



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:00 AM UTC

PDB ID : 5INI / pdb_00005ini
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)

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 ⓘ 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:

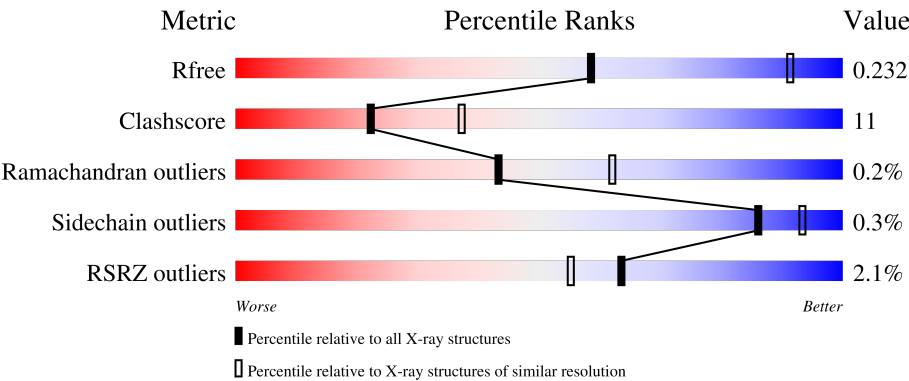
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 $\leq 5\%$. 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	% 74% 15% • 10%
1	B	538	% 75% 14% 11%
1	C	538	% 72% 16% 11%
1	D	538	2% 75% 16% • 8%
1	E	538	3% 74% 17% 8%

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Mol	Chain	Length	Quality of chain
1	F	538	4% 72% 21% • 5%

2 Entry composition

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

There are 36 discrepancies between the modelled and reference sequences:

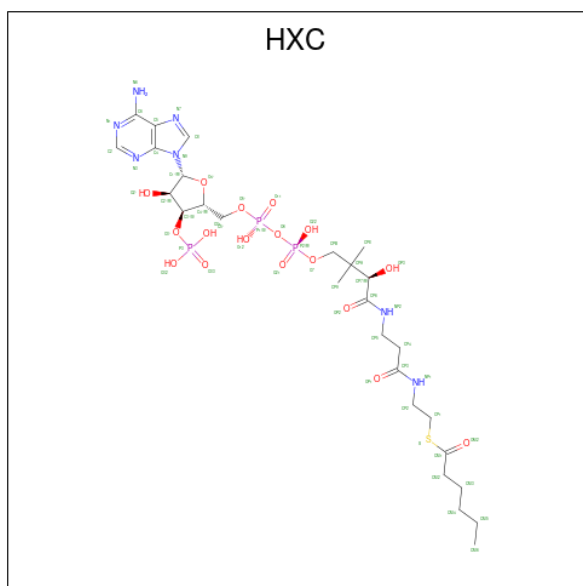
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP A0ACI9
A	-4	ILE	-	expression tag	UNP A0ACI9
A	-3	ASP	-	expression tag	UNP A0ACI9
A	-2	PRO	-	expression tag	UNP A0ACI9
A	-1	PHE	-	expression tag	UNP A0ACI9
A	0	THR	-	expression tag	UNP A0ACI9
B	-5	GLY	-	expression tag	UNP A0ACI9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

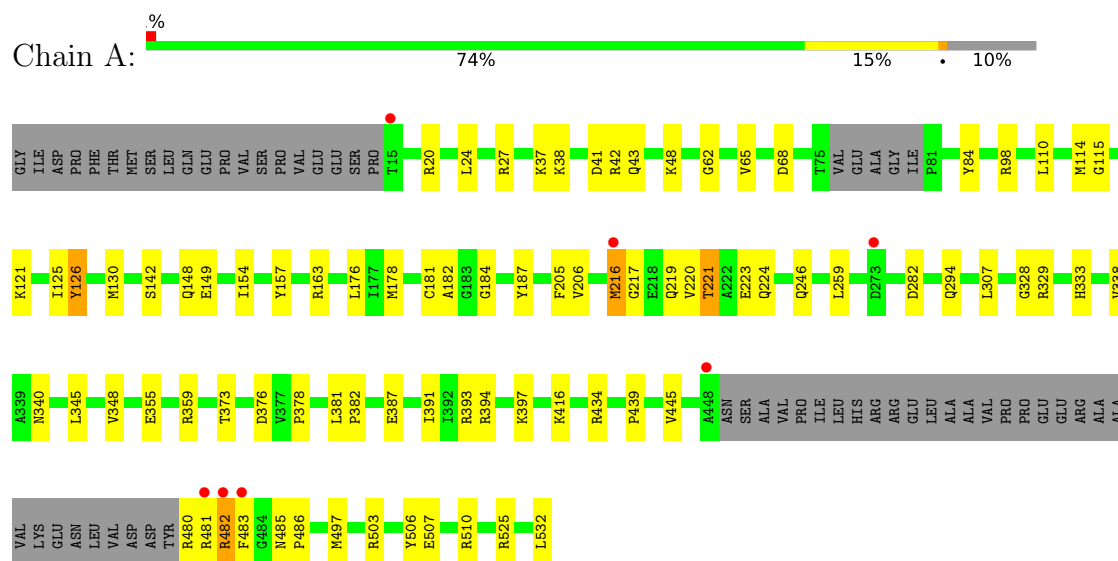
- Molecule 3 is water.

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		

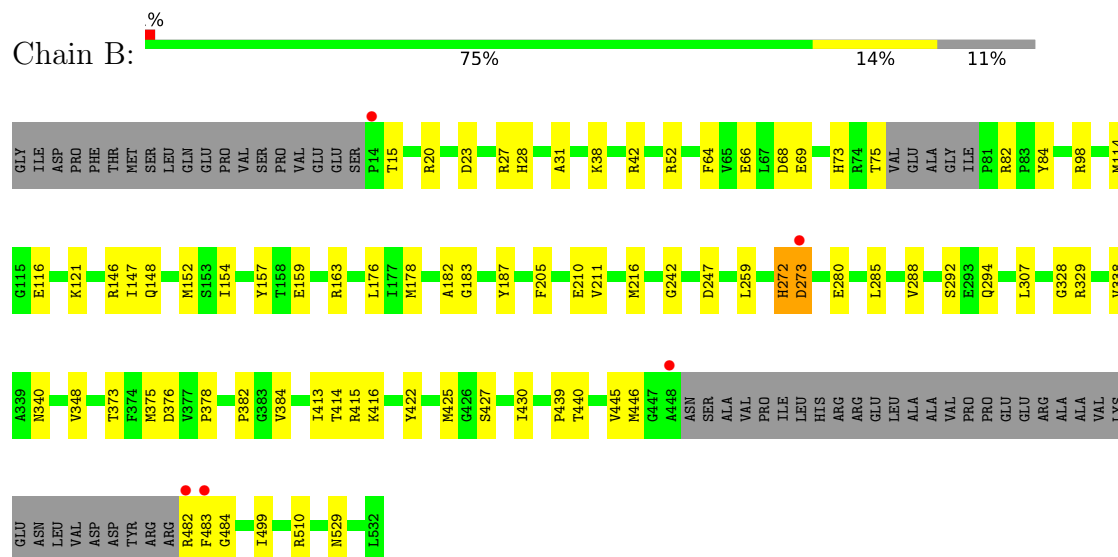
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

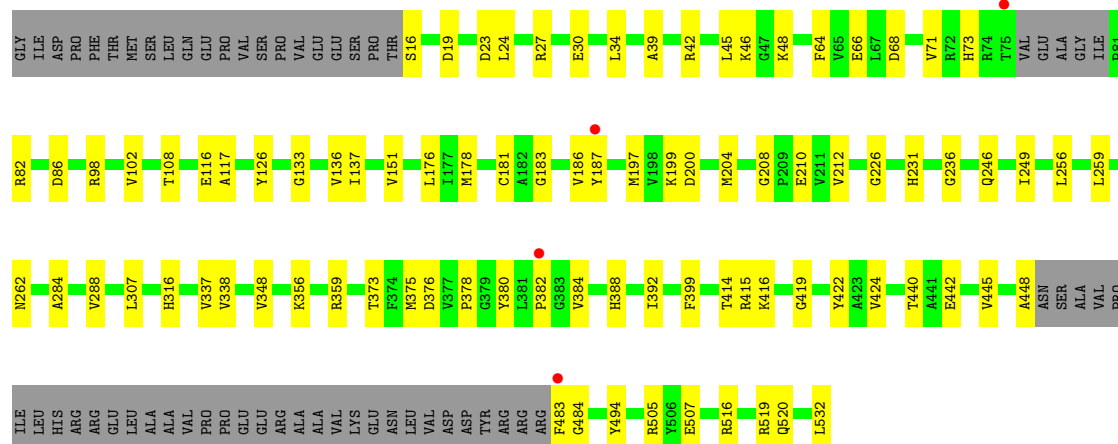
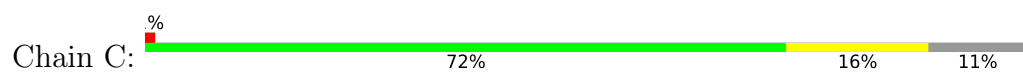
- Molecule 1: Putative carboxyl transferase



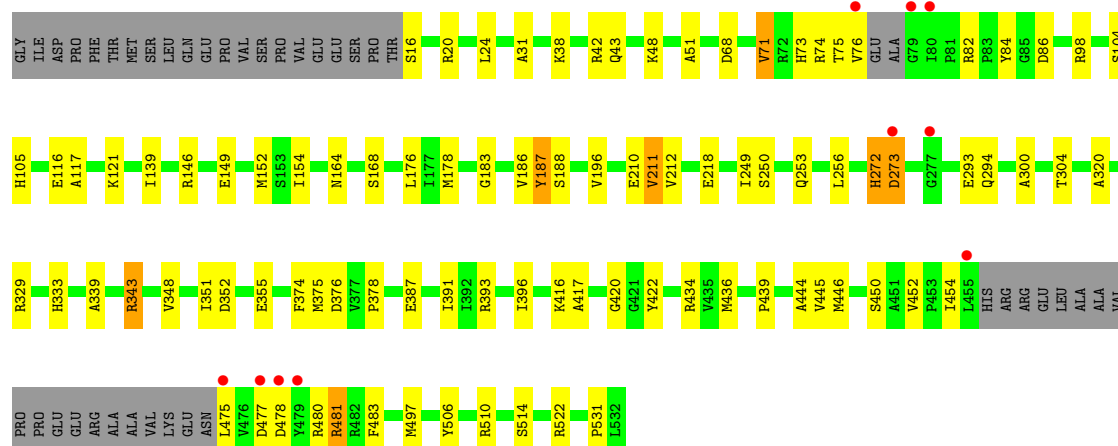
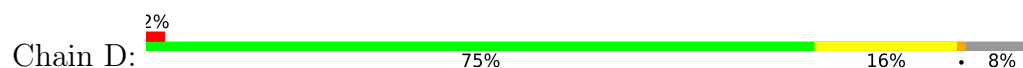
- Molecule 1: Putative carboxyl transferase



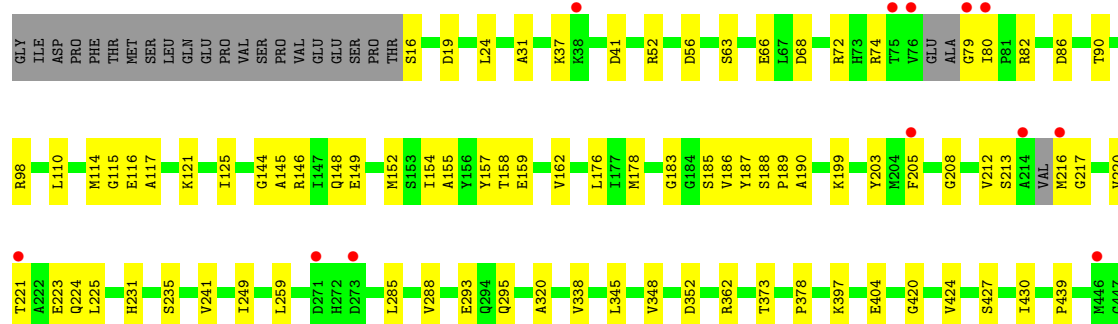
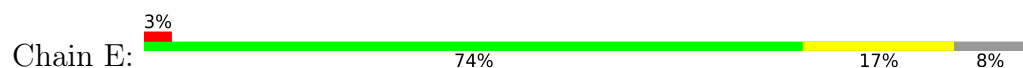
- Molecule 1: Putative carboxyl transferase

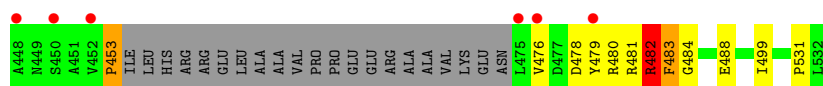


• Molecule 1: Putative carboxyl transferase

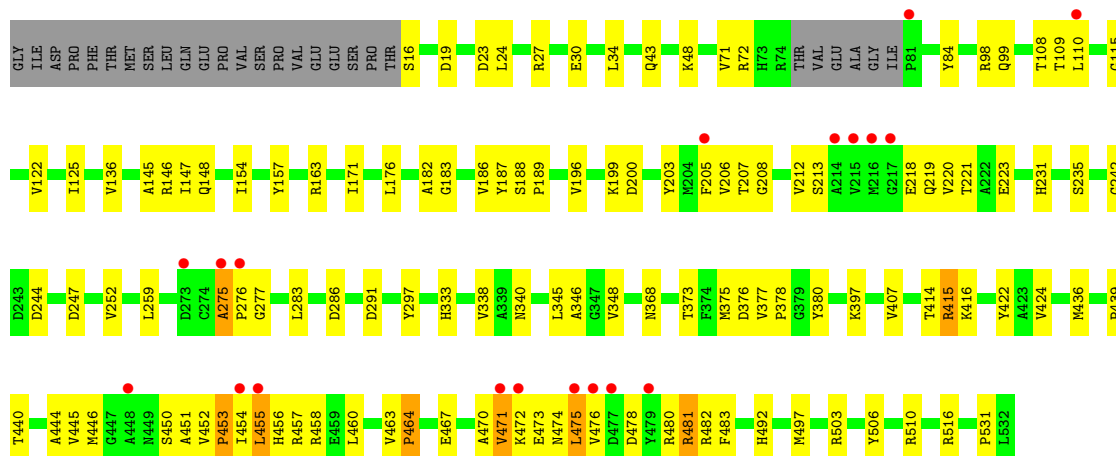
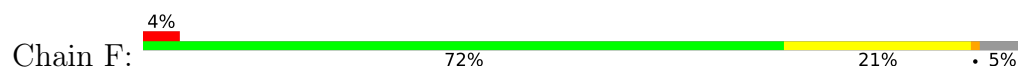


• Molecule 1: Putative carboxyl transferase





• Molecule 1: Putative carboxyl transferase



4 Data and refinement statistics

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 58.23 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (58.23-2.85) 95.5 (58.23-2.85)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.173 , 0.232 0.175 , 0.232	Depositor DCC
R_{free} test set	2000 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.26	1/3730 (0.0%)	0.48	1/5066 (0.0%)
1	B	0.22	0/3716	0.50	2/5049 (0.0%)
1	C	0.19	0/3690	0.45	0/5014
1	D	0.26	0/3836	0.60	7/5214 (0.1%)
1	E	0.40	4/3812 (0.1%)	0.58	5/5179 (0.1%)
1	F	0.37	3/3966 (0.1%)	0.63	7/5390 (0.1%)
All	All	0.29	8/22750 (0.0%)	0.55	22/30912 (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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	453	PRO	CA-CB	-8.32	1.36	1.53
1	E	453	PRO	CG-CD	7.44	1.76	1.50
1	F	464	PRO	N-CA	-6.96	1.36	1.46
1	F	471	VAL	CB-CG1	-5.73	1.33	1.52
1	A	221	THR	CB-CG2	-5.38	1.34	1.52
1	E	453	PRO	N-CD	-5.28	1.40	1.47
1	E	453	PRO	CA-C	5.18	1.63	1.52
1	F	464	PRO	CG-CD	5.04	1.67	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	464	PRO	N-CA-CB	12.32	109.63	103.22
1	F	471	VAL	N-CA-C	10.37	123.79	108.45
1	E	453	PRO	N-CA-CB	9.36	113.30	103.00
1	D	343	ARG	CG-CD-NE	-8.38	93.58	112.00
1	B	272	HIS	CA-C-N	7.16	134.59	121.70
1	B	272	HIS	C-N-CA	7.16	134.59	121.70
1	D	272	HIS	CA-C-N	6.74	133.84	121.70
1	D	272	HIS	C-N-CA	6.74	133.84	121.70
1	F	464	PRO	N-CD-CG	-6.62	93.27	103.20
1	F	455	LEU	N-CA-C	-6.47	92.88	111.00
1	E	482	ARG	CB-CG-CD	-6.46	96.44	111.30
1	E	453	PRO	N-CD-CG	-5.87	94.40	103.20
1	D	343	ARG	CB-CG-CD	-5.77	98.02	111.30
1	F	475	LEU	CD1-CG-CD2	-5.72	98.22	110.80
1	A	216	MET	N-CA-C	5.40	120.88	113.97
1	E	482	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	E	483	PHE	CA-CB-CG	5.31	119.11	113.80
1	D	211	VAL	CG1-CB-CG2	-5.30	99.13	110.80
1	D	187	TYR	CA-C-N	-5.25	109.00	121.80
1	D	187	TYR	C-N-CA	-5.25	109.00	121.80
1	F	275	ALA	CA-C-N	5.08	125.48	119.99
1	F	275	ALA	C-N-CA	5.08	125.48	119.99

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 ⓘ

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	74	0
1	B	3639	0	3581	77	0
1	C	3614	0	3553	67	0
1	D	3758	0	3705	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3735	0	3673	93	0
1	F	3884	0	3829	115	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	7	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	474	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 11.

All (474) 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:O4'	2:B:601:HXC:C1'	1.67	1.18
2:E:601:HXC:O4'	2:E:601:HXC:C1'	1.67	1.17
2:F:601:HXC:C1'	2:F:601:HXC:O4'	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
1:D:20:ARG:NH2	1:E:484:GLY:O	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:375:MET:HE1	1:C:422:TYR:HD1	1.48	0.77
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:C:197:MET:HE1	1:C:231:HIS:HD2	1.51	0.75
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: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:E:482:ARG:HD3	1:E:482:ARG:C	2.17	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:VAL:HG11	1:F:220:VAL:HG11	1.75	0.68
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:E:293:GLU:CD	1:E:293:GLU:H	2.03	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:D:375:MET:CE	1:D:422:TYR:HA	2.26	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: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:A:130:MET:HE1	1:A:163:ARG:HB3	1.79	0.63
1:C:42:ARG:HD2	1:C:46:LYS:HZ1	1.63	0.63
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:B:375:MET:HE1	1:B:422:TYR:HD1	1.64	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:D:452:VAL:C	1:D:454:ILE:H	2.06	0.63
1:D:375:MET:HE1	1:D:422:TYR:HA	1.79	0.63
1:C:483:PHE:N	3:C:608:HOH:O	2.32	0.63
1:D:434:ARG:HD2	1:D:497:MET:HE2	1.81	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:436:MET:HB3	1:D:497:MET:HE3	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
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:176:LEU:HD22	1:C:178:MET:HE3	1.82	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:B:378:PRO:HD3	1:B:416:LYS:HZ2	1.67	0.59
1:A:503:ARG:HG2	1:A:503:ARG:HH11	1.68	0.59
1:B:272:HIS:HB2	1:B:273:ASP:HB2	1.83	0.59
1:E:116:GLU:HB3	1:E:152:MET:HE3	1.84	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:OE1	1:C:246:GLN:N	2.30	0.58
1:F:163:ARG:HG3	1:F:163:ARG:HH11	1.68	0.58
1:D:164:ASN:OD1	1:D:188:SER:HB3	2.03	0.58
1:D:300:ALA:O	1:D:304:THR:HG23	2.04	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:246:GLN:CD	1:A:246:GLN:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:419:GLY:HA2	2:E:601:HXC:HP12	1.87	0.56
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:197:MET:HE1	1:C:231:HIS:CD2	2.38	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:B:176:LEU:HD22	1:B:178:MET:HE3	1.88	0.55
1:F:436:MET:HB3	1:F:497:MET:HE3	1.87	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: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:ND1	2.24	0.53
1:C:384:VAL:HG13	1:C:388:HIS:CE1	2.43	0.53
1:D:38:LYS:HZ1	1:D:42:ARG:HG3	1.71	0.53
1:C:181:CYS:HB3	1:C:204:MET:HG2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:ALA:O	1:C:288:VAL:HG23	2.09	0.52
1:B:378:PRO:CD	1:B:416:LYS:HZ2	2.21	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
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:F:414:THR:O	1:F:440:THR:OG1	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: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:20:ARG:NH2	1:B:484:GLY:O	2.43	0.50
1:A:480:ARG:HH12	1:A:483:PHE:HB2	1.75	0.50
2:B:601:HXC:O3'	1:F:455:LEU:HD11	2.11	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
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:A:223:GLU:CD	1:A:223:GLU:H	2.19	0.50
1:B:384:VAL:CG1	1:F:220:VAL:HG11	2.42	0.50
1:E:72:ARG:HH21	1:E:82:ARG:HG3	1.75	0.50
1:E:203:TYR:HE1	1:E:223:GLU:HG3	1.76	0.50
1:A:394:ARG:HA	1:A:397:LYS:HE3	1.94	0.50
1:B:375:MET:HE2	1:B:413:ILE:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ILE:HD11	1:F:445:VAL:HA	1.95	0.49
1:F:345:LEU:O	1:F:348:VAL:HG22	2.12	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:532:LEU:HD22	1:E:397:LYS:HD2	1.93	0.49
1:D:454:ILE:HG22	1:D:454:ILE:O	2.13	0.49
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:B:210:GLU:CD	1:B:210:GLU:H	2.18	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:A:130:MET:HE1	1:A:163:ARG:CB	2.44	0.47
1:D:210:GLU:CD	1:D:211:VAL:N	2.72	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:NE2	1:E:148:GLN:H	2.12	0.47
1:D:343:ARG:HE	1:D:343:ARG:HB3	0.84	0.47
1:E:148:GLN:H	1:E:148:GLN:CD	2.23	0.47
1:F:223:GLU:CD	1:F:223:GLU:H	2.22	0.47
1:A:126:TYR:HD2	1:A:130:MET:HE2	1.80	0.47
1:C:236:GLY:O	1:C:316:HIS:HE1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:ILE:O	1:D:253:GLN:HG3	2.14	0.47
1:E:203:TYR:CE1	1:E:223:GLU:HG3	2.48	0.47
1:F:163:ARG:HG3	1:F:163:ARG:NH1	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:A:176:LEU:HD22	1:A:178:MET:HE3	1.97	0.47
1:C:210:GLU:H	1:C:210:GLU:CD	2.23	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:F:470:ALA:C	1:F:471:VAL:HG13	2.38	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:F:223:GLU:CD	1:F:223:GLU:N	2.73	0.46
1:C:419:GLY:CA	2:E:601:HXC:HP12	2.45	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: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
1:A:497:MET:HE1	1:A:507:GLU:OE1	2.15	0.46
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: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:E:293:GLU:CD	1:E:293:GLU:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:LYS:HE2	1:F:200:ASP:OD1	2.16	0.45
1:A:125:ILE:HD12	1:A:125:ILE:HA	1.79	0.45
1:A:221:THR:HB	1:A:224:GLN:CD	2.42	0.45
1:A:482:ARG:HA	1:A:482:ARG:NH1	2.32	0.45
1:D:375:MET:HE3	1:D:422:TYR:HA	1.96	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:D:176:LEU:HD22	1:D:178:MET:HE3	1.97	0.44
1:B:147:ILE:CG2	1:F:454:ILE:HG12	2.48	0.44
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:HG3	1:A:163:ARG:NH1	2.33	0.44
1:B:98:ARG:NH2	1:B:259:LEU:O	2.39	0.44
1:E:176:LEU:HD22	1:E:178:MET:HE3	2.00	0.44
1:B:152:MET:HE3	1:F:492:HIS:CE1	2.52	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:C:178:MET:HE1	1:C:249:ILE:HG13	2.00	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:C:197:MET:HE3	1:C:204:MET:HG3	1.98	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:148:GLN:OE1	2:A:601:HXC:H2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:PRO:HB3	1:A:416:LYS:HD2	1.99	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:F:450:SER:C	1:F:452:VAL:N	2.76	0.43
1:C:181:CYS:O	1:C:204:MET:HA	2.18	0.43
1:D:210:GLU:CD	1:D:211:VAL:H	2.26	0.43
1:E:63:SER:HA	1:F:510:ARG:HH12	1.84	0.43
1:F:16:SER:HB3	1:F:19:ASP:CG	2.43	0.43
1:F:182:ALA:HB3	2:F:601:HXC:HP91	1.99	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:F:297:TYR:OH	1:F:376:ASP:OD2	2.28	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:HD23	1:C:45:LEU:O	2.18	0.43
1:D:348:VAL:HG12	1:D:378:PRO:HG2	2.01	0.43
1:E:178:MET:HE1	1:E:249:ILE:HG13	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:D:446:MET:HE3	1:D:446:MET:HB2	1.91	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:HA	1:A:219:GLN:NE2	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:B:338:VAL:O	1:B:373:THR:HA	2.19	0.43
1:D:16:SER:O	1:D:20:ARG:HG3	2.19	0.42
1:E:16:SER:OG	1:F:291:ASP:OD1	2.25	0.42
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: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: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: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:OE1	1:B:148:GLN:N	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:481:ARG:NE	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:HG3	1:B:329:ARG:HH11	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:B:446:MET:HE2	1:F:147:ILE:HD13	2.01	0.42
1:C:399:PHE:HD2	1:C:424:VAL:HG12	1.85	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:149:GLU:HB3	1:D:152:MET:HE3	2.02	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
1:E:199:LYS:HD2	1:E:241:VAL:HG11	2.02	0.41
1:A:130:MET:HE1	1:A:163:ARG:CG	2.49	0.41
1:B:159:GLU:HG3	1:B:163:ARG:NH1	2.36	0.41
1:D:31:ALA:HB2	1:D:84:TYR:CD2	2.55	0.41
1:D:104:SER:HA	1:D:139:ILE:HB	2.02	0.41
1:F:244:ASP:OD1	1:F:244:ASP:N	2.52	0.41
1:C:199:LYS:NZ	1:C:200:ASP:OD2	2.50	0.41
1:F:148:GLN:OE1	2:F:601:HXC:H2	2.20	0.41
1:F:242:GLY:HA2	1:F:247:ASP:OD2	2.20	0.41
1:D:51:ALA:HB2	1:D:105:HIS:O	2.21	0.41
1:D:178:MET:HE1	1:D:249:ILE:HG13	2.02	0.41
1:E:52:ARG:HH22	1:E:66:GLU:CD	2.26	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:HD12	1:D:396:ILE:HA	1.91	0.41
1:F:375:MET:HG3	1:F:377:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ARG:O	1:C:42:ARG:HG3	2.18	0.41
1:D:477:ASP:OD1	1:D:477:ASP:C	2.64	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:E:481:ARG:O	1:E:482:ARG:C	2.63	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:142:SER:O	1:A:181:CYS:HA	2.21	0.41
1:A:187:TYR:HB3	2:A:601:HXC:HM52	2.03	0.41
1:B:422:TYR:HD2	1:F:154:ILE:HG21	1.86	0.41
1:C:48:LYS:NZ	3:C:607:HOH:O	2.30	0.41
1:D:187:TYR:N	1:D:187:TYR:CD1	2.88	0.41
1:D:375:MET:HE2	1:D:417:ALA:CB	2.51	0.41
1:D:446:MET:HG2	1:D:450:SER:HB2	2.03	0.41
1:C:392:ILE:HG22	1:E:190:ALA:HB2	2.03	0.41
1:D:439:PRO:HG3	1:F:24:LEU:HD22	2.02	0.41
1:F:231:HIS:HA	1:F:235:SER:OG	2.20	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:OE2	1:E:223:GLU:N	2.46	0.40
1:F:275:ALA:HA	1:F:276:PRO:HD3	1.83	0.40
1:D:480:ARG:C	1:D:481:ARG:HD3	2.46	0.40
1:E:125:ILE:HA	1:E:125:ILE:HD13	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:B:216:MET:HE3	1:B:216:MET:HB3	1.93	0.40
1:B:376:ASP:CG	1:B:415:ARG:HB3	2.46	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
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:375:MET:HE1	1:B:422:TYR:CD1	2.49	0.40
1:A:154:ILE:HG21	1:D:422:TYR:HD2	1.86	0.40
1:B:28:HIS:ND1	1:B:69:GLU:OE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:LYS:HE3	1:B:416:LYS:HB2	1.87	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%)	43	62
1	C	472/538 (88%)	457 (97%)	15 (3%)	0	100	100
1	D	490/538 (91%)	465 (95%)	24 (5%)	1 (0%)	43	62
1	E	485/538 (90%)	465 (96%)	19 (4%)	1 (0%)	43	62
1	F	507/538 (94%)	480 (95%)	25 (5%)	2 (0%)	30	48
All	All	2905/3228 (90%)	2783 (96%)	117 (4%)	5 (0%)	43	62

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%)	380 (100%)	2 (0%)	81	90
1	B	381/430 (89%)	381 (100%)	0	100	100
1	C	378/430 (88%)	378 (100%)	0	100	100
1	D	394/430 (92%)	393 (100%)	1 (0%)	86	93
1	E	391/430 (91%)	390 (100%)	1 (0%)	86	93
1	F	406/430 (94%)	403 (99%)	3 (1%)	76	87
All	All	2332/2580 (90%)	2325 (100%)	7 (0%)	86	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	TYR
1	A	482	ARG
1	D	71	VAL
1	E	295	GLN
1	F	71	VAL
1	F	108	THR
1	F	482	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	44	HIS
1	A	166	HIS
1	A	340	ASN
1	A	344	HIS
1	A	492	HIS
1	B	73	HIS
1	B	166	HIS
1	B	272	HIS
1	B	333	HIS
1	B	340	ASN
1	C	164	ASN
1	C	295	GLN
1	C	344	HIS

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Mol	Chain	Res	Type
1	D	43	GLN
1	D	44	HIS
1	D	92	HIS
1	D	224	GLN
1	D	253	GLN
1	D	295	GLN
1	E	43	GLN
1	E	73	HIS
1	E	148	GLN
1	E	237	ASN
1	E	344	HIS
1	E	492	HIS
1	F	333	HIS
1	F	340	ASN
1	F	449	ASN
1	F	456	HIS
1	F	492	HIS

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 oligosaccharides 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	-	55,57,57	2.56	9 (16%)	77,83,83	1.80	14 (18%)
2	HXC	E	601	-	55,57,57	2.56	10 (18%)	77,83,83	1.84	15 (19%)
2	HXC	F	601	-	55,57,57	2.60	10 (18%)	77,83,83	1.73	13 (16%)
2	HXC	B	601	-	55,57,57	2.57	10 (18%)	77,83,83	1.78	16 (20%)

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	-	-	19/56/72/72	0/3/3/3
2	HXC	E	601	-	-	13/56/72/72	0/3/3/3
2	HXC	F	601	-	-	19/56/72/72	0/3/3/3
2	HXC	B	601	-	-	16/56/72/72	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	HXC	O4'-C1'	11.21	1.67	1.42
2	E	601	HXC	O4'-C1'	11.20	1.67	1.42
2	B	601	HXC	O4'-C1'	11.12	1.67	1.42
2	A	601	HXC	O4'-C1'	10.99	1.67	1.42
2	A	601	HXC	C2'-C1'	-8.41	1.27	1.53
2	F	601	HXC	C2'-C1'	-8.24	1.27	1.53
2	B	601	HXC	C2'-C1'	-8.23	1.27	1.53
2	E	601	HXC	C2'-C1'	-8.23	1.27	1.53
2	A	601	HXC	O4'-C4'	-6.73	1.30	1.45
2	E	601	HXC	O4'-C4'	-6.49	1.30	1.45
2	F	601	HXC	O4'-C4'	-6.49	1.30	1.45
2	B	601	HXC	O4'-C4'	-6.19	1.31	1.45
2	A	601	HXC	CP6-NP2	5.70	1.47	1.33
2	F	601	HXC	CP6-NP2	5.65	1.46	1.33
2	E	601	HXC	CP6-NP2	5.47	1.46	1.33
2	B	601	HXC	CP6-NP2	5.39	1.46	1.33
2	A	601	HXC	CP3-NP1	4.66	1.44	1.33
2	F	601	HXC	CP3-NP1	4.66	1.44	1.33
2	B	601	HXC	CP3-NP1	4.56	1.44	1.33
2	E	601	HXC	CP3-NP1	4.38	1.43	1.33
2	F	601	HXC	C6-N6	3.51	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HXC	C6-N6	3.48	1.43	1.34
2	B	601	HXC	C6-N6	3.47	1.43	1.34
2	E	601	HXC	C6-N6	3.42	1.42	1.34
2	F	601	HXC	O3'-C3'	-3.36	1.32	1.44
2	E	601	HXC	O3'-C3'	-3.34	1.32	1.44
2	A	601	HXC	O3'-C3'	-3.31	1.32	1.44
2	B	601	HXC	O3'-C3'	-3.09	1.33	1.44
2	B	601	HXC	C2'-C3'	3.08	1.59	1.53
2	B	601	HXC	CM2-CM1	2.78	1.53	1.50
2	F	601	HXC	CM2-CM1	2.74	1.53	1.50
2	B	601	HXC	O2'-C2'	2.71	1.49	1.43
2	F	601	HXC	O2'-C2'	2.57	1.49	1.43
2	F	601	HXC	C2'-C3'	2.56	1.58	1.53
2	E	601	HXC	O2'-C2'	2.54	1.49	1.43
2	E	601	HXC	C2'-C3'	2.45	1.58	1.53
2	E	601	HXC	CM2-CM1	2.39	1.53	1.50
2	A	601	HXC	C2'-C3'	2.28	1.58	1.53
2	A	601	HXC	O2'-C2'	2.13	1.48	1.43

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	HXC	CM2-CM1-S	6.63	121.31	113.40
2	F	601	HXC	CM2-CM1-S	6.10	120.68	113.40
2	A	601	HXC	CM2-CM1-S	6.10	120.67	113.40
2	B	601	HXC	CM2-CM1-S	5.66	120.15	113.40
2	F	601	HXC	N1-C2-N3	-5.28	120.58	128.58
2	A	601	HXC	N1-C2-N3	-5.19	120.73	128.58
2	B	601	HXC	N1-C2-N3	-5.11	120.84	128.58
2	B	601	HXC	C5-C4-N3	-5.05	119.76	126.72
2	E	601	HXC	OM2-CM1-CM2	-5.03	118.17	123.98
2	A	601	HXC	OM2-CM1-CM2	-4.92	118.30	123.98
2	F	601	HXC	C5-C4-N3	-4.90	119.97	126.72
2	A	601	HXC	C5-C4-N3	-4.84	120.05	126.72
2	E	601	HXC	N1-C2-N3	-4.77	121.36	128.58
2	E	601	HXC	C5-C4-N3	-4.60	120.38	126.72
2	F	601	HXC	OM2-CM1-CM2	-3.81	119.58	123.98
2	A	601	HXC	N9-C8-N7	-3.64	108.77	113.94
2	A	601	HXC	N3-C4-N9	3.64	133.36	127.17
2	B	601	HXC	N3-C4-N9	3.61	133.30	127.17
2	B	601	HXC	N9-C8-N7	-3.61	108.82	113.94
2	E	601	HXC	N9-C8-N7	-3.55	108.91	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	HXC	C2-N3-C4	3.50	120.37	111.83
2	F	601	HXC	N9-C8-N7	-3.47	109.02	113.94
2	B	601	HXC	C2-N3-C4	3.46	120.28	111.83
2	F	601	HXC	N3-C4-N9	3.42	132.98	127.17
2	A	601	HXC	CP5-CP4-CP3	3.40	118.06	112.39
2	A	601	HXC	C2-N3-C4	3.39	120.12	111.83
2	B	601	HXC	C5-N7-C8	3.30	108.64	103.45
2	E	601	HXC	N3-C4-N9	3.23	132.65	127.17
2	E	601	HXC	C2-N3-C4	3.19	119.62	111.83
2	E	601	HXC	CP1-S-CM1	3.12	111.06	101.84
2	A	601	HXC	C5-N7-C8	3.04	108.23	103.45
2	F	601	HXC	C5-N7-C8	3.04	108.23	103.45
2	B	601	HXC	C4-C5-N7	-2.94	107.22	110.58
2	E	601	HXC	C5-N7-C8	2.93	108.05	103.45
2	A	601	HXC	CP1-S-CM1	2.86	110.29	101.84
2	E	601	HXC	CP2-NP1-CP3	-2.83	117.55	122.82
2	A	601	HXC	C4-N9-C8	2.82	108.70	105.74
2	B	601	HXC	OM2-CM1-CM2	-2.82	120.73	123.98
2	B	601	HXC	OM2-CM1-S	-2.80	119.12	122.68
2	F	601	HXC	C4-C5-N7	-2.71	107.48	110.58
2	E	601	HXC	CP4-CP3-NP1	2.64	121.16	116.34
2	F	601	HXC	CP1-S-CM1	2.56	109.41	101.84
2	E	601	HXC	C4-C5-N7	-2.55	107.67	110.58
2	E	601	HXC	C4-N9-C8	2.54	108.41	105.74
2	A	601	HXC	CP4-CP5-NP2	-2.54	106.59	112.00
2	B	601	HXC	C4-N9-C8	2.52	108.39	105.74
2	A	601	HXC	C4-C5-N7	-2.52	107.71	110.58
2	F	601	HXC	C4-N9-C8	2.37	108.23	105.74
2	F	601	HXC	OM2-CM1-S	-2.31	119.74	122.68
2	B	601	HXC	CP1-S-CM1	2.31	108.66	101.84
2	A	601	HXC	O2'-C2'-C3'	-2.31	104.73	111.19
2	B	601	HXC	O4'-C1'-C2'	-2.17	101.97	106.62
2	B	601	HXC	O7-CPB-CPA	-2.14	107.10	110.55
2	E	601	HXC	CP5-CP4-CP3	-2.09	108.91	112.39
2	B	601	HXC	C2'-C3'-C4'	-2.08	99.60	103.24
2	B	601	HXC	O4'-C1'-N9	2.07	112.06	108.09
2	E	601	HXC	CP5-NP2-CP6	-2.04	118.88	122.55
2	F	601	HXC	CP9-CPA-CP7	2.02	112.21	108.77

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HXC	CPB-O7-P2-O6
2	A	601	HXC	CPB-O7-P2-O22
2	A	601	HXC	CP7-CPA-CPB-O7
2	A	601	HXC	CP9-CPA-CPB-O7
2	A	601	HXC	CP8-CPA-CPB-O7
2	A	601	HXC	CP6-CP7-CPA-CPB
2	A	601	HXC	OP3-CP7-CPA-CP9
2	A	601	HXC	CP6-CP7-CPA-CP9
2	A	601	HXC	CP6-CP7-CPA-CP8
2	A	601	HXC	CP1-CP2-NP1-CP3
2	A	601	HXC	S-CP1-CP2-NP1
2	A	601	HXC	CP2-CP1-S-CM1
2	A	601	HXC	CM1-CM2-CM3-CM4
2	B	601	HXC	C5'-O5'-P1-O12
2	B	601	HXC	C5'-O5'-P1-O6
2	B	601	HXC	CPB-O7-P2-O6
2	B	601	HXC	CPB-O7-P2-O21
2	B	601	HXC	CPB-O7-P2-O22
2	B	601	HXC	CP7-CPA-CPB-O7
2	B	601	HXC	CP9-CPA-CPB-O7
2	B	601	HXC	CP8-CPA-CPB-O7
2	B	601	HXC	CP2-CP1-S-CM1
2	E	601	HXC	C3'-C4'-C5'-O5'
2	E	601	HXC	O4'-C4'-C5'-O5'
2	E	601	HXC	CP7-CPA-CPB-O7
2	E	601	HXC	CP9-CPA-CPB-O7
2	E	601	HXC	CP8-CPA-CPB-O7
2	E	601	HXC	S-CP1-CP2-NP1
2	E	601	HXC	CM1-CM2-CM3-CM4
2	F	601	HXC	O4'-C4'-C5'-O5'
2	F	601	HXC	C5'-O5'-P1-O11
2	F	601	HXC	C5'-O5'-P1-O6
2	F	601	HXC	CP7-CPA-CPB-O7
2	F	601	HXC	CP9-CPA-CPB-O7
2	F	601	HXC	CP8-CPA-CPB-O7
2	F	601	HXC	OP3-CP7-CPA-CPB
2	F	601	HXC	CP6-CP7-CPA-CPB
2	F	601	HXC	OP3-CP7-CPA-CP9
2	F	601	HXC	S-CP1-CP2-NP1
2	F	601	HXC	CM1-CM2-CM3-CM4
2	B	601	HXC	O4'-C4'-C5'-O5'
2	F	601	HXC	C3'-C4'-C5'-O5'
2	A	601	HXC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A	601	HXC	CP3-CP4-CP5-NP2
2	F	601	HXC	CM3-CM4-CM5-CM6
2	A	601	HXC	OP3-CP7-CPA-CP8
2	F	601	HXC	OP3-CP7-CPA-CP8
2	B	601	HXC	C3'-O3'-P3-O31
2	B	601	HXC	C3'-C4'-C5'-O5'
2	B	601	HXC	CM3-CM4-CM5-CM6
2	E	601	HXC	NP2-CP6-CP7-OP3
2	F	601	HXC	CP1-CP2-NP1-CP3
2	E	601	HXC	OM2-CM1-S-CP1
2	A	601	HXC	C3'-C4'-C5'-O5'
2	E	601	HXC	CM2-CM1-S-CP1
2	F	601	HXC	CM2-CM3-CM4-CM5
2	F	601	HXC	CP6-CP7-CPA-CP9
2	E	601	HXC	CM2-CM3-CM4-CM5
2	E	601	HXC	OP2-CP6-CP7-OP3
2	E	601	HXC	CP2-CP1-S-CM1
2	A	601	HXC	OP3-CP7-CPA-CPB
2	F	601	HXC	C5'-O5'-P1-O12
2	B	601	HXC	C3'-O3'-P3-O33
2	A	601	HXC	P1-O6-P2-O22
2	F	601	HXC	CP6-CP7-CPA-CP8
2	B	601	HXC	C3'-O3'-P3-O32
2	B	601	HXC	CP1-CP2-NP1-CP3

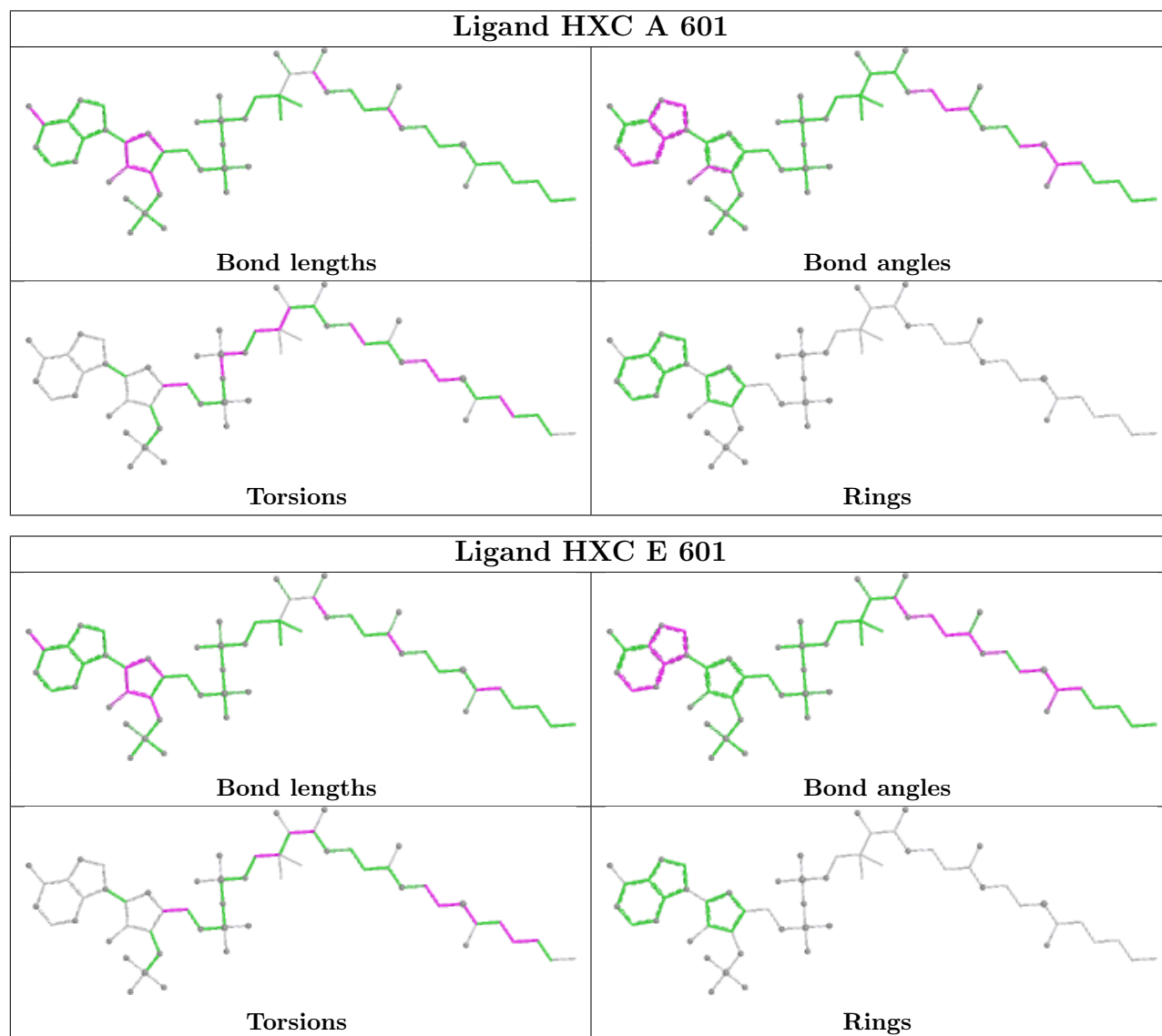
There are no ring outliers.

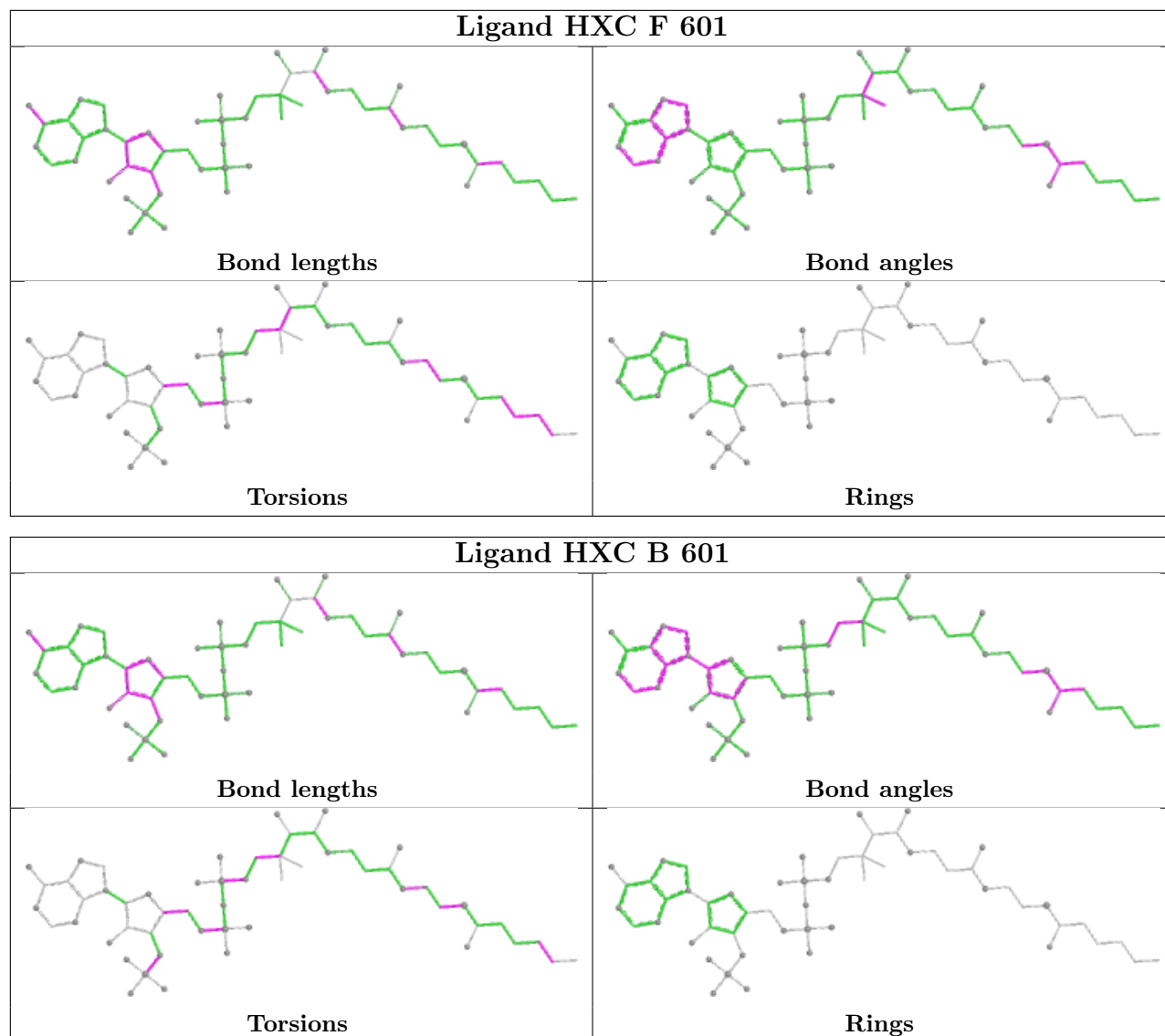
4 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HXC	5	0
2	E	601	HXC	11	0
2	F	601	HXC	10	0
2	B	601	HXC	5	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 than 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.





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, 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%)	-0.45	7 (1%) 72 65	7, 18, 41, 68	0
1	B	481/538 (89%)	-0.42	5 (1%) 79 74	8, 19, 45, 67	0
1	C	478/538 (88%)	-0.35	4 (0%) 82 78	9, 22, 45, 74	0
1	D	496/538 (92%)	-0.36	10 (2%) 65 57	6, 18, 48, 75	0
1	E	493/538 (91%)	-0.14	18 (3%) 45 35	10, 25, 61, 88	0
1	F	511/538 (94%)	-0.21	19 (3%) 45 35	9, 22, 62, 84	0
All	All	2941/3228 (91%)	-0.32	63 (2%) 63 55	6, 21, 51, 88	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	454	ILE	5.5
1	F	472	LYS	5.5
1	E	80	ILE	4.7
1	D	475	LEU	4.4
1	F	448	ALA	3.9
1	F	476	VAL	3.8
1	C	483	PHE	3.7
1	F	455	LEU	3.7
1	F	275	ALA	3.7
1	B	483	PHE	3.4
1	F	477	ASP	3.4
1	C	382	PRO	3.3
1	D	479	TYR	3.3
1	F	471	VAL	3.2
1	F	479	TYR	3.2
1	E	76	VAL	3.2
1	C	75	THR	3.2
1	E	216	MET	3.2
1	B	14	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	476	VAL	3.0
1	E	479	TYR	3.0
1	D	76	VAL	2.9
1	F	273	ASP	2.9
1	E	475	LEU	2.9
1	B	273	ASP	2.8
1	E	450	SER	2.8
1	E	214	ALA	2.8
1	D	478	ASP	2.7
1	E	448	ALA	2.6
1	D	79	GLY	2.6
1	E	271	ASP	2.6
1	E	452	VAL	2.6
1	A	448	ALA	2.6
1	B	482	ARG	2.6
1	D	455	LEU	2.6
1	F	217	GLY	2.6
1	A	216	MET	2.6
1	D	273	ASP	2.5
1	D	80	ILE	2.5
1	B	448	ALA	2.5
1	F	110	LEU	2.5
1	A	482	ARG	2.5
1	A	15	THR	2.5
1	C	187	TYR	2.4
1	F	81	PRO	2.3
1	A	481	ARG	2.3
1	F	215	VAL	2.3
1	F	205	PHE	2.3
1	F	475	LEU	2.3
1	D	277	GLY	2.3
1	E	79	GLY	2.3
1	F	216	MET	2.3
1	E	38	LYS	2.2
1	F	214	ALA	2.2
1	E	273	ASP	2.2
1	F	276	PRO	2.2
1	E	205	PHE	2.2
1	A	273	ASP	2.1
1	D	477	ASP	2.1
1	E	75	THR	2.1
1	E	221	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	446	MET	2.0
1	A	483	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

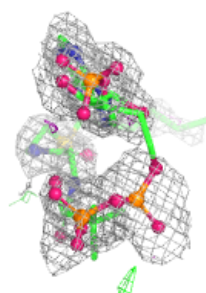
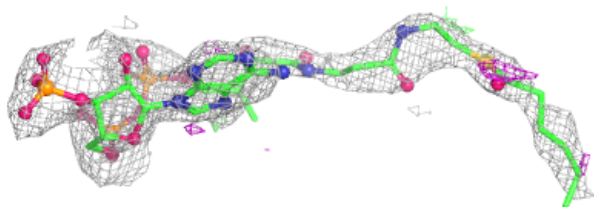
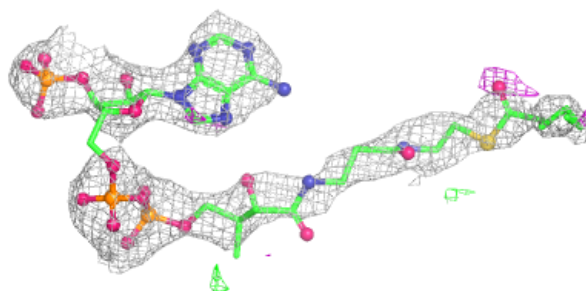
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HXC	F	601	55/55	0.78	0.15	23,63,98,106	0
2	HXC	E	601	55/55	0.82	0.14	36,70,97,100	0
2	HXC	A	601	55/55	0.92	0.10	13,37,60,73	0
2	HXC	B	601	55/55	0.94	0.09	15,40,60,64	0

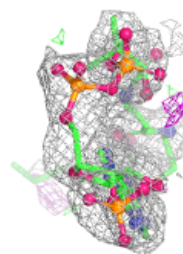
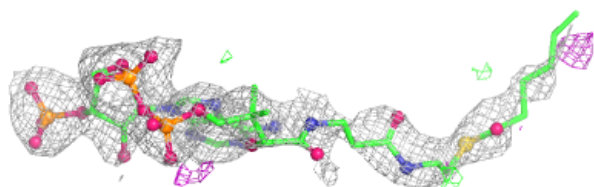
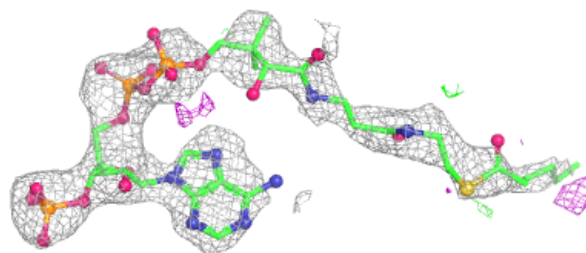
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HXC F 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

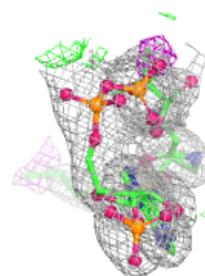
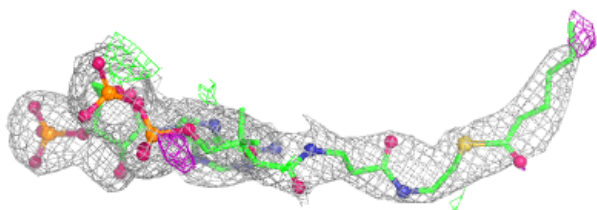
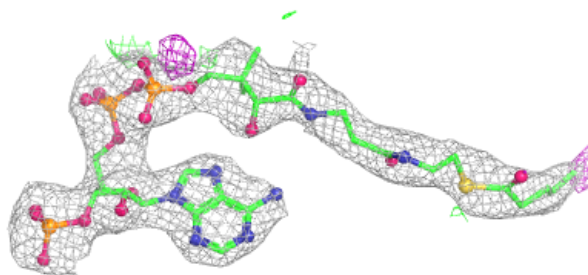
**Electron density around HXC E 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

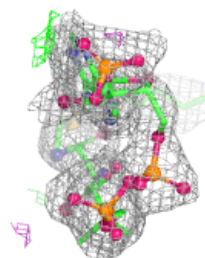
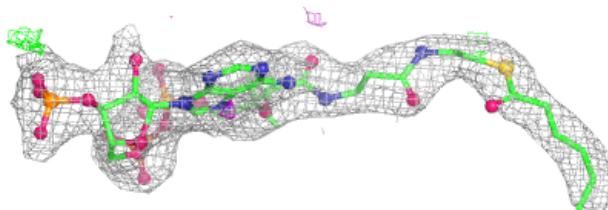
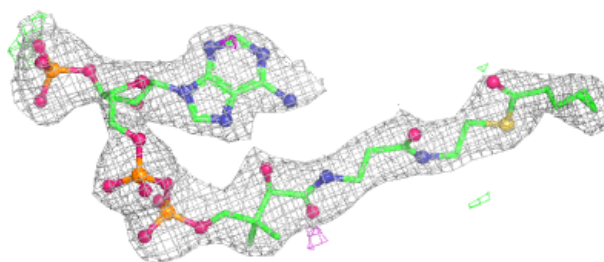


Electron density around HXC A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around HXC B 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.