1970	0	1993	25	0
2	A	54	0	36	13	0
2	B	54	0	36	5	0
2	C	54	0	36	10	0
2	E	54	0	36	7	0
2	F	54	0	36	5	0
3	A	112	0	0	2	0
3	B	101	0	0	1	0
3	C	79	0	0	1	0
3	D	101	0	0	3	1
3	E	110	0	0	3	0
3	F	92	0	0	1	0
All	All	12706	0	12161	191	1

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 8.

All (191) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:VAL:HG22	1:B:206:ALA:HB1	1.56	0.86
1:B:261:LYS:HD3	1:F:262:LEU:HD21	1.59	0.84
1:C:224:GLN:HG2	3:C:376:HOH:O	1.80	0.81
1:C:183:VAL:HG22	1:C:206:ALA:HB1	1.63	0.81
1:E:183:VAL:HG22	1:E:206:ALA:HB1	1.67	0.76
1:C:117:LEU:HD11	2:C:300:CAA:H4'2	1.68	0.74
1:C:129:PRO:HG2	1:C:229:ILE:HG21	1.70	0.74
1:C:127:LYS:HD2	1:D:115:LYS:HE2	1.71	0.72
1:E:103:MET:HG2	1:E:116:PHE:HZ	1.55	0.72
1:C:183:VAL:HG13	1:C:187:LEU:HB3	1.73	0.71
1:E:183:VAL:HG13	1:E:187:LEU:HB3	1.72	0.71
1:B:262:LEU:HD21	1:F:261:LYS:HD3	1.71	0.71
1:A:183:VAL:HG13	1:A:187:LEU:HB3	1.73	0.70
1:B:104:GLN:OE1	1:C:280:VAL:HG21	1.91	0.70
1:F:163:PRO:HG2	2:F:300:CAA:H31	1.74	0.70
1:C:262:LEU:HD21	1:E:261:LYS:HD3	1.76	0.68
1:A:267:PHE:HA	1:A:272:ARG:HD3	1.76	0.68
1:F:167:LEU:HD11	2:F:300:CAA:H21	1.75	0.68
1:B:117:LEU:HD11	2:B:300:CAA:H4'2	1.76	0.67
1:F:183:VAL:HG22	1:F:206:ALA:HB1	1.77	0.66
1:A:183:VAL:HG22	1:A:206:ALA:HB1	1.76	0.66
2:C:300:CAA:H8A	2:C:300:CAA:OAP	1.96	0.66
1:D:183:VAL:HG22	1:D:206:ALA:HB1	1.77	0.65
1:B:183:VAL:HG22	1:B:206:ALA:CB	2.26	0.65
1:D:78:GLU:O	1:D:80:PRO:HD3	1.97	0.64
1:C:54:ARG:H	1:C:59:ASN:ND2	1.95	0.64
3:A:394:HOH:O	1:B:205:GLN:HG3	1.99	0.63
1:D:290:HIS:HB3	3:D:376:HOH:O	1.98	0.62
1:E:56:LYS:O	2:E:300:CAA:H4B	2.00	0.62
1:C:127:LYS:CD	1:D:115:LYS:HE2	2.28	0.62
1:D:117:LEU:O	1:D:120:TRP:HB2	2.00	0.62
1:F:183:VAL:HG13	1:F:187:LEU:HB3	1.81	0.61
1:C:261:LYS:HD3	1:E:262:LEU:HD21	1.82	0.61
1:C:37:ILE:HD11	1:C:53:ASN:ND2	2.16	0.61
1:C:54:ARG:N	1:C:55:PRO:HD3	2.16	0.60
1:D:183:VAL:HG13	1:D:187:LEU:HB3	1.82	0.60
1:A:103:MET:HG2	1:A:116:PHE:HZ	1.66	0.60
1:D:101:LYS:H	1:D:101:LYS:HD2	1.65	0.60
1:E:183:VAL:HG22	1:E:206:ALA:CB	2.32	0.59
1:B:183:VAL:HG13	1:B:187:LEU:HB3	1.84	0.59
1:A:262:LEU:HD21	1:D:261:LYS:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:VAL:HG22	1:C:206:ALA:CB	2.31	0.59
1:A:183:VAL:CG1	1:A:187:LEU:HB3	2.33	0.59
1:E:183:VAL:CG1	1:E:187:LEU:HB3	2.33	0.58
1:E:167:LEU:HD11	2:E:300:CAA:H21	1.83	0.58
1:A:163:PRO:HG2	2:A:300:CAA:H31	1.85	0.58
1:D:163:PRO:HD3	3:D:319:HOH:O	2.04	0.58
1:F:58:LEU:HD12	2:F:300:CAA:H8A	1.87	0.57
1:E:101:LYS:HE2	3:E:392:HOH:O	2.04	0.57
1:A:261:LYS:HD3	1:D:262:LEU:HD21	1.86	0.57
1:C:117:LEU:HD22	1:C:120:TRP:NE1	2.20	0.57
1:C:54:ARG:O	1:C:54:ARG:HG2	2.03	0.57
1:C:58:LEU:HD12	2:C:300:CAA:H8A	1.85	0.57
1:E:103:MET:HG2	1:E:116:PHE:CZ	2.39	0.57
1:E:267:PHE:HA	1:E:272:ARG:HD3	1.87	0.56
1:E:117:LEU:HG	1:E:120:TRP:CD1	2.41	0.56
1:D:183:VAL:HG22	1:D:206:ALA:CB	2.36	0.56
1:C:183:VAL:CG1	1:C:187:LEU:HB3	2.35	0.55
1:D:54:ARG:N	1:D:55:PRO:HD3	2.23	0.54
1:C:117:LEU:O	1:C:120:TRP:HB2	2.07	0.54
1:A:58:LEU:HD11	2:A:300:CAA:H122	1.90	0.54
2:A:300:CAA:O5B	2:A:300:CAA:H2B	2.08	0.54
1:B:125:ARG:HH22	1:E:125:ARG:NH1	2.05	0.54
1:F:183:VAL:HG22	1:F:206:ALA:CB	2.38	0.53
2:C:300:CAA:O5B	2:C:300:CAA:H2B	2.08	0.53
1:F:54:ARG:O	1:F:54:ARG:HG2	2.08	0.51
1:A:117:LEU:O	1:A:120:TRP:HB2	2.11	0.51
2:B:300:CAA:H2B	2:B:300:CAA:O5B	2.12	0.50
2:E:300:CAA:H32	2:E:300:CAA:O1	2.11	0.50
1:F:117:LEU:O	1:F:120:TRP:HB2	2.11	0.50
1:D:84:ALA:HB3	1:D:226:ALA:HB1	1.93	0.50
1:B:104:GLN:O	1:C:272:ARG:NH2	2.44	0.50
1:A:52:LEU:HD22	1:A:65:LEU:HD11	1.93	0.50
1:A:262:LEU:O	1:A:265:SER:HB2	2.12	0.50
1:A:183:VAL:HG22	1:A:206:ALA:CB	2.42	0.50
2:E:300:CAA:H2B	2:E:300:CAA:O5B	2.12	0.50
1:A:57:ALA:HA	2:A:300:CAA:O4B	2.12	0.50
1:B:82:VAL:O	1:B:234:LYS:HE2	2.12	0.50
1:B:183:VAL:CG1	1:B:187:LEU:HB3	2.42	0.49
1:F:46:SER:HA	1:F:81:ALA:O	2.13	0.49
1:C:129:PRO:HA	1:C:150:ASP:OD2	2.14	0.48
1:B:117:LEU:O	1:B:120:TRP:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:300:CAA:H141	2:C:300:CAA:N8P	2.28	0.48
1:F:159:GLN:NE2	1:F:197:ARG:HD2	2.29	0.48
1:C:108:PHE:HZ	1:D:239:MET:HE2	1.79	0.48
1:C:52:LEU:HD21	1:C:87:LEU:HD11	1.95	0.47
1:D:129:PRO:HG2	1:D:229:ILE:HG21	1.95	0.47
1:F:137:TYR:CE2	2:F:300:CAA:H121	2.50	0.47
1:E:117:LEU:O	1:E:120:TRP:HB2	2.14	0.47
1:A:79:ASP:OD2	1:A:82:VAL:HG23	2.14	0.47
1:E:119:HIS:HB2	3:E:402:HOH:O	2.13	0.47
1:C:111:CYS:HA	1:C:116:PHE:HB2	1.96	0.47
1:C:216:GLU:CD	1:C:216:GLU:H	2.17	0.47
1:D:183:VAL:CG1	1:D:187:LEU:HB3	2.44	0.47
1:A:46:SER:O	1:A:82:VAL:HA	2.15	0.47
1:E:46:SER:HA	1:E:81:ALA:O	2.14	0.47
1:C:80:PRO:O	1:C:234:LYS:HE2	2.15	0.47
1:D:280:VAL:HG21	1:F:104:GLN:OE1	2.15	0.47
1:E:43:LYS:O	1:E:44:ASN:HB2	2.15	0.46
1:A:252:LEU:HB3	1:C:249:GLU:OE2	2.15	0.46
1:D:62:CYS:HB2	1:D:102:GLU:OE2	2.15	0.46
1:E:146:ALA:O	1:E:149:CYS:HB2	2.15	0.46
1:E:157:LYS:HB2	3:E:356:HOH:O	2.16	0.46
1:E:35:TYR:HB3	1:E:65:LEU:HD22	1.97	0.46
1:A:263:PHE:CE1	2:C:300:CAA:H4'3	2.51	0.46
1:D:58:LEU:HD12	1:D:58:LEU:HA	1.79	0.46
1:C:140:GLY:HA2	1:C:164:GLU:OE2	2.16	0.46
1:B:116:PHE:O	1:B:117:LEU:HB2	2.15	0.46
1:A:117:LEU:HD21	2:A:300:CAA:H4'2	1.97	0.46
1:E:58:LEU:CD1	2:E:300:CAA:H122	2.46	0.46
1:B:147:MET:HE1	1:B:175:GLY:HA2	1.97	0.46
1:A:111:CYS:HA	1:A:116:PHE:HB2	1.97	0.45
1:B:265:SER:HB3	1:E:108:PHE:HZ	1.81	0.45
1:B:111:CYS:HB3	1:C:264:TYR:CD1	2.52	0.45
1:A:46:SER:HA	1:A:81:ALA:O	2.16	0.45
1:C:115:LYS:O	1:C:118:SER:HB2	2.17	0.45
1:B:249:GLU:OE2	1:C:252:LEU:HB3	2.17	0.45
1:D:252:LEU:HB3	1:F:249:GLU:OE2	2.17	0.45
1:C:140:GLY:HA3	2:C:300:CAA:H32	1.98	0.45
1:D:271:ASP:OD1	1:D:287:PHE:HA	2.17	0.45
1:C:159:GLN:NE2	1:C:197:ARG:HD2	2.32	0.45
2:A:300:CAA:H62	2:A:300:CAA:H62A	1.82	0.44
1:D:276:MET:O	1:D:280:VAL:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:CAA:H8A	2:B:300:CAA:OAP	2.17	0.44
1:F:35:TYR:HB3	1:F:65:LEU:HD22	1.99	0.44
1:A:172:GLY:H	2:A:300:CAA:C4	2.30	0.44
1:B:260:LYS:O	1:B:263:PHE:HB3	2.17	0.44
1:D:280:VAL:HG21	1:F:104:GLN:CD	2.38	0.44
3:D:349:HOH:O	1:F:184:GLY:HA2	2.17	0.44
1:E:54:ARG:N	1:E:55:PRO:CD	2.80	0.44
1:A:41:LYS:O	1:A:45:SER:HA	2.18	0.44
1:B:42:GLY:HA2	1:B:227:GLU:OE2	2.17	0.44
1:C:53:ASN:C	1:C:55:PRO:HD3	2.38	0.44
1:A:58:LEU:CD1	2:A:300:CAA:H122	2.48	0.44
1:A:35:TYR:HB3	1:A:65:LEU:HD22	1.99	0.43
1:B:265:SER:HB3	1:E:108:PHE:CZ	2.53	0.43
1:D:264:TYR:CD1	1:F:111:CYS:HB3	2.53	0.43
1:C:129:PRO:HG2	1:C:229:ILE:CG2	2.43	0.43
1:B:79:ASP:HA	1:B:80:PRO:HD2	1.86	0.43
1:B:108:PHE:HZ	1:E:239:MET:HE2	1.82	0.43
1:B:117:LEU:CD1	2:B:300:CAA:H4'2	2.46	0.43
1:D:54:ARG:N	1:D:55:PRO:CD	2.82	0.43
1:C:54:ARG:N	1:C:55:PRO:CD	2.82	0.43
1:A:257:LYS:HB2	3:A:361:HOH:O	2.19	0.43
2:C:300:CAA:O5B	2:C:300:CAA:C2B	2.65	0.43
1:A:78:GLU:O	1:A:80:PRO:HD3	2.19	0.43
1:B:262:LEU:HA	1:B:262:LEU:HD23	1.89	0.43
1:E:41:LYS:O	1:E:45:SER:HA	2.19	0.43
1:A:108:PHE:HZ	1:F:239:MET:HE2	1.84	0.43
1:B:111:CYS:HA	1:B:116:PHE:HB2	2.00	0.43
1:A:172:GLY:H	2:A:300:CAA:H4'1	1.83	0.43
2:A:300:CAA:O5B	2:A:300:CAA:C2B	2.66	0.43
1:E:43:LYS:HZ2	1:E:44:ASN:HD21	1.66	0.43
1:D:140:GLY:HA2	1:D:164:GLU:OE2	2.19	0.43
1:F:159:GLN:HE22	1:F:197:ARG:HH11	1.67	0.42
1:D:43:LYS:HE2	1:D:43:LYS:HB3	1.86	0.42
1:B:98:ALA:CB	2:B:300:CAA:H2'1	2.49	0.42
1:E:159:GLN:NE2	1:E:197:ARG:HD2	2.35	0.42
1:A:249:GLU:OE2	1:B:252:LEU:HB3	2.18	0.42
2:E:300:CAA:C2B	2:E:300:CAA:O5B	2.67	0.42
1:E:57:ALA:HA	2:E:300:CAA:O4B	2.19	0.42
1:E:43:LYS:NZ	1:E:44:ASN:HD21	2.18	0.42
1:B:143:CYS:O	1:B:147:MET:HG3	2.20	0.42
1:F:167:LEU:CD1	2:F:300:CAA:H21	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:LEU:HG	1:E:120:TRP:CG	2.56	0.41
1:B:274:GLU:OE2	1:B:285:ALA:HA	2.20	0.41
1:D:190:GLU:OE2	1:E:211:LYS:HE2	2.20	0.41
1:A:43:LYS:HG3	1:A:44:ASN:ND2	2.35	0.41
1:F:79:ASP:HA	1:F:80:PRO:HD3	1.78	0.41
1:C:163:PRO:HG2	2:C:300:CAA:H31	2.02	0.41
1:E:98:ALA:HB2	1:E:120:TRP:CH2	2.56	0.41
1:F:80:PRO:HA	3:F:305:HOH:O	2.20	0.41
1:F:103:MET:O	1:F:106:ARG:HB2	2.21	0.41
1:A:79:ASP:HA	1:A:80:PRO:HD3	1.90	0.41
1:B:211:LYS:NZ	3:B:341:HOH:O	2.43	0.41
1:A:58:LEU:HG	2:A:300:CAA:H52A	2.01	0.41
1:C:98:ALA:CB	2:C:300:CAA:H2'1	2.51	0.41
1:A:167:LEU:HD11	2:A:300:CAA:C2P	2.51	0.41
1:D:101:LYS:HD2	1:D:101:LYS:N	2.34	0.41
1:D:155:GLY:HA2	1:D:213:PHE:O	2.21	0.41
1:E:111:CYS:HA	1:E:116:PHE:HB2	2.03	0.41
1:A:116:PHE:O	1:A:117:LEU:HB2	2.21	0.41
1:E:59:ASN:HB2	1:E:95:ALA:HA	2.03	0.41
1:C:147:MET:HE1	1:C:175:GLY:HA2	2.03	0.41
1:B:159:GLN:NE2	1:B:197:ARG:HD2	2.36	0.41
1:B:59:ASN:HB2	1:B:95:ALA:HA	2.04	0.40
1:C:99:ASP:O	1:C:103:MET:HG3	2.21	0.40
1:D:270:ASP:OD2	1:D:290:HIS:ND1	2.53	0.40
1:A:98:ALA:HB2	1:A:120:TRP:CH2	2.57	0.40
1:A:167:LEU:CD1	2:A:300:CAA:H22	2.52	0.40
1:D:108:PHE:HB2	1:E:268:ALA:HB2	2.04	0.40

All (1) 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)
1:D:56:LYS:NZ	3:D:351:HOH:O[4_566]	2.16	0.04

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	258/261 (99%)	250 (97%)	8 (3%)	0	100	100
1	B	257/261 (98%)	249 (97%)	8 (3%)	0	100	100
1	C	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	D	258/261 (99%)	250 (97%)	8 (3%)	0	100	100
1	E	258/261 (99%)	254 (98%)	4 (2%)	0	100	100
1	F	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
All	All	1545/1566 (99%)	1503 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	204/205 (100%)	199 (98%)	5 (2%)	55	82
1	B	204/205 (100%)	198 (97%)	6 (3%)	50	77
1	C	204/205 (100%)	197 (97%)	7 (3%)	44	72
1	D	205/205 (100%)	198 (97%)	7 (3%)	44	72
1	E	205/205 (100%)	197 (96%)	8 (4%)	39	66
1	F	204/205 (100%)	199 (98%)	5 (2%)	55	82
All	All	1226/1230 (100%)	1188 (97%)	38 (3%)	47	75

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	106	ARG
1	A	183	VAL

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Mol	Chain	Res	Type
1	A	211	LYS
1	A	272	ARG
1	B	65	LEU
1	B	106	ARG
1	B	183	VAL
1	B	211	LYS
1	B	272	ARG
1	B	273	ARG
1	C	44	ASN
1	C	65	LEU
1	C	205	GLN
1	C	211	LYS
1	C	272	ARG
1	C	286	ASN
1	C	290	HIS
1	D	58	LEU
1	D	65	LEU
1	D	92	LYS
1	D	106	ARG
1	D	183	VAL
1	D	211	LYS
1	D	272	ARG
1	E	65	LEU
1	E	112	TYR
1	E	113	SER
1	E	117	LEU
1	E	183	VAL
1	E	211	LYS
1	E	272	ARG
1	E	277	SER
1	F	65	LEU
1	F	106	ARG
1	F	183	VAL
1	F	211	LYS
1	F	272	ARG

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	159	GLN
1	B	122	HIS
1	B	159	GLN

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Mol	Chain	Res	Type
1	C	53	ASN
1	C	59	ASN
1	C	159	GLN
1	C	224	GLN
1	D	159	GLN
1	E	44	ASN
1	E	122	HIS
1	E	159	GLN
1	E	162	GLN
1	E	224	GLN
1	F	122	HIS
1	F	159	GLN
1	F	201	GLN
1	F	224	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	CAA	A	300	-	45,56,56	1.27	6 (13%)	58,83,83	1.74	12 (20%)
2	CAA	B	300	-	45,56,56	1.39	6 (13%)	58,83,83	1.91	13 (22%)
2	CAA	C	300	-	45,56,56	1.40	5 (11%)	58,83,83	1.98	12 (20%)
2	CAA	E	300	-	45,56,56	1.21	4 (8%)	58,83,83	1.75	13 (22%)
2	CAA	F	300	-	45,56,56	1.34	7 (15%)	58,83,83	1.86	13 (22%)

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	CAA	A	300	-	-	0/50/71/71	0/3/3/3
2	CAA	B	300	-	-	0/50/71/71	0/3/3/3
2	CAA	C	300	-	-	0/50/71/71	0/3/3/3
2	CAA	E	300	-	-	0/50/71/71	0/3/3/3
2	CAA	F	300	-	-	0/50/71/71	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	CAA	C3P-N4P	-2.67	1.39	1.46
2	A	300	CAA	C3P-N4P	-2.58	1.40	1.46
2	A	300	CAA	C7P-N8P	-2.56	1.40	1.46
2	F	300	CAA	C7P-N8P	-2.54	1.40	1.46
2	F	300	CAA	C3P-N4P	-2.54	1.40	1.46
2	E	300	CAA	C7P-N8P	-2.39	1.40	1.46
2	B	300	CAA	C3P-N4P	-2.31	1.40	1.46
2	A	300	CAA	P3B-O3B	-2.21	1.53	1.60
2	C	300	CAA	C7P-N8P	-2.16	1.41	1.46
2	E	300	CAA	C5A-C4A	-2.08	1.35	1.40
2	A	300	CAA	O4B-C1B	2.22	1.44	1.41
2	B	300	CAA	C4A-N3A	2.30	1.39	1.35
2	A	300	CAA	C5P-N4P	2.32	1.38	1.33
2	F	300	CAA	O4B-C1B	2.38	1.44	1.41
2	F	300	CAA	OAP-CAP	2.60	1.47	1.42
2	E	300	CAA	C9P-N8P	2.66	1.39	1.33
2	C	300	CAA	C9P-N8P	2.99	1.39	1.33
2	F	300	CAA	O1-C1	3.03	1.25	1.21
2	F	300	CAA	C5P-N4P	3.07	1.40	1.33
2	B	300	CAA	C9P-N8P	3.13	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	300	CAA	C9P-N8P	3.39	1.40	1.33
2	B	300	CAA	C5P-N4P	3.49	1.41	1.33
2	C	300	CAA	O1-C1	3.64	1.26	1.21
2	A	300	CAA	C9P-N8P	3.77	1.41	1.33
2	B	300	CAA	O1-C1	3.82	1.27	1.21
2	E	300	CAA	C5P-N4P	4.04	1.43	1.33
2	B	300	CAA	O4B-C1B	4.36	1.46	1.41
2	C	300	CAA	O4B-C1B	4.64	1.47	1.41

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	300	CAA	O1-C1-S1P	-9.95	114.94	122.83
2	B	300	CAA	O1-C1-S1P	-9.31	115.44	122.83
2	E	300	CAA	O1-C1-S1P	-5.51	118.46	122.83
2	F	300	CAA	O1-C1-S1P	-5.26	118.66	122.83
2	F	300	CAA	C2B-C1B-N9A	-4.86	106.87	114.29
2	B	300	CAA	C2B-C1B-N9A	-4.53	107.38	114.29
2	E	300	CAA	C2B-C1B-N9A	-4.47	107.46	114.29
2	A	300	CAA	O1-C1-S1P	-4.23	119.48	122.83
2	F	300	CAA	C6P-C5P-N4P	-4.12	109.29	116.46
2	A	300	CAA	C2B-C1B-N9A	-4.06	108.09	114.29
2	F	300	CAA	O3-C3-C4	-4.00	111.42	121.31
2	B	300	CAA	O3-C3-C4	-3.61	112.39	121.31
2	A	300	CAA	OAP-CAP-C9P	-3.61	102.09	110.38
2	A	300	CAA	C6P-C5P-N4P	-3.59	110.22	116.46
2	C	300	CAA	C2P-C3P-N4P	-3.59	105.19	112.36
2	C	300	CAA	O3-C3-C4	-3.45	112.80	121.31
2	A	300	CAA	O3-C3-C4	-3.34	113.06	121.31
2	E	300	CAA	O3-C3-C4	-3.34	113.06	121.31
2	C	300	CAA	C2B-C1B-N9A	-3.31	109.24	114.29
2	C	300	CAA	C6P-C5P-N4P	-3.19	110.92	116.46
2	B	300	CAA	C2B-C3B-C4B	-3.03	97.60	103.29
2	C	300	CAA	OAP-CAP-C9P	-2.93	103.65	110.38
2	E	300	CAA	C2B-C3B-C4B	-2.92	97.81	103.29
2	F	300	CAA	C2B-C3B-C4B	-2.70	98.22	103.29
2	A	300	CAA	C2B-C3B-C4B	-2.60	98.41	103.29
2	E	300	CAA	OAP-CAP-C9P	-2.50	104.65	110.38
2	C	300	CAA	C2B-C3B-C4B	-2.46	98.66	103.29
2	E	300	CAA	C6P-C5P-N4P	-2.13	112.77	116.46
2	B	300	CAA	C2P-C3P-N4P	-2.11	108.14	112.36
2	F	300	CAA	C4B-O4B-C1B	-2.09	107.42	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	300	CAA	C6P-C5P-N4P	-2.08	112.84	116.46
2	F	300	CAA	OAP-CAP-C9P	-2.01	105.76	110.38
2	F	300	CAA	C4-C3-C2	2.01	126.02	118.35
2	B	300	CAA	C3P-C2P-S1P	2.08	116.92	111.36
2	E	300	CAA	C3-C2-C1	2.09	122.81	114.06
2	C	300	CAA	O4B-C1B-N9A	2.10	112.49	108.10
2	E	300	CAA	O4B-C1B-N9A	2.11	112.52	108.10
2	C	300	CAA	C3P-C2P-S1P	2.14	117.10	111.36
2	C	300	CAA	C2-C1-S1P	2.18	115.67	113.50
2	F	300	CAA	O4B-C1B-N9A	2.21	112.72	108.10
2	F	300	CAA	O5P-C5P-N4P	2.21	127.33	122.94
2	F	300	CAA	C3-C2-C1	2.30	123.69	114.06
2	B	300	CAA	O4B-C1B-N9A	2.30	112.92	108.10
2	A	300	CAA	C3-C2-C1	2.30	123.71	114.06
2	B	300	CAA	N3A-C2A-N1A	2.33	130.68	128.89
2	A	300	CAA	O3A-P1A-O5B	2.37	109.21	102.94
2	B	300	CAA	O3A-P1A-O5B	2.48	109.51	102.94
2	B	300	CAA	C3-C2-C1	2.50	124.54	114.06
2	E	300	CAA	O3A-P1A-O5B	2.53	109.64	102.94
2	B	300	CAA	O3A-P2A-O6A	2.65	109.97	102.94
2	E	300	CAA	C2P-S1P-C1	2.77	111.95	102.09
2	E	300	CAA	C3P-C2P-S1P	2.77	118.77	111.36
2	E	300	CAA	O3A-P2A-O6A	2.79	110.33	102.94
2	C	300	CAA	O3A-P2A-O6A	2.84	110.46	102.94
2	C	300	CAA	C3-C2-C1	2.85	125.98	114.06
2	A	300	CAA	O3A-P2A-O6A	2.94	110.74	102.94
2	B	300	CAA	C2-C1-S1P	2.95	116.44	113.50
2	F	300	CAA	O3A-P2A-O6A	3.11	111.20	102.94
2	A	300	CAA	C2-C1-S1P	3.13	116.62	113.50
2	A	300	CAA	C3P-C2P-S1P	3.71	121.30	111.36
2	A	300	CAA	C2P-S1P-C1	3.85	115.81	102.09
2	E	300	CAA	C2-C1-S1P	5.18	118.67	113.50
2	F	300	CAA	C2-C1-S1P	5.45	118.93	113.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	CAA	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	300	CAA	5	0
2	C	300	CAA	10	0
2	E	300	CAA	7	0
2	F	300	CAA	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	260/261 (99%)	-0.17	6 (2%) 64 67	3, 17, 44, 76	0
1	B	259/261 (99%)	-0.28	3 (1%) 81 83	4, 16, 46, 59	0
1	C	259/261 (99%)	-0.03	8 (3%) 52 57	3, 20, 46, 59	0
1	D	260/261 (99%)	-0.20	6 (2%) 64 67	2, 17, 47, 74	0
1	E	260/261 (99%)	-0.21	11 (4%) 40 45	3, 16, 44, 76	0
1	F	259/261 (99%)	-0.33	2 (0%) 87 89	4, 15, 45, 63	0
All	All	1557/1566 (99%)	-0.20	36 (2%) 64 67	2, 17, 46, 76	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	31	ALA	10.2
1	A	280	VAL	6.6
1	E	118	SER	5.2
1	A	31	ALA	4.6
1	A	115	LYS	4.5
1	E	115	LYS	4.1
1	A	43	LYS	3.9
1	F	32	ASN	3.9
1	E	31	ALA	3.8
1	D	105	ASN	3.7
1	C	212	ILE	3.6
1	E	119	HIS	3.4
1	C	280	VAL	3.3
1	B	56	LYS	3.0
1	C	281	GLU	3.0
1	D	32	ASN	3.0
1	E	116	PHE	2.9
1	E	32	ASN	2.9
1	E	43	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	117	LEU	2.7
1	D	98	ALA	2.6
1	C	286	ASN	2.6
1	C	57	ALA	2.6
1	E	114	GLY	2.5
1	D	104	GLN	2.5
1	C	115	LYS	2.5
1	D	280	VAL	2.5
1	B	105	ASN	2.4
1	C	101	LYS	2.3
1	E	125	ARG	2.3
1	F	104	GLN	2.1
1	A	284	LYS	2.1
1	B	33	PHE	2.1
1	A	42	GLY	2.1
1	C	277	SER	2.1
1	E	42	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CAA	F	300	54/54	0.87	0.22	1.63	15,31,50,54	0
2	CAA	C	300	54/54	0.87	0.27	1.24	15,32,51,56	0
2	CAA	B	300	54/54	0.87	0.25	0.97	16,32,51,53	0
2	CAA	E	300	54/54	0.96	0.13	-0.42	11,21,40,47	0
2	CAA	A	300	54/54	0.96	0.13	-0.68	11,23,43,47	0

6.5 Other polymers (i)

There are no such residues in this entry.