WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 28, 2016 – 03:06 PM EST

PDB ID	:	5INI
Title	:	Structural basis for acyl-CoA carboxylase-mediated assembly of unusual polyketide synthase extender units incorporated into the stambomycin antibiotics
Authors	:	Valentic, T.R.; Ray, L.; Miyazawa, T.; Withall, D.M.; Song, L.; Milligan, J.C.; Osada, H.; Tsai, S.C.; Challis, G.L.
Deposited on	:	2016-03-07
Resolution	:	2.85 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

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 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
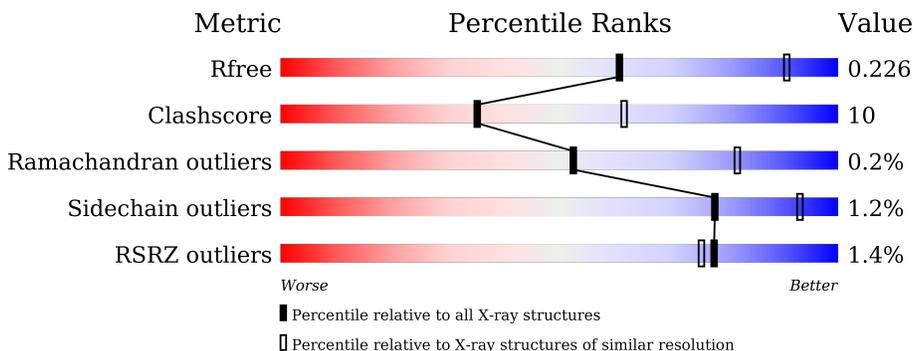
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	538	% 75% 14% • 10%
1	B	538	% 75% 13% • 11%
1	C	538	73% 15% 11%
1	D	538	% 75% 15% • 8%
1	E	538	3% 75% 16% • 8%
1	F	538	3% 73% 20% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HXC	E	601	-	-	-	X
2	HXC	F	601	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22896 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 Putative carboxyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total 3654	C 2299	N 646	O 690	S 19	0	0	0
1	B	481	Total 3639	C 2292	N 639	O 689	S 19	0	0	0
1	C	478	Total 3614	C 2277	N 633	O 685	S 19	0	0	0
1	D	496	Total 3758	C 2368	N 661	O 710	S 19	0	0	0
1	E	493	Total 3735	C 2351	N 658	O 707	S 19	0	0	0
1	F	511	Total 3884	C 2443	N 689	O 733	S 19	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP A0ACI9
A	-4	ILE	-	expression tag	UNP A0ACI9
A	-3	ASP	-	expression tag	UNP A0ACI9
A	-2	PRO	-	expression tag	UNP A0ACI9
A	-1	PHE	-	expression tag	UNP A0ACI9
A	0	THR	-	expression tag	UNP A0ACI9
B	-5	GLY	-	expression tag	UNP A0ACI9
B	-4	ILE	-	expression tag	UNP A0ACI9
B	-3	ASP	-	expression tag	UNP A0ACI9
B	-2	PRO	-	expression tag	UNP A0ACI9
B	-1	PHE	-	expression tag	UNP A0ACI9
B	0	THR	-	expression tag	UNP A0ACI9
C	-5	GLY	-	expression tag	UNP A0ACI9
C	-4	ILE	-	expression tag	UNP A0ACI9
C	-3	ASP	-	expression tag	UNP A0ACI9
C	-2	PRO	-	expression tag	UNP A0ACI9
C	-1	PHE	-	expression tag	UNP A0ACI9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	THR	-	expression tag	UNP A0ACI9
D	-5	GLY	-	expression tag	UNP A0ACI9
D	-4	ILE	-	expression tag	UNP A0ACI9
D	-3	ASP	-	expression tag	UNP A0ACI9
D	-2	PRO	-	expression tag	UNP A0ACI9
D	-1	PHE	-	expression tag	UNP A0ACI9
D	0	THR	-	expression tag	UNP A0ACI9
E	-5	GLY	-	expression tag	UNP A0ACI9
E	-4	ILE	-	expression tag	UNP A0ACI9
E	-3	ASP	-	expression tag	UNP A0ACI9
E	-2	PRO	-	expression tag	UNP A0ACI9
E	-1	PHE	-	expression tag	UNP A0ACI9
E	0	THR	-	expression tag	UNP A0ACI9
F	-5	GLY	-	expression tag	UNP A0ACI9
F	-4	ILE	-	expression tag	UNP A0ACI9
F	-3	ASP	-	expression tag	UNP A0ACI9
F	-2	PRO	-	expression tag	UNP A0ACI9
F	-1	PHE	-	expression tag	UNP A0ACI9
F	0	THR	-	expression tag	UNP A0ACI9

- Molecule 2 is HEXANOYL-COENZYME A (three-letter code: HXC) (formula: $C_{27}H_{46}N_7O_{17}P_3S$).
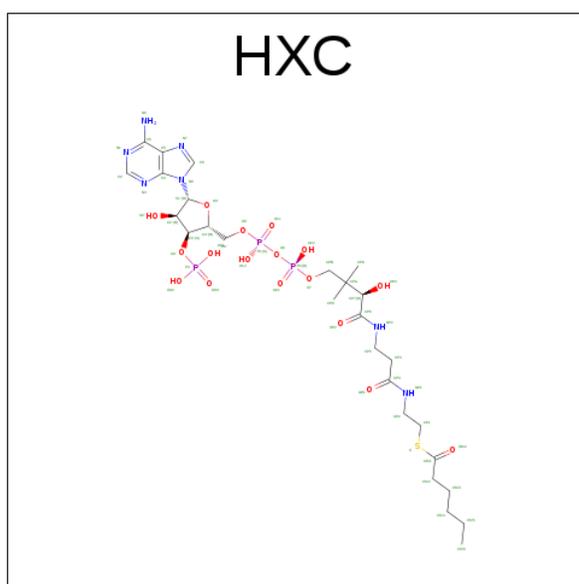
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	0
			69	69		
3	B	71	Total	O	0	0
			71	71		
3	C	58	Total	O	0	0
			58	58		
3	D	80	Total	O	0	0
			80	80		
3	E	61	Total	O	0	0
			61	61		
3	F	53	Total	O	0	0
			53	53		

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: Putative carboxyl transferase
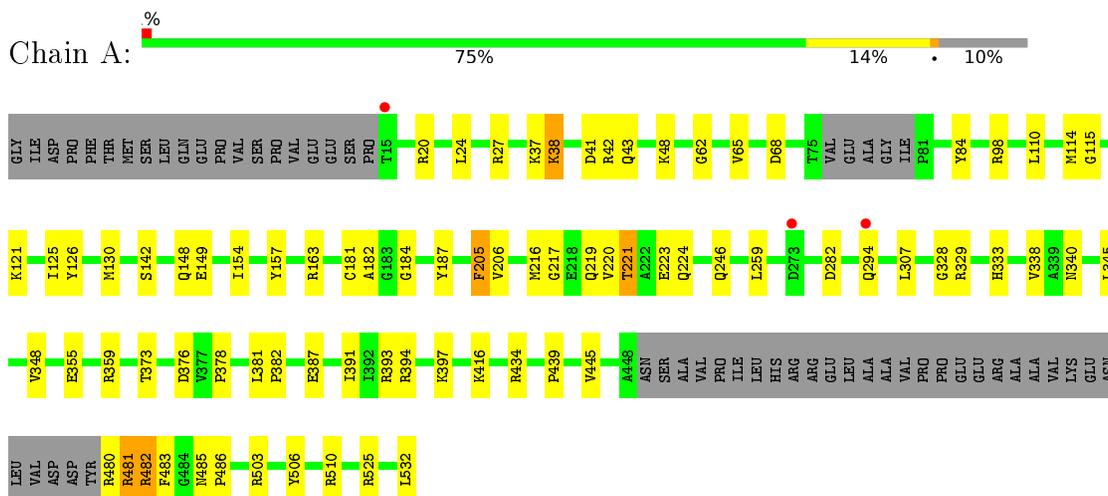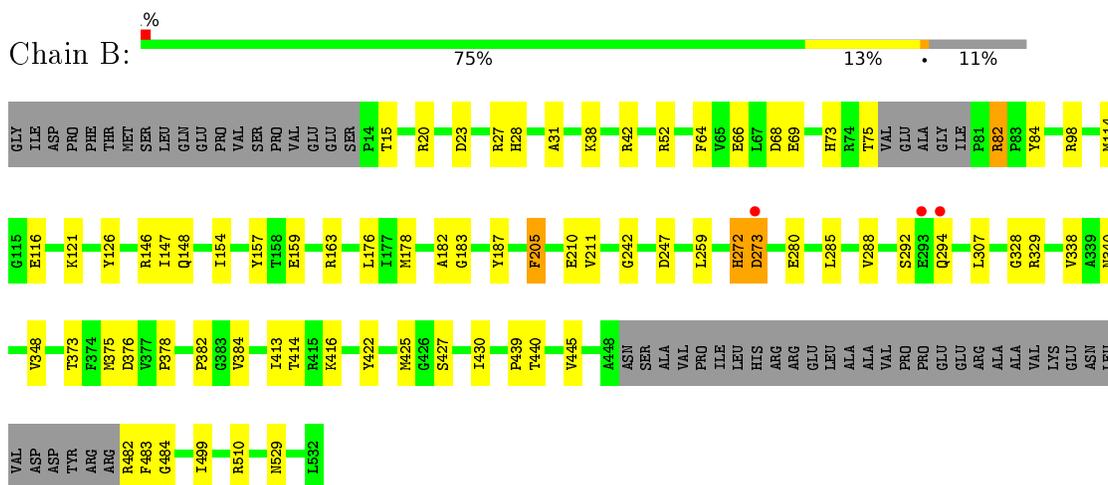
- Molecule 1: Putative carboxyl transferase

- Molecule 1: Putative carboxyl transferase

• Molecule 1: Putative carboxyl transferase

Chain D:

• Molecule 1: Putative carboxyl transferase

Chain E:

• Molecule 1: Putative carboxyl transferase

Chain F:
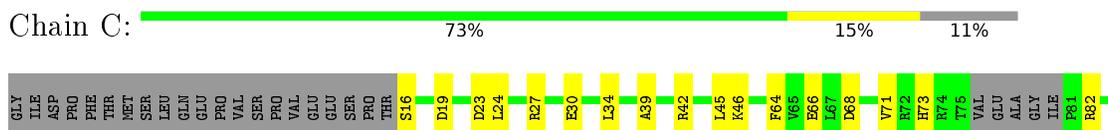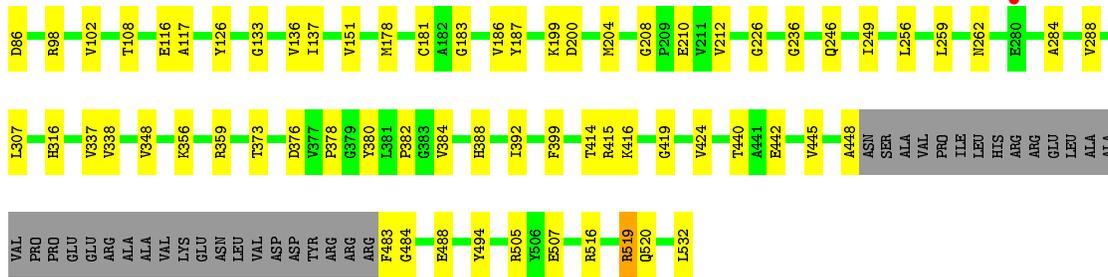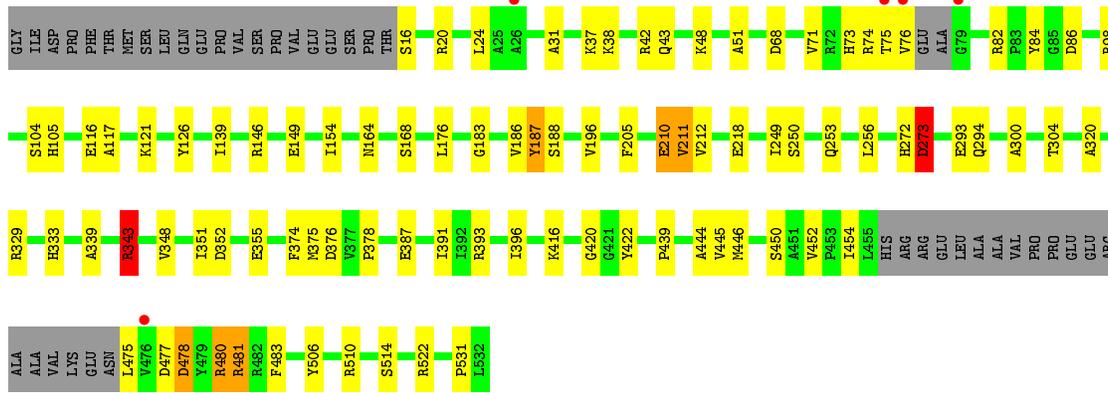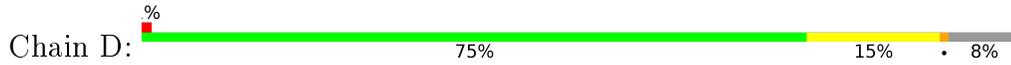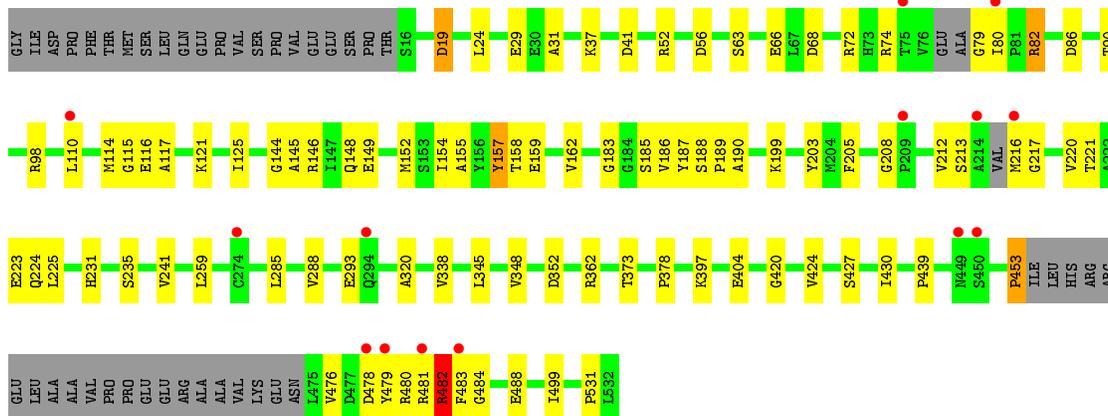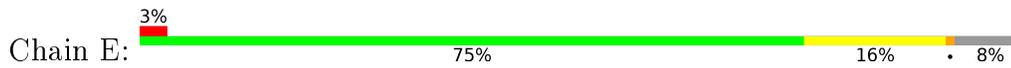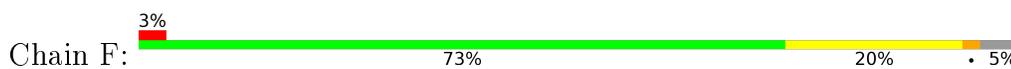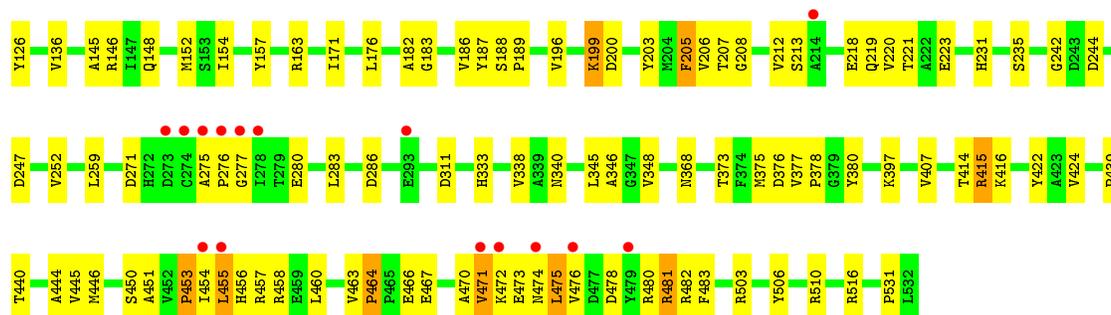
4　Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.98Å　　161.53Å　　187.29Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	58.23　–　2.85 65.43　–　2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (58.23-2.85) 95.5 (65.43-2.85)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.84 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.173　,　0.232 0.171　,　0.226	Depositor DCC
R_{free} test set	1914 reflections (2.53%)	DCC
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22896	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.33	1/3730 (0.0%)	0.52	0/5066
1	B	0.31	0/3716	0.51	1/5049 (0.0%)
1	C	0.29	0/3690	0.50	0/5014
1	D	0.34	0/3836	0.60	5/5214 (0.1%)
1	E	0.47	4/3812 (0.1%)	0.60	5/5179 (0.1%)
1	F	0.46	7/3966 (0.2%)	0.59	5/5390 (0.1%)
All	All	0.38	12/22750 (0.1%)	0.56	16/30912 (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	D	0	1
1	F	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	471	VAL	CB-CG1	-9.15	1.33	1.52
1	E	453	PRO	CA-CB	-8.38	1.36	1.53
1	F	466	GLU	CD-OE1	-7.71	1.17	1.25
1	E	453	PRO	CG-CD	7.69	1.76	1.50
1	F	466	GLU	CD-OE2	-6.42	1.18	1.25
1	F	280	GLU	CD-OE1	-6.30	1.18	1.25
1	F	464	PRO	N-CA	-6.24	1.36	1.47
1	E	453	PRO	CA-C	5.48	1.63	1.52
1	E	453	PRO	N-CD	-5.35	1.40	1.47
1	A	221	THR	CB-CG2	-5.32	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	464	PRO	CG-CD	5.22	1.67	1.50
1	F	280	GLU	CD-OE2	-5.02	1.20	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	482	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	D	343	ARG	CG-CD-NE	-8.68	93.58	111.80
1	E	453	PRO	N-CA-CB	8.33	113.30	103.30
1	D	211	VAL	CG1-CB-CG2	-7.36	99.13	110.90
1	F	475	LEU	CB-CG-CD1	7.08	123.04	111.00
1	F	455	LEU	N-CA-C	-6.71	92.88	111.00
1	F	464	PRO	N-CD-CG	-6.62	93.27	103.20
1	E	482	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	E	453	PRO	N-CD-CG	-5.87	94.40	103.20
1	E	482	ARG	CB-CG-CD	-5.83	96.44	111.60
1	F	471	VAL	CA-CB-CG1	-5.48	102.67	110.90
1	D	480	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	F	464	PRO	N-CA-CB	5.27	109.63	103.30
1	D	343	ARG	CB-CG-CD	-5.22	98.02	111.60
1	B	272	HIS	C-N-CA	5.16	134.59	121.70
1	D	187	TYR	C-N-CA	-5.08	109.00	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	481	ARG	Peptide
1	F	481	ARG	Peptide

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	3654	0	3599	69	0
1	B	3639	0	3581	70	0
1	C	3614	0	3553	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3758	0	3705	70	0
1	E	3735	0	3673	88	0
1	F	3884	0	3829	109	0
2	A	55	0	41	5	0
2	B	55	0	42	5	0
2	E	55	0	42	11	0
2	F	55	0	42	10	0
3	A	69	0	0	4	0
3	B	71	0	0	4	0
3	C	58	0	0	6	0
3	D	80	0	0	3	0
3	E	61	0	0	2	0
3	F	53	0	0	1	0
All	All	22896	0	22107	438	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 10.

All (438) 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:453:PRO:CD	1:E:453:PRO:CG	1.76	1.59
2:B:601:HXC:C1'	2:B:601:HXC:O4'	1.67	1.18
2:E:601:HXC:O4'	2:E:601:HXC:C1'	1.67	1.17
2:F:601:HXC:O4'	2:F:601:HXC:C1'	1.67	1.15
2:A:601:HXC:C1'	2:A:601:HXC:O4'	1.67	1.15
1:A:480:ARG:HB3	1:A:481:ARG:NH1	1.68	1.09
1:B:510:ARG:NH1	3:B:701:HOH:O	1.87	1.06
1:C:73:HIS:O	1:C:82:ARG:NH1	1.89	1.04
1:D:506:TYR:OH	1:D:510:ARG:NH1	1.92	1.03
1:B:38:LYS:HE2	1:B:42:ARG:NH1	1.76	0.99
1:F:218:GLU:OE2	3:F:701:HOH:O	1.82	0.98
1:A:434:ARG:NH1	3:A:701:HOH:O	1.83	0.97
1:B:340:ASN:HD22	1:B:376:ASP:H	1.09	0.95
1:D:210:GLU:OE2	1:D:211:VAL:HG23	1.67	0.93
1:A:481:ARG:NH2	3:A:703:HOH:O	2.03	0.91
1:E:144:GLY:O	1:E:157:TYR:HE1	1.53	0.91
1:B:210:GLU:OE1	3:B:702:HOH:O	1.90	0.90
1:E:148:GLN:HE22	2:E:601:HXC:H2	1.37	0.89
1:E:37:LYS:NZ	1:E:41:ASP:OD1	2.06	0.88
1:D:272:HIS:HB2	1:D:273:ASP:HB2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ARG:NH2	1:E:484:GLY:O	2.07	0.88
1:E:480:ARG:NH1	1:E:483:PHE:CE1	2.43	0.86
1:A:282:ASP:OD2	3:A:702:HOH:O	1.94	0.85
1:A:37:LYS:NZ	1:A:41:ASP:OD2	2.11	0.83
1:C:505:ARG:NH1	3:C:601:HOH:O	2.11	0.83
1:B:38:LYS:HE2	1:B:42:ARG:HH11	1.42	0.83
1:E:203:TYR:OH	1:E:223:GLU:OE1	1.97	0.82
1:C:516:ARG:NH1	3:C:602:HOH:O	2.13	0.82
1:F:471:VAL:HA	1:F:473:GLU:H	1.46	0.81
1:E:157:TYR:HB3	2:E:601:HXC:HM32	1.61	0.81
1:A:154:ILE:HD11	1:D:445:VAL:HA	1.61	0.80
1:F:348:VAL:HG12	1:F:378:PRO:HG2	1.64	0.80
1:F:471:VAL:HG11	1:F:475:LEU:HD12	1.64	0.79
1:B:482:ARG:HG3	1:B:483:PHE:H	1.48	0.77
1:E:144:GLY:O	1:E:157:TYR:CE1	2.39	0.76
1:E:56:ASP:OD1	3:E:701:HOH:O	2.05	0.74
1:F:456:HIS:O	1:F:460:LEU:HB2	1.87	0.74
1:B:114:MET:HB3	1:B:157:TYR:HE1	1.52	0.74
1:F:471:VAL:HG11	1:F:475:LEU:CD1	2.18	0.74
1:B:340:ASN:ND2	1:B:376:ASP:H	1.82	0.73
1:D:375:MET:HE3	1:D:422:TYR:HA	1.69	0.73
1:F:446:MET:O	1:F:480:ARG:NH2	2.21	0.72
1:A:340:ASN:HD22	1:A:376:ASP:H	1.37	0.72
1:F:471:VAL:HA	1:F:473:GLU:N	2.05	0.71
1:F:464:PRO:HD2	1:F:467:GLU:HB2	1.72	0.71
1:E:31:ALA:O	3:E:702:HOH:O	2.09	0.71
1:A:480:ARG:N	3:A:704:HOH:O	2.23	0.71
1:A:62:GLY:O	3:B:701:HOH:O	2.09	0.71
1:D:506:TYR:CZ	1:D:510:ARG:NH1	2.59	0.71
1:E:480:ARG:NH1	1:E:483:PHE:CZ	2.59	0.70
1:C:494:TYR:OH	1:E:152:MET:HG3	1.91	0.70
1:F:333:HIS:CD2	1:F:516:ARG:NH1	2.60	0.70
1:B:38:LYS:CE	1:B:42:ARG:NH1	2.53	0.70
1:B:445:VAL:HG23	1:F:154:ILE:HD11	1.75	0.69
1:F:109:THR:HG22	1:F:110:LEU:HD12	1.75	0.69
1:B:73:HIS:HD2	1:B:75:THR:HG22	1.57	0.69
1:F:444:ALA:HB2	1:F:483:PHE:HB3	1.76	0.68
1:E:145:ALA:O	2:E:601:HXC:N6	2.23	0.68
1:B:414:THR:O	1:B:440:THR:OG1	2.11	0.68
1:F:471:VAL:HG11	1:F:475:LEU:HB2	1.75	0.68
1:B:384:VAL:HG11	1:F:220:VAL:HG11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:471:VAL:CG1	1:F:475:LEU:HB2	2.24	0.68
1:C:86:ASP:OD2	1:C:117:ALA:HB3	1.94	0.67
1:C:42:ARG:HD2	1:C:46:LYS:NZ	2.09	0.67
1:D:293:GLU:HG3	1:D:294:GLN:HG3	1.75	0.67
1:F:446:MET:HG3	1:F:450:SER:OG	1.96	0.66
1:D:444:ALA:HB2	1:D:483:PHE:HB3	1.78	0.66
1:A:43:GLN:HE22	1:A:48:LYS:HE2	1.60	0.65
1:C:183:GLY:O	1:C:186:VAL:HG22	1.95	0.65
1:B:210:GLU:HG2	1:B:211:VAL:H	1.62	0.65
1:B:529:ASN:OD1	3:B:703:HOH:O	2.13	0.65
1:E:148:GLN:HE22	2:E:601:HXC:C2	2.10	0.65
1:C:126:TYR:CE2	1:C:136:VAL:HG11	2.31	0.65
1:A:114:MET:HB3	1:A:157:TYR:CE2	2.31	0.64
1:A:348:VAL:HG12	1:A:378:PRO:HG2	1.80	0.64
1:A:480:ARG:HB3	1:A:481:ARG:HH12	1.60	0.64
1:E:482:ARG:C	1:E:482:ARG:HD3	2.17	0.64
1:D:375:MET:CE	1:D:422:TYR:HA	2.26	0.64
1:D:477:ASP:O	1:D:480:ARG:HB2	1.97	0.64
1:C:376:ASP:OD1	1:C:416:LYS:NZ	2.27	0.64
1:C:507:GLU:OE2	3:C:603:HOH:O	2.16	0.64
1:E:348:VAL:HG12	1:E:378:PRO:HG2	1.80	0.63
1:C:414:THR:O	1:C:440:THR:OG1	2.14	0.63
1:F:471:VAL:CG1	1:F:475:LEU:HD12	2.28	0.63
1:F:471:VAL:CB	1:F:472:LYS:HA	2.27	0.63
1:C:483:PHE:N	3:C:608:HOH:O	2.32	0.63
1:A:157:TYR:HB3	2:A:601:HXC:HM21	1.79	0.62
1:F:98:ARG:NH2	1:F:259:LEU:O	2.27	0.62
1:C:98:ARG:NH2	1:C:259:LEU:O	2.31	0.62
1:E:293:GLU:H	1:E:293:GLU:CD	2.03	0.62
1:C:519:ARG:NE	1:C:520:GLN:H	1.97	0.62
1:F:346:ALA:O	1:F:416:LYS:NZ	2.32	0.62
1:A:38:LYS:HG3	1:A:42:ARG:HH21	1.65	0.61
1:C:348:VAL:HG12	1:C:378:PRO:HG2	1.81	0.61
1:E:68:ASP:HB2	1:E:121:LYS:HE3	1.81	0.61
1:E:480:ARG:CZ	1:E:483:PHE:CE1	2.83	0.61
1:F:187:TYR:HD1	2:F:601:HXC:HM31	1.65	0.61
1:A:445:VAL:HA	1:D:154:ILE:HD11	1.83	0.61
1:E:208:GLY:O	1:E:212:VAL:HG23	2.01	0.61
1:E:52:ARG:NH2	1:E:66:GLU:OE1	2.31	0.61
1:F:203:TYR:HB3	1:F:205:PHE:CZ	2.36	0.61
1:B:272:HIS:HA	1:B:273:ASP:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ARG:NH1	1:A:532:LEU:O	2.34	0.60
1:D:73:HIS:CE1	1:D:82:ARG:HG2	2.37	0.60
1:D:475:LEU:HD12	1:D:477:ASP:HB3	1.84	0.60
1:A:24:LEU:HD22	1:B:439:PRO:HG3	1.83	0.60
1:A:27:ARG:NH1	1:A:84:TYR:OH	2.34	0.60
1:C:448:ALA:O	3:C:604:HOH:O	2.17	0.59
1:F:470:ALA:O	1:F:474:ASN:N	2.35	0.59
1:B:73:HIS:CD2	1:B:75:THR:HG22	2.36	0.59
1:E:148:GLN:NE2	2:E:601:HXC:H2	2.15	0.59
1:C:186:VAL:HG23	1:C:187:TYR:HD2	1.68	0.59
1:E:478:ASP:O	1:E:481:ARG:HG3	2.03	0.59
1:A:294:GLN:O	1:A:294:GLN:HG2	2.02	0.59
1:B:272:HIS:HB2	1:B:273:ASP:CB	2.32	0.59
1:A:503:ARG:HH11	1:A:503:ARG:HG2	1.68	0.59
1:B:272:HIS:HB2	1:B:273:ASP:HB2	1.83	0.59
1:D:24:LEU:HD22	1:E:439:PRO:HG3	1.85	0.58
1:D:16:SER:N	3:D:604:HOH:O	2.36	0.58
1:C:208:GLY:O	1:C:212:VAL:HG23	2.03	0.58
1:C:246:GLN:N	1:C:246:GLN:OE1	2.30	0.58
1:F:163:ARG:HH11	1:F:163:ARG:HG3	1.68	0.58
1:D:164:ASN:OD1	1:D:188:SER:HB3	2.03	0.58
1:B:378:PRO:HD3	1:B:416:LYS:HZ2	1.67	0.58
1:D:300:ALA:O	1:D:304:THR:HG23	2.04	0.58
1:D:452:VAL:C	1:D:454:ILE:H	2.06	0.58
1:E:90:THR:HB	1:E:125:ILE:HG13	1.83	0.58
1:E:144:GLY:HA2	1:E:185:SER:HB2	1.85	0.58
1:E:480:ARG:HB3	1:E:483:PHE:HD1	1.68	0.58
1:F:340:ASN:HD22	1:F:376:ASP:H	1.52	0.58
1:A:221:THR:CG2	1:A:223:GLU:OE2	2.51	0.57
1:A:221:THR:HG21	1:A:223:GLU:OE2	2.04	0.57
1:D:272:HIS:CB	1:D:273:ASP:HB2	2.29	0.57
1:B:272:HIS:CA	1:B:273:ASP:HB2	2.35	0.57
1:D:68:ASP:HB2	1:D:121:LYS:HE3	1.85	0.57
2:A:601:HXC:OM2	1:D:420:GLY:HA2	2.05	0.57
1:A:130:MET:HE1	1:A:163:ARG:HB3	1.87	0.57
1:A:98:ARG:NH2	1:A:259:LEU:O	2.34	0.57
1:F:109:THR:CG2	1:F:110:LEU:HD12	2.34	0.56
1:F:145:ALA:H	2:F:601:HXC:HP41	1.70	0.56
1:C:186:VAL:HG23	1:C:187:TYR:CD2	2.40	0.56
1:D:376:ASP:OD1	1:D:416:LYS:HB2	2.05	0.56
1:C:23:ASP:O	1:C:27:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:LYS:NZ	1:D:42:ARG:HG3	2.20	0.56
1:F:471:VAL:HB	1:F:472:LYS:HA	1.87	0.56
1:C:419:GLY:HA2	2:E:601:HXC:HP12	1.87	0.56
1:B:116:GLU:OE2	1:E:74:ARG:NH2	2.26	0.56
1:C:445:VAL:HA	1:E:154:ILE:HD11	1.87	0.56
1:D:478:ASP:HA	1:D:481:ARG:HG2	1.88	0.56
1:E:285:LEU:O	1:E:288:VAL:HG12	2.06	0.56
1:B:114:MET:HB3	1:B:157:TYR:CE1	2.37	0.56
1:E:24:LEU:HD22	1:F:439:PRO:HG3	1.88	0.56
1:A:355:GLU:OE1	1:A:394:ARG:HB3	2.06	0.55
1:F:157:TYR:HB3	2:F:601:HXC:HM41	1.88	0.55
1:F:213:SER:OG	1:F:219:GLN:OE1	2.13	0.55
1:F:23:ASP:OD2	1:F:27:ARG:HD2	2.07	0.55
1:F:453:PRO:O	1:F:455:LEU:HA	2.06	0.55
1:A:307:LEU:HD13	1:A:328:GLY:HA3	1.90	0.54
1:D:212:VAL:HG12	1:D:218:GLU:HB2	1.89	0.54
1:B:146:ARG:HG2	1:B:148:GLN:OE1	2.07	0.54
1:B:375:MET:HE2	1:B:413:ILE:HG23	1.89	0.54
1:F:30:GLU:HG3	1:F:34:LEU:HD12	1.90	0.54
1:B:482:ARG:CG	1:B:483:PHE:H	2.21	0.54
1:C:116:GLU:OE1	1:D:74:ARG:NH2	2.41	0.54
1:D:38:LYS:HD2	1:D:38:LYS:O	2.08	0.54
1:F:115:GLY:HA3	1:F:146:ARG:HH21	1.73	0.54
1:F:43:GLN:HE22	1:F:48:LYS:HE2	1.72	0.53
1:C:384:VAL:HG13	1:C:388:HIS:CE1	2.43	0.53
1:C:384:VAL:HG13	1:C:388:HIS:ND1	2.24	0.53
1:C:181:CYS:HB3	1:C:204:MET:HG2	1.90	0.53
1:A:246:GLN:H	1:A:246:GLN:CD	2.12	0.53
1:B:147:ILE:HB	1:F:454:ILE:HG12	1.90	0.53
1:A:503:ARG:HG2	1:A:503:ARG:NH1	2.23	0.53
1:E:220:VAL:HG22	1:E:224:GLN:HB2	1.91	0.53
1:C:284:ALA:O	1:C:288:VAL:HG23	2.09	0.52
1:B:378:PRO:CD	1:B:416:LYS:HZ2	2.22	0.52
1:E:183:GLY:O	1:E:186:VAL:HG22	2.09	0.52
1:F:340:ASN:ND2	1:F:376:ASP:H	2.08	0.52
1:F:463:VAL:HG12	1:F:467:GLU:O	2.10	0.52
1:C:16:SER:HB3	1:C:19:ASP:OD2	2.09	0.52
1:E:476:VAL:HG12	1:E:479:TYR:HB2	1.92	0.52
1:F:473:GLU:HA	1:F:476:VAL:HG22	1.92	0.52
1:F:503:ARG:NH1	1:F:506:TYR:CE2	2.78	0.52
1:E:187:TYR:HB3	2:E:601:HXC:HM63	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:LEU:HD23	1:F:196:VAL:HB	1.92	0.51
1:F:199:LYS:HD2	1:F:200:ASP:N	2.24	0.51
1:B:68:ASP:HB2	1:B:121:LYS:HE3	1.91	0.51
1:F:23:ASP:O	1:F:27:ARG:HG3	2.10	0.51
1:E:397:LYS:HD3	1:E:531:PRO:O	2.10	0.51
1:F:457:ARG:HG3	1:F:458:ARG:N	2.25	0.51
1:C:42:ARG:HD2	1:C:46:LYS:HZ1	1.76	0.51
1:E:158:THR:O	1:E:162:VAL:HG23	2.10	0.51
1:B:210:GLU:HG2	1:B:211:VAL:N	2.26	0.50
1:C:68:ASP:HB3	1:C:71:VAL:CG2	2.41	0.50
1:A:480:ARG:HH12	1:A:483:PHE:HB2	1.75	0.50
1:A:20:ARG:NH2	1:B:484:GLY:O	2.43	0.50
1:C:519:ARG:HE	1:C:520:GLN:H	1.59	0.50
1:E:221:THR:CG2	1:E:223:GLU:OE2	2.59	0.50
2:B:601:HXC:O3'	1:F:455:LEU:HD11	2.11	0.50
1:F:463:VAL:HG12	1:F:464:PRO:CD	2.41	0.50
1:B:15:THR:O	1:B:20:ARG:NH1	2.45	0.50
1:B:285:LEU:HA	1:B:288:VAL:HG23	1.93	0.50
1:A:387:GLU:HA	1:A:391:ILE:HG22	1.92	0.50
1:B:384:VAL:CG1	1:F:220:VAL:HG11	2.42	0.50
1:E:203:TYR:HE1	1:E:223:GLU:HG3	1.76	0.50
1:E:72:ARG:HH21	1:E:82:ARG:HG3	1.75	0.50
1:A:394:ARG:HA	1:A:397:LYS:HE3	1.94	0.50
1:C:151:VAL:HG22	1:E:488:GLU:OE2	2.12	0.50
1:F:187:TYR:OH	1:F:206:VAL:HG13	2.12	0.50
1:A:480:ARG:NH1	1:A:483:PHE:CD1	2.80	0.50
1:F:503:ARG:NH1	1:F:506:TYR:CD2	2.80	0.50
1:B:242:GLY:HA2	1:B:247:ASP:OD2	2.11	0.49
1:E:72:ARG:NH2	1:E:82:ARG:HG3	2.26	0.49
1:D:38:LYS:HZ1	1:D:42:ARG:HG3	1.75	0.49
1:F:345:LEU:O	1:F:348:VAL:HG22	2.12	0.49
1:B:154:ILE:HD11	1:F:445:VAL:HA	1.95	0.49
1:D:351:ILE:O	1:D:355:GLU:HG3	2.12	0.49
1:C:380:TYR:O	1:C:382:PRO:HD3	2.11	0.49
1:D:250:SER:HA	1:D:253:GLN:HE21	1.77	0.49
1:F:375:MET:SD	1:F:422:TYR:HA	2.53	0.49
1:B:272:HIS:CB	1:B:273:ASP:HB2	2.43	0.49
1:B:375:MET:SD	1:B:425:MET:HB2	2.53	0.49
1:C:178:MET:HE3	1:C:249:ILE:HG13	1.94	0.49
1:D:454:ILE:HG22	1:D:454:ILE:O	2.13	0.49
1:C:532:LEU:HD22	1:E:397:LYS:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:GLY:HA3	2:F:601:HXC:OP1	2.12	0.49
1:C:30:GLU:HA	1:C:34:LEU:HD12	1.95	0.49
1:F:474:ASN:O	1:F:478:ASP:OD1	2.31	0.49
1:E:187:TYR:HD1	2:E:601:HXC:HM42	1.78	0.48
1:E:98:ARG:NH2	1:E:259:LEU:O	2.31	0.48
1:B:348:VAL:HG12	1:B:378:PRO:HG2	1.94	0.48
1:C:133:GLY:O	1:C:262:ASN:ND2	2.37	0.48
1:A:65:VAL:HG22	1:B:510:ARG:CZ	2.43	0.48
1:D:387:GLU:HA	1:D:391:ILE:HG22	1.94	0.48
1:A:439:PRO:HG3	1:C:24:LEU:HD22	1.95	0.48
1:B:38:LYS:CE	1:B:42:ARG:HH12	2.27	0.48
1:F:451:ALA:O	1:F:456:HIS:HB2	2.14	0.48
1:D:210:GLU:OE2	1:D:211:VAL:CG2	2.50	0.48
1:A:184:GLY:HA2	1:A:187:TYR:HB2	1.95	0.48
1:A:340:ASN:ND2	1:A:376:ASP:H	2.09	0.48
1:B:52:ARG:NH2	1:B:66:GLU:OE1	2.47	0.48
1:C:316:HIS:HB2	1:C:356:LYS:HE3	1.94	0.48
1:E:362:ARG:NH1	1:E:404:GLU:OE1	2.44	0.48
1:D:74:ARG:O	3:D:602:HOH:O	2.20	0.47
1:E:480:ARG:HA	1:E:482:ARG:N	2.30	0.47
1:F:333:HIS:HD2	1:F:516:ARG:NH1	2.12	0.47
1:A:115:GLY:HA2	1:A:149:GLU:OE2	2.14	0.47
1:E:148:GLN:H	1:E:148:GLN:NE2	2.12	0.47
1:D:343:ARG:HE	1:D:343:ARG:HB3	0.84	0.47
1:D:249:ILE:O	1:D:253:GLN:HG3	2.14	0.47
1:C:236:GLY:O	1:C:316:HIS:HE1	1.97	0.47
1:E:203:TYR:CE1	1:E:223:GLU:HG3	2.48	0.47
1:F:163:ARG:NH1	1:F:163:ARG:HG3	2.30	0.47
1:F:276:PRO:HA	1:F:277:GLY:HA2	1.64	0.47
1:A:525:ARG:NH1	1:D:168:SER:O	2.46	0.47
1:D:76:VAL:HA	1:D:82:ARG:HD2	1.96	0.47
1:F:221:THR:HB	1:F:223:GLU:OE1	2.15	0.47
1:A:154:ILE:HG13	1:D:445:VAL:HG22	1.96	0.46
1:A:220:VAL:CG1	1:A:224:GLN:HB2	2.44	0.46
1:E:427:SER:O	1:E:430:ILE:HG22	2.15	0.46
1:F:146:ARG:HG3	1:F:148:GLN:OE1	2.16	0.46
1:D:393:ARG:O	1:D:396:ILE:HG22	2.14	0.46
1:E:320:ALA:HB2	1:E:352:ASP:HB3	1.96	0.46
1:C:419:GLY:CA	2:E:601:HXC:HP12	2.45	0.46
1:B:187:TYR:HB3	2:B:601:HXC:HM52	1.96	0.46
1:F:199:LYS:O	1:F:200:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:VAL:HA	1:C:137:ILE:O	2.16	0.46
1:C:137:ILE:HD11	1:C:256:LEU:HD11	1.96	0.46
1:E:345:LEU:O	1:E:348:VAL:HG22	2.16	0.46
1:F:115:GLY:CA	1:F:146:ARG:HH21	2.28	0.46
1:E:115:GLY:HA2	1:E:149:GLU:OE2	2.15	0.46
1:A:480:ARG:NH1	1:A:483:PHE:HB2	2.31	0.46
1:B:23:ASP:OD2	1:B:27:ARG:HD2	2.17	0.45
1:D:176:LEU:HD23	1:D:196:VAL:HB	1.98	0.45
1:E:480:ARG:CZ	1:E:483:PHE:CD1	2.99	0.45
1:A:223:GLU:H	1:A:223:GLU:CD	2.19	0.45
1:A:485:ASN:HB2	1:A:486:PRO:HD2	1.99	0.45
1:E:231:HIS:HA	1:E:235:SER:OG	2.16	0.45
1:C:338:VAL:O	1:C:373:THR:HA	2.16	0.45
1:D:522:ARG:NH1	3:D:601:HOH:O	2.08	0.45
1:F:115:GLY:N	1:F:146:ARG:HH21	2.13	0.45
1:B:176:LEU:HD22	1:B:178:MET:HE3	1.98	0.45
1:E:480:ARG:HG2	1:E:483:PHE:CD1	2.52	0.45
1:F:154:ILE:CD1	2:F:601:HXC:HP12	2.47	0.45
1:F:283:LEU:HD23	1:F:286:ASP:OD2	2.17	0.45
1:A:506:TYR:O	1:A:510:ARG:HG3	2.16	0.45
1:F:145:ALA:O	2:F:601:HXC:N6	2.41	0.45
1:F:199:LYS:HE2	1:F:200:ASP:OD1	2.16	0.45
1:A:125:ILE:HA	1:A:125:ILE:HD12	1.79	0.45
1:A:482:ARG:HA	1:A:482:ARG:NH1	2.32	0.45
1:F:478:ASP:HA	1:F:481:ARG:HG3	1.97	0.45
1:B:147:ILE:HB	1:F:454:ILE:HG21	1.99	0.45
1:B:378:PRO:HD3	1:B:416:LYS:NZ	2.32	0.45
1:B:292:SER:OG	1:B:294:GLN:HG3	2.17	0.45
1:B:439:PRO:HD3	1:B:499:ILE:O	2.17	0.45
1:A:163:ARG:HG3	1:A:163:ARG:HH11	1.82	0.45
1:E:213:SER:O	1:E:217:GLY:HA2	2.17	0.45
1:B:183:GLY:HA3	2:B:601:HXC:OP1	2.16	0.44
1:C:39:ALA:HA	1:C:108:THR:HG21	1.99	0.44
1:F:463:VAL:CG1	1:F:464:PRO:HD3	2.47	0.44
1:B:382:PRO:HB3	1:F:207:THR:HG22	1.97	0.44
1:C:483:PHE:N	3:C:614:HOH:O	2.50	0.44
1:F:450:SER:HA	1:F:453:PRO:HD2	1.99	0.44
2:B:601:HXC:O2'	1:F:455:LEU:HD12	2.17	0.44
1:C:442:GLU:HG2	1:C:484:GLY:O	2.17	0.44
1:A:38:LYS:HG3	1:A:42:ARG:NH2	2.32	0.44
1:B:147:ILE:CG2	1:F:454:ILE:HG12	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:481:ARG:O	1:E:483:PHE:N	2.50	0.44
1:E:188:SER:HB3	1:E:189:PRO:HD3	2.00	0.44
1:F:376:ASP:OD1	1:F:416:LYS:HE3	2.18	0.44
1:A:163:ARG:NH1	1:A:163:ARG:HG3	2.33	0.44
1:B:98:ARG:NH2	1:B:259:LEU:O	2.39	0.44
1:D:86:ASP:OD1	1:D:146:ARG:NH2	2.43	0.44
1:E:420:GLY:O	1:E:424:VAL:HG23	2.18	0.44
1:B:482:ARG:HG3	1:B:483:PHE:N	2.24	0.44
1:F:176:LEU:HD21	1:F:252:VAL:HG21	1.99	0.44
1:B:182:ALA:HA	1:B:205:PHE:O	2.18	0.43
1:E:221:THR:HG22	1:E:223:GLU:OE2	2.16	0.43
1:E:480:ARG:HG2	1:E:483:PHE:CE1	2.52	0.43
1:F:471:VAL:HG12	1:F:475:LEU:HB2	1.98	0.43
1:A:378:PRO:HB3	1:A:416:LYS:HD2	1.99	0.43
1:A:148:GLN:OE1	2:A:601:HXC:H2	2.18	0.43
1:D:329:ARG:HA	1:D:333:HIS:O	2.18	0.43
1:E:439:PRO:HD3	1:E:499:ILE:O	2.19	0.43
1:C:181:CYS:O	1:C:204:MET:HA	2.18	0.43
1:F:182:ALA:HB3	2:F:601:HXC:HP91	1.99	0.43
1:E:63:SER:HA	1:F:510:ARG:HH12	1.84	0.43
1:B:64:PHE:CE2	1:B:66:GLU:HB2	2.54	0.43
1:E:146:ARG:HA	2:E:601:HXC:N1	2.34	0.43
1:E:479:TYR:O	1:E:479:TYR:CD2	2.71	0.43
1:A:182:ALA:HA	1:A:205:PHE:O	2.19	0.43
1:C:45:LEU:O	1:C:45:LEU:HD23	2.18	0.43
1:D:348:VAL:HG12	1:D:378:PRO:HG2	2.01	0.43
1:F:183:GLY:O	1:F:186:VAL:HG22	2.19	0.43
1:F:338:VAL:O	1:F:373:THR:HA	2.19	0.43
1:A:216:MET:H	1:A:217:GLY:HA2	1.84	0.43
1:E:212:VAL:HG13	1:E:216:MET:SD	2.58	0.43
1:C:359:ARG:NE	1:E:531:PRO:HA	2.34	0.43
1:E:221:THR:N	1:E:224:GLN:OE1	2.29	0.43
1:A:219:GLN:NE2	1:A:219:GLN:HA	2.34	0.43
1:A:381:LEU:HD12	1:A:382:PRO:HD2	2.01	0.43
1:D:98:ARG:NH2	1:D:256:LEU:O	2.52	0.43
1:F:414:THR:O	1:F:440:THR:OG1	2.24	0.43
1:B:338:VAL:O	1:B:373:THR:HA	2.19	0.43
1:C:42:ARG:HD2	1:C:46:LYS:HZ2	1.84	0.43
1:F:244:ASP:N	1:F:244:ASP:OD1	2.52	0.43
1:D:16:SER:O	1:D:20:ARG:HG3	2.19	0.42
1:D:210:GLU:CD	1:D:211:VAL:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:GLY:O	1:F:212:VAL:HG23	2.19	0.42
1:D:187:TYR:HD1	1:D:187:TYR:N	2.18	0.42
1:E:115:GLY:CA	1:E:149:GLU:OE2	2.67	0.42
1:D:86:ASP:OD2	1:D:117:ALA:HB3	2.19	0.42
1:E:148:GLN:H	1:E:148:GLN:CD	2.23	0.42
1:E:86:ASP:OD2	1:E:117:ALA:HB3	2.18	0.42
1:F:182:ALA:CB	2:F:601:HXC:HP91	2.48	0.42
1:F:223:GLU:H	1:F:223:GLU:CD	2.22	0.42
1:A:329:ARG:HA	1:A:333:HIS:O	2.20	0.42
1:F:380:TYR:OH	1:F:424:VAL:HG21	2.19	0.42
1:F:470:ALA:C	1:F:471:VAL:HG13	2.38	0.42
1:C:204:MET:O	1:C:226:GLY:HA3	2.19	0.42
1:C:382:PRO:HD2	1:E:216:MET:CE	2.50	0.42
1:B:148:GLN:N	1:B:148:GLN:OE1	2.42	0.42
1:B:427:SER:O	1:B:430:ILE:HG22	2.20	0.42
1:D:320:ALA:HB2	1:D:352:ASP:HB3	2.01	0.42
1:E:19:ASP:OD1	1:E:19:ASP:N	2.52	0.42
1:F:136:VAL:HG23	1:F:171:ILE:HD12	2.02	0.42
1:A:481:ARG:NE	1:A:481:ARG:N	2.67	0.42
1:B:31:ALA:HB2	1:B:84:TYR:CD2	2.55	0.42
1:E:110:LEU:HA	1:E:110:LEU:HD23	1.75	0.42
1:A:187:TYR:OH	1:A:206:VAL:HG13	2.20	0.42
1:B:280:GLU:OE2	1:B:280:GLU:N	2.53	0.42
1:B:329:ARG:HH11	1:B:329:ARG:HG3	1.85	0.42
1:C:307:LEU:HD11	1:C:337:VAL:HG21	2.02	0.42
1:E:221:THR:HG22	1:E:223:GLU:H	1.84	0.42
1:F:122:VAL:O	1:F:125:ILE:HG22	2.20	0.42
1:A:110:LEU:HD22	1:A:148:GLN:HE22	1.84	0.42
1:C:210:GLU:H	1:C:210:GLU:CD	2.23	0.42
1:C:42:ARG:HG3	1:C:42:ARG:O	2.18	0.42
1:C:399:PHE:HD2	1:C:424:VAL:HG12	1.85	0.42
1:F:152:MET:HE3	1:F:152:MET:HB2	1.90	0.42
1:F:223:GLU:N	1:F:223:GLU:CD	2.73	0.42
1:F:72:ARG:HD2	1:F:84:TYR:CE1	2.55	0.42
1:A:345:LEU:O	1:A:348:VAL:HG22	2.20	0.41
1:D:116:GLU:N	1:D:149:GLU:OE1	2.53	0.41
1:D:183:GLY:O	1:D:186:VAL:HG22	2.19	0.41
1:D:514:SER:HB2	1:F:99:GLN:OE1	2.20	0.41
1:F:188:SER:HB2	1:F:189:PRO:HD3	2.01	0.41
1:F:378:PRO:HD3	1:F:416:LYS:NZ	2.35	0.41
1:D:339:ALA:HB2	1:D:374:PHE:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:LYS:HD2	1:E:241:VAL:HG11	2.02	0.41
1:B:159:GLU:HG3	1:B:163:ARG:NH1	2.36	0.41
1:D:104:SER:HA	1:D:139:ILE:HB	2.02	0.41
1:D:31:ALA:HB2	1:D:84:TYR:CD2	2.55	0.41
1:C:199:LYS:NZ	1:C:200:ASP:OD2	2.50	0.41
1:F:242:GLY:HA2	1:F:247:ASP:OD2	2.20	0.41
1:F:148:GLN:OE1	2:F:601:HXC:H2	2.20	0.41
1:D:51:ALA:HB2	1:D:105:HIS:O	2.21	0.41
1:E:116:GLU:HB3	1:E:152:MET:HE3	2.02	0.41
1:E:205:PHE:CD2	1:E:225:LEU:HG	2.56	0.41
1:D:71:VAL:CG1	1:D:117:ALA:HB1	2.51	0.41
1:D:396:ILE:HA	1:D:396:ILE:HD12	1.91	0.41
1:F:375:MET:HG3	1:F:377:VAL:HG12	2.02	0.41
1:E:79:GLY:HA2	1:E:80:ILE:HA	1.73	0.41
1:B:73:HIS:O	1:B:82:ARG:NH2	2.47	0.41
1:D:73:HIS:CE1	1:D:75:THR:HG23	2.55	0.41
1:F:368:ASN:HA	1:F:407:VAL:CG1	2.51	0.41
1:F:415:ARG:HB3	1:F:416:LYS:H	1.67	0.41
1:A:187:TYR:HB3	2:A:601:HXC:HM52	2.03	0.41
1:A:142:SER:O	1:A:181:CYS:HA	2.21	0.41
1:D:187:TYR:CD1	1:D:187:TYR:N	2.88	0.41
1:D:446:MET:HG2	1:D:450:SER:HB2	2.03	0.41
1:B:422:TYR:HD2	1:F:154:ILE:HG21	1.86	0.41
1:C:392:ILE:HG22	1:E:190:ALA:HB2	2.03	0.41
1:F:231:HIS:HA	1:F:235:SER:OG	2.20	0.41
1:D:439:PRO:HG3	1:F:24:LEU:HD22	2.02	0.41
1:A:68:ASP:HB2	1:A:121:LYS:HE3	2.03	0.40
1:C:415:ARG:HH21	1:C:416:LYS:HZ1	1.68	0.40
1:D:475:LEU:CD1	1:D:477:ASP:HB3	2.51	0.40
1:E:155:ALA:O	1:E:159:GLU:HG2	2.22	0.40
1:E:223:GLU:N	1:E:223:GLU:OE2	2.46	0.40
1:E:293:GLU:CD	1:E:293:GLU:N	2.74	0.40
1:F:275:ALA:HA	1:F:276:PRO:HD3	1.83	0.40
1:E:125:ILE:HD13	1:E:125:ILE:HA	1.82	0.40
1:F:460:LEU:HD11	1:F:472:LYS:O	2.21	0.40
1:A:359:ARG:NE	1:D:531:PRO:HA	2.36	0.40
1:C:64:PHE:CE2	1:C:66:GLU:HB2	2.56	0.40
1:D:452:VAL:O	1:D:454:ILE:N	2.54	0.40
1:E:114:MET:CE	1:E:157:TYR:CE2	3.04	0.40
1:E:338:VAL:O	1:E:373:THR:HA	2.21	0.40
1:F:397:LYS:HE2	1:F:531:PRO:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:THR:HB	1:A:224:GLN:CD	2.42	0.40
1:A:338:VAL:O	1:A:373:THR:HA	2.22	0.40
1:B:272:HIS:HB2	1:B:273:ASP:HB3	2.02	0.40
1:B:307:LEU:HD13	1:B:328:GLY:HA3	2.03	0.40
1:B:416:LYS:HE3	1:B:416:LYS:HB2	1.87	0.40
1:B:28:HIS:ND1	1:B:69:GLU:OE2	2.54	0.40
1:A:154:ILE:HG21	1:D:422:TYR:HD2	1.86	0.40
1:D:43:GLN:HE22	1:D:48:LYS:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/538 (88%)	457 (96%)	19 (4%)	0	100	100
1	B	475/538 (88%)	459 (97%)	15 (3%)	1 (0%)	52	82
1	C	472/538 (88%)	457 (97%)	15 (3%)	0	100	100
1	D	490/538 (91%)	465 (95%)	24 (5%)	1 (0%)	52	82
1	E	485/538 (90%)	465 (96%)	19 (4%)	1 (0%)	52	82
1	F	507/538 (94%)	480 (95%)	25 (5%)	2 (0%)	39	71
All	All	2905/3228 (90%)	2783 (96%)	117 (4%)	5 (0%)	52	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	ASP
1	D	273	ASP
1	E	482	ARG
1	F	453	PRO
1	F	415	ARG

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	382/430 (89%)	377 (99%)	5 (1%)	76	92
1	B	381/430 (89%)	378 (99%)	3 (1%)	86	96
1	C	378/430 (88%)	376 (100%)	2 (0%)	92	97
1	D	394/430 (92%)	387 (98%)	7 (2%)	66	89
1	E	391/430 (91%)	386 (99%)	5 (1%)	76	92
1	F	406/430 (94%)	400 (98%)	6 (2%)	72	91
All	All	2332/2580 (90%)	2304 (99%)	28 (1%)	78	93

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	126	TYR
1	A	205	PHE
1	A	481	ARG
1	A	482	ARG
1	B	82	ARG
1	B	126	TYR
1	B	205	PHE
1	C	488	GLU
1	C	519	ARG
1	D	37	LYS
1	D	126	TYR
1	D	205	PHE
1	D	210	GLU
1	D	273	ASP
1	D	343	ARG
1	D	478	ASP
1	E	19	ASP
1	E	29	GLU
1	E	82	ARG
1	E	157	TYR
1	E	482	ARG

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Mol	Chain	Res	Type
1	F	126	TYR
1	F	199	LYS
1	F	205	PHE
1	F	271	ASP
1	F	311	ASP
1	F	482	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	340	ASN
1	B	73	HIS
1	B	340	ASN
1	B	520	GLN
1	C	295	GLN
1	D	44	HIS
1	D	253	GLN
1	D	295	GLN
1	E	148	GLN
1	F	333	HIS
1	F	340	ASN

5.3.3　RNA (i)

There are no RNA molecules in this entry.

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

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

5.5　Carbohydrates (i)

There are no carbohydrates in this entry.

5.6　Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	HXC	A	601	-	48,57,57	4.02	9 (18%)	58,83,83	2.35	10 (17%)
2	HXC	B	601	-	48,57,57	4.01	10 (20%)	58,83,83	2.16	6 (10%)
2	HXC	E	601	-	48,57,57	4.02	10 (20%)	58,83,83	2.42	10 (17%)
2	HXC	F	601	-	48,57,57	4.05	10 (20%)	58,83,83	2.26	7 (12%)

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	HXC	A	601	-	-	0/52/72/72	0/3/3/3
2	HXC	B	601	-	-	0/52/72/72	0/3/3/3
2	HXC	E	601	-	-	0/52/72/72	0/3/3/3
2	HXC	F	601	-	-	0/52/72/72	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HXC	C2'-C1'	-16.74	1.27	1.53
2	F	601	HXC	C2'-C1'	-16.39	1.27	1.53
2	B	601	HXC	C2'-C1'	-16.37	1.27	1.53
2	E	601	HXC	C2'-C1'	-16.36	1.27	1.53
2	A	601	HXC	O4'-C4'	-6.54	1.30	1.45
2	E	601	HXC	O4'-C4'	-6.32	1.30	1.45
2	F	601	HXC	O4'-C4'	-6.31	1.30	1.45
2	B	601	HXC	O4'-C4'	-6.02	1.31	1.45
2	F	601	HXC	O3'-C3'	-3.63	1.32	1.44
2	E	601	HXC	O3'-C3'	-3.60	1.32	1.44
2	A	601	HXC	O3'-C3'	-3.58	1.32	1.44
2	B	601	HXC	O3'-C3'	-3.34	1.33	1.44
2	E	601	HXC	C6-N6	2.16	1.42	1.34
2	A	601	HXC	C2'-C3'	2.16	1.58	1.53
2	B	601	HXC	C6-N6	2.19	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HXC	C6-N6	2.20	1.43	1.34
2	F	601	HXC	C6-N6	2.21	1.43	1.34
2	A	601	HXC	O2'-C2'	2.24	1.48	1.43
2	E	601	HXC	C2'-C3'	2.33	1.58	1.53
2	F	601	HXC	C2'-C3'	2.44	1.58	1.53
2	E	601	HXC	O2'-C2'	2.67	1.49	1.43
2	F	601	HXC	O2'-C2'	2.70	1.49	1.43
2	B	601	HXC	O2'-C2'	2.85	1.49	1.43
2	B	601	HXC	C2'-C3'	2.94	1.59	1.53
2	E	601	HXC	CM2-CM1	2.97	1.53	1.50
2	F	601	HXC	CM2-CM1	3.39	1.53	1.50
2	B	601	HXC	CM2-CM1	3.43	1.53	1.50
2	E	601	HXC	CP3-NP1	4.29	1.43	1.33
2	B	601	HXC	CP3-NP1	4.46	1.44	1.33
2	F	601	HXC	CP3-NP1	4.56	1.44	1.33
2	A	601	HXC	CP3-NP1	4.56	1.44	1.33
2	B	601	HXC	CP6-NP2	6.09	1.46	1.33
2	E	601	HXC	CP6-NP2	6.18	1.46	1.33
2	F	601	HXC	CP6-NP2	6.38	1.46	1.33
2	A	601	HXC	CP6-NP2	6.44	1.47	1.33
2	A	601	HXC	O4'-C1'	18.33	1.67	1.41
2	B	601	HXC	O4'-C1'	18.53	1.67	1.41
2	E	601	HXC	O4'-C1'	18.67	1.67	1.41
2	F	601	HXC	O4'-C1'	18.69	1.67	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	HXC	N3-C2-N1	-10.55	120.58	128.87
2	A	601	HXC	N3-C2-N1	-10.36	120.73	128.87
2	B	601	HXC	N3-C2-N1	-10.22	120.84	128.87
2	E	601	HXC	N3-C2-N1	-9.57	121.36	128.87
2	E	601	HXC	OM2-CM1-CM2	-8.38	118.17	123.94
2	A	601	HXC	OM2-CM1-CM2	-8.19	118.30	123.94
2	F	601	HXC	OM2-CM1-CM2	-6.33	119.58	123.94
2	B	601	HXC	OM2-CM1-S	-4.68	119.12	122.83
2	B	601	HXC	OM2-CM1-CM2	-4.66	120.73	123.94
2	F	601	HXC	OM2-CM1-S	-3.90	119.74	122.83
2	F	601	HXC	C4'-O4'-C1'	-3.81	105.61	109.64
2	E	601	HXC	CM3-CM2-CM1	-3.46	108.01	113.12
2	E	601	HXC	OM2-CM1-S	-2.94	120.50	122.83
2	E	601	HXC	C4'-O4'-C1'	-2.67	106.81	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	HXC	CP2-NP1-CP3	-2.65	117.55	122.79
2	A	601	HXC	C4'-O4'-C1'	-2.54	106.95	109.64
2	A	601	HXC	CP4-CP5-NP2	-2.39	106.59	111.94
2	E	601	HXC	CP8-CPA-CPB	-2.34	105.47	108.50
2	A	601	HXC	OM2-CM1-S	-2.28	121.03	122.83
2	A	601	HXC	CP2-CP1-S	-2.27	105.44	111.47
2	A	601	HXC	O2'-C2'-C3'	-2.22	104.73	111.13
2	F	601	HXC	CP9-CPA-CPB	-2.01	105.90	108.50
2	F	601	HXC	CP1-S-CM1	2.05	109.41	102.09
2	B	601	HXC	O3'-P3-O33	2.09	112.47	107.48
2	B	601	HXC	O4'-C1'-N9	2.09	112.06	108.11
2	A	601	HXC	CP1-S-CM1	2.30	110.29	102.09
2	E	601	HXC	CP1-S-CM1	2.52	111.06	102.09
2	E	601	HXC	CP4-CP3-NP1	2.70	121.16	116.46
2	A	601	HXC	CP5-CP4-CP3	3.41	118.06	112.22
2	B	601	HXC	CM2-CM1-S	7.56	120.15	113.36
2	A	601	HXC	CM2-CM1-S	8.13	120.67	113.36
2	F	601	HXC	CM2-CM1-S	8.14	120.68	113.36
2	E	601	HXC	CM2-CM1-S	8.84	121.31	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HXC	5	0
2	B	601	HXC	5	0
2	E	601	HXC	11	0
2	F	601	HXC	10	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	482/538 (89%)	-0.27	3 (0%)	90	89	7, 18, 41, 68	0
1	B	481/538 (89%)	-0.40	3 (0%)	90	89	8, 19, 45, 67	0
1	C	478/538 (88%)	-0.31	1 (0%)	95	95	9, 22, 45, 74	0
1	D	496/538 (92%)	-0.36	5 (1%)	84	81	6, 18, 48, 75	0
1	E	493/538 (91%)	0.01	14 (2%)	56	51	10, 25, 61, 88	0
1	F	511/538 (94%)	-0.13	15 (2%)	55	49	9, 22, 62, 84	0
All	All	2941/3228 (91%)	-0.24	41 (1%)	78	75	6, 21, 51, 88	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	472	LYS	6.6
1	D	76	VAL	5.5
1	F	479	TYR	4.4
1	F	274	CYS	3.9
1	F	277	GLY	3.7
1	F	454	ILE	3.7
1	F	455	LEU	3.4
1	E	479	TYR	3.3
1	F	275	ALA	3.1
1	A	15	THR	3.1
1	F	273	ASP	3.1
1	F	471	VAL	3.1
1	F	476	VAL	3.1
1	E	478	ASP	2.9
1	E	483	PHE	2.9
1	E	450	SER	2.8
1	E	214	ALA	2.5
1	E	216	MET	2.5
1	A	273	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	79	GLY	2.4
1	F	276	PRO	2.4
1	E	80	ILE	2.4
1	F	214	ALA	2.3
1	E	75	THR	2.3
1	D	476	VAL	2.3
1	B	273	ASP	2.3
1	F	293	GLU	2.2
1	F	474	ASN	2.2
1	E	274	CYS	2.2
1	E	209	PRO	2.1
1	B	294	GLN	2.1
1	E	481	ARG	2.1
1	D	26	ALA	2.1
1	E	294	GLN	2.1
1	F	278	ILE	2.1
1	A	294	GLN	2.0
1	C	280	GLU	2.0
1	D	75	THR	2.0
1	B	293	GLU	2.0
1	E	110	LEU	2.0
1	E	449	ASN	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, 95th 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	HXC	F	601	55/55	0.86	0.33	2.62	23,63,98,106	0
2	HXC	E	601	55/55	0.90	0.38	2.22	36,70,97,100	0
2	HXC	A	601	55/55	0.95	0.22	1.28	13,37,60,73	0
2	HXC	B	601	55/55	0.96	0.16	-0.29	15,40,60,64	0

6.5 Other polymers (i)

There are no such residues in this entry.