



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:16 AM GMT

PDB ID : 1HV5
Title : CRYSTAL STRUCTURE OF THE STROMELYSIN-3 (MMP-11) CATALYTIC DOMAIN COMPLEXED WITH A PHOSPHINIC INHIBITOR
Authors : Gall, A.L.; Ruff, M.; Kannan, R.; Cuniasse, P.; Yiotakis, A.; Dive, V.; Rio, M.C.; Basset, P.; Moras, D.
Deposited on : 2001-01-08
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

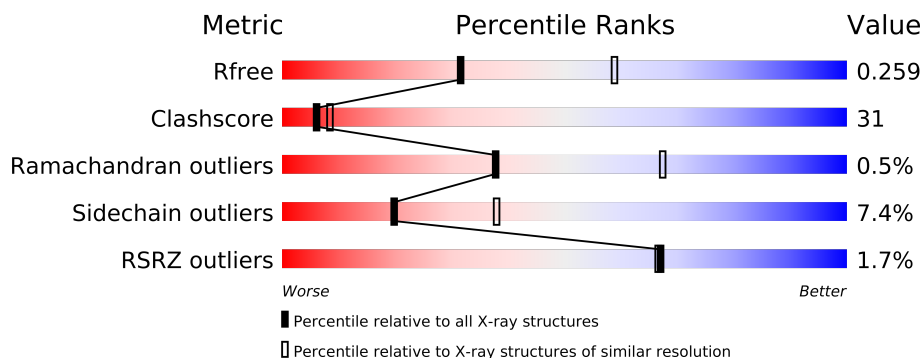
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	165	
1	B	165	
1	C	165	
1	D	165	
1	E	165	
1	F	165	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	CPS	B	5002	-	X
4	CPS	E	5005	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	CPS	F	5091	-	X
5	RXP	A	6001	-	X
5	RXP	B	6002	-	X
5	RXP	C	6003	-	X
5	RXP	D	6004	-	X
5	RXP	E	6005	-	X
5	RXP	F	6006	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10772 atoms, of which 0 are hydrogen and 0 are deuterium.

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 STROMELYSIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			
1	B	164	Total	C	N	O	S	0	0	0
			1342	863	236	240	3			
1	C	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			
1	D	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			
1	E	165	Total	C	N	O	S	0	0	0
			1352	868	238	243	3			
1	F	162	Total	C	N	O	S	0	0	0
			1324	852	231	238	3			

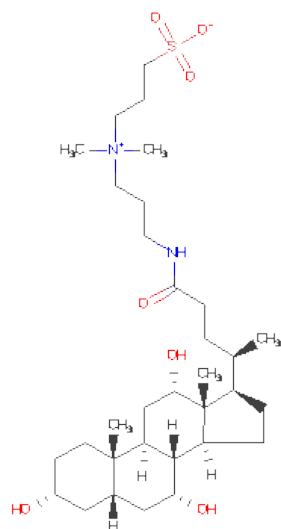
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



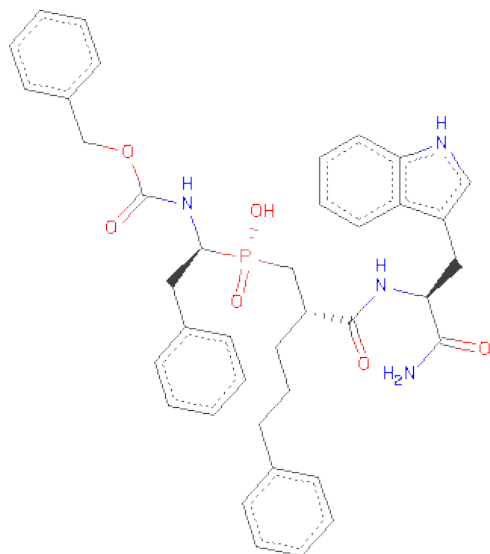
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 26 23 3	4	0
4	B	1	Total C O 26 23 3	4	0
4	C	1	Total C O 26 23 3	4	0
4	D	1	Total C O 26 23 3	4	0
4	E	1	Total C O 26 23 3	4	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O			4	0
			26	23	3				
4	B	1	Total	C	O			4	0
			26	23	3				
4	C	1	Total	C	O			4	0
			26	23	3				
4	D	1	Total	C	O			4	0
			26	23	3				
4	E	1	Total	C	O			4	0
			26	23	3				
4	F	1	Total	C	O			4	0
			26	23	3				
4	F	1	Total	C	N	O	S	0	0
			42	32	2	7	1		

- Molecule 5 is 1-BENZYLOXYCARBONYLAMINO-2-PHENYL-ETHYL)-{2-[1-CARBAMOYL-2-(1H-INDOL-3-YL)-ETHYLCARBAMOYL]-5-PHENYL-PENTYL}-PHOSPHINIC ACID (three-letter code: RXP) (formula: C₃₉H₄₃N₄O₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	B	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	C	1	Total	C	N	O	P	0	0
			50	39	4	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	E	1	Total	C	N	O	P	0	0
			50	39	4	6	1		
5	F	1	Total	C	N	O	P	0	0
			50	39	4	6	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	376	Total	O	0	0
			376	376		
6	B	318	Total	O	0	0
			318	318		
6	C	367	Total	O	0	0
			367	367		
6	D	341	Total	O	0	0
			341	341		
6	E	353	Total	O	0	0
			353	353		
6	F	381	Total	O	0	0
			381	381		

3 Residue-property plots

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.

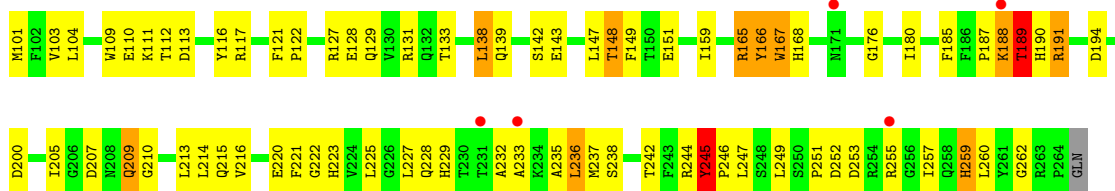
• Molecule 1: STROMELYSIN 3

Chain A: 



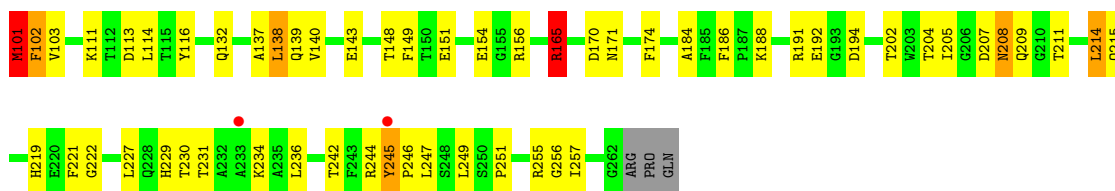
• Molecule 1: STROMELYSIN 3

Chain B: 



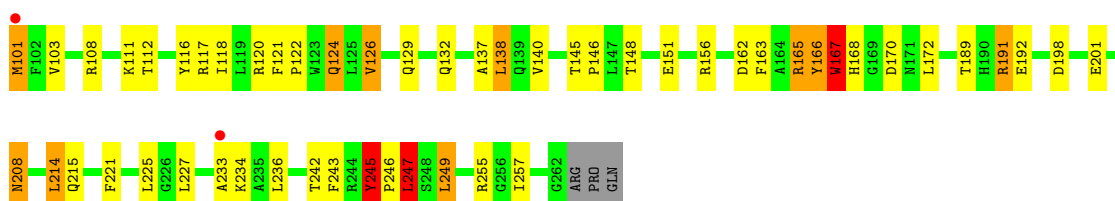
• Molecule 1: STROMELYSIN 3

Chain C: 



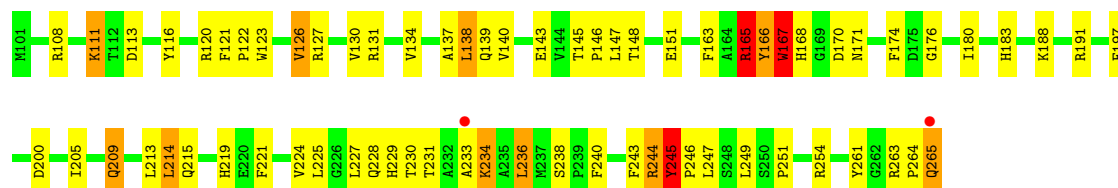
• Molecule 1: STROMELYSIN 3

Chain D: 



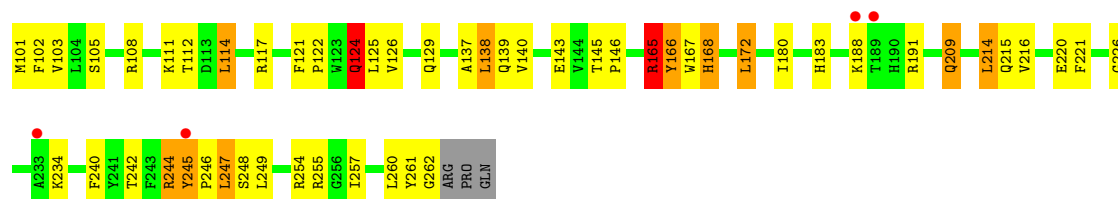
- Molecule 1: STROMELYSIN 3

Chain E:



- Molecule 1: STROMELYSIN 3

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.10Å 148.50Å 91.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.60 19.89 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.89-2.60) 96.8 (19.89-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.50 (at 2.59Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.262 0.213 , 0.259	Depositor DCC
R_{free} test set	5828 reflections (10.16%)	DCC
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 59596 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10772	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RXP, ZN, CPS, CA

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	0.70	1/1367 (0.1%)	0.87	5/1861 (0.3%)
1	B	0.70	3/1386 (0.2%)	0.99	11/1887 (0.6%)
1	C	0.63	0/1367	0.94	9/1861 (0.5%)
1	D	0.79	3/1367 (0.2%)	0.97	11/1861 (0.6%)
1	E	0.66	1/1396 (0.1%)	0.88	5/1899 (0.3%)
1	F	0.75	3/1367 (0.2%)	0.94	7/1861 (0.4%)
All	All	0.70	11/8250 (0.1%)	0.93	48/11230 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	3
1	E	0	1
1	F	0	1
All	All	0	6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	TYR	C-N	-15.08	0.99	1.34
1	E	167	TRP	N-CA	11.29	1.69	1.46
1	A	167	TRP	N-CA	9.55	1.65	1.46
1	F	165	ARG	C-N	-9.54	1.12	1.34
1	F	168	HIS	C-N	-7.49	1.19	1.33
1	B	188	LYS	C-N	-5.82	1.20	1.34
1	D	101	MET	C-N	-5.56	1.21	1.34
1	B	167	TRP	CA-C	-5.18	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	TYR	CA-C	-5.15	1.39	1.52
1	F	166	TYR	C-N	-5.12	1.22	1.34
1	B	167	TRP	C-N	-5.00	1.22	1.34

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	LYS	CB-CA-C	12.47	135.34	110.40
1	F	245	TYR	C-N-CD	10.84	151.17	128.40
1	C	245	TYR	C-N-CD	10.81	151.10	128.40
1	D	101	MET	N-CA-C	8.98	135.24	111.00
1	C	102	PHE	O-C-N	-8.87	108.51	122.70
1	B	245	TYR	C-N-CD	8.84	146.97	128.40
1	D	245	TYR	C-N-CD	8.70	146.66	128.40
1	D	166	TYR	O-C-N	-8.37	109.31	122.70
1	B	245	TYR	N-CA-C	7.77	131.99	111.00
1	A	167	TRP	N-CA-C	7.76	131.96	111.00
1	C	165	ARG	N-CA-C	7.74	131.90	111.00
1	F	168	HIS	N-CA-CB	-7.73	96.68	110.60
1	F	166	TYR	CB-CA-C	-7.65	95.10	110.40
1	C	165	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	E	245	TYR	N-CA-C	7.54	131.35	111.00
1	E	165	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	F	165	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	F	245	TYR	C-N-CA	-7.48	90.59	122.00
1	E	245	TYR	C-N-CD	7.43	144.01	128.40
1	A	165	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	D	165	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	B	191	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	E	167	TRP	N-CA-C	7.12	130.21	111.00
1	B	165	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	D	167	TRP	C-N-CA	6.95	139.08	121.70
1	B	166	TYR	CA-CB-CG	-6.94	100.21	113.40
1	D	245	TYR	N-CA-C	6.71	129.11	111.00
1	A	191	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	E	245	TYR	C-N-CA	-6.59	94.33	122.00
1	F	245	TYR	N-CA-C	6.51	128.58	111.00
1	B	166	TYR	CD1-CG-CD2	6.41	124.95	117.90
1	C	103	VAL	N-CA-C	6.26	127.89	111.00
1	D	101	MET	CG-SD-CE	6.13	110.01	100.20
1	B	166	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	D	167	TRP	N-CA-C	6.02	127.24	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	245	TYR	N-CA-C	5.96	127.10	111.00
1	B	166	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	C	101	MET	CG-SD-CE	5.79	109.46	100.20
1	D	245	TYR	CA-CB-CG	-5.78	102.42	113.40
1	C	245	TYR	C-N-CA	-5.63	98.34	122.00
1	C	103	VAL	N-CA-CB	-5.62	99.14	111.50
1	A	167	TRP	N-CA-CB	-5.59	100.53	110.60
1	A	138	LEU	CA-CB-CG	5.55	128.06	115.30
1	B	189	THR	N-CA-CB	-5.38	100.07	110.30
1	F	124	GLN	CB-CA-C	-5.37	99.67	110.40
1	B	166	TYR	CG-CD2-CE2	-5.21	117.13	121.30
1	D	247	LEU	CA-CB-CG	5.09	127.00	115.30
1	D	168	HIS	N-CA-C	5.04	124.59	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	TYR	Peptide
1	D	166	TYR	Mainchain,Peptide
1	D	245	TYR	Sidechain
1	E	166	TYR	Peptide
1	F	165	ARG	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1324	0	1253	70	0
1	B	1342	0	1272	77	0
1	C	1324	0	1253	77	0
1	D	1324	0	1252	58	0
1	E	1352	0	1281	85	0
1	F	1324	0	1252	68	1
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	52	0	70	16	0
4	B	52	0	70	15	0
4	C	52	0	70	15	0
4	D	52	0	70	9	0
4	E	52	0	70	16	0
4	F	68	0	91	30	0
5	A	50	0	42	5	0
5	B	50	0	42	4	0
5	C	50	0	42	1	0
5	D	50	0	42	1	0
5	E	50	0	42	9	0
5	F	50	0	42	2	0
6	A	376	0	0	35	0
6	B	318	0	0	30	0
6	C	367	0	0	31	0
6	D	341	0	0	28	0
6	E	353	0	0	31	1
6	F	381	0	0	34	0
All	All	10772	0	8256	517	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (517) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:5004:CPS:C10	4:D:5004:CPS:C5	1.75	1.65
4:B:5007:CPS:C10	4:B:5007:CPS:C5	1.74	1.64
4:A:5006:CPS:C10	4:A:5006:CPS:C5	1.75	1.63
4:F:5091:CPS:C19	4:F:5091:CPS:C18	1.75	1.63
4:F:5011:CPS:C5	4:F:5011:CPS:C10	1.76	1.61
4:C:5008:CPS:C5	4:C:5008:CPS:C10	1.75	1.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:5001:CPS:C10	4:A:5001:CPS:C5	1.76	1.60
4:E:5005:CPS:C5	4:E:5005:CPS:C10	1.76	1.59
4:B:5002:CPS:C5	4:B:5002:CPS:C10	1.76	1.59
4:E:5010:CPS:C5	4:E:5010:CPS:C10	1.75	1.59
4:D:5009:CPS:C10	4:D:5009:CPS:C5	1.75	1.56
4:C:5003:CPS:C5	4:C:5003:CPS:C10	1.76	1.56
1:E:167:TRP:CA	1:E:167:TRP:N	1.68	1.55
4:F:5091:CPS:C5	4:F:5091:CPS:C10	1.84	1.53
1:B:189:THR:HG22	6:B:6013:HOH:O	1.22	1.37
1:F:240:PHE:CD2	4:F:5091:CPS:H29B	1.60	1.34
1:D:167:TRP:HZ3	6:F:742:HOH:O	1.00	1.31
4:F:5091:CPS:C29	6:F:1547:HOH:O	1.78	1.25
1:A:217:ALA:HA	6:A:6365:HOH:O	1.36	1.21
5:E:6005:RXP:H231	6:E:6108:HOH:O	1.37	1.20
6:A:6072:HOH:O	1:C:102:PHE:CE1	1.94	1.18
1:D:167:TRP:CZ3	6:F:742:HOH:O	1.77	1.07
1:B:222:GLY:HA3	1:B:237:MET:HE1	1.33	1.04
6:A:6072:HOH:O	1:C:102:PHE:HE1	1.34	1.03
1:F:240:PHE:CD2	4:F:5091:CPS:C29	2.42	1.02
1:C:165:ARG:O	6:C:6105:HOH:O	1.83	0.97
1:F:101:MET:HG3	1:F:112:THR:H	1.29	0.97
1:E:166:TYR:O	1:E:168:HIS:ND1	1.97	0.97
1:F:240:PHE:HD2	4:F:5091:CPS:H29B	1.26	0.96
1:E:131:ARG:HD2	6:E:6031:HOH:O	1.63	0.95
1:B:222:GLY:HA3	1:B:237:MET:CE	1.96	0.95
1:A:197:PHE:CZ	6:A:6365:HOH:O	2.18	0.94
1:C:132:GLN:NE2	6:C:6024:HOH:O	2.01	0.94
1:A:165:ARG:HG2	6:A:6022:HOH:O	1.67	0.94
1:D:245:TYR:O	1:D:247:LEU:N	2.01	0.93
1:C:113:ASP:HA	1:C:148:THR:HG22	1.49	0.92
6:A:6089:HOH:O	1:E:165:ARG:HG2	1.68	0.91
1:B:216:VAL:HB	6:B:6277:HOH:O	1.68	0.91
4:F:5091:CPS:H29	6:F:1547:HOH:O	1.49	0.87
4:C:5008:CPS:C6	4:C:5008:CPS:C10	2.54	0.86
1:B:166:TYR:HB3	1:B:167:TRP:CE3	2.10	0.86
1:E:265:GLN:CD	1:E:265:GLN:H	1.78	0.86
4:A:5006:CPS:C9	4:A:5006:CPS:C10	2.52	0.86
1:C:256:GLY:HA2	6:C:6365:HOH:O	1.75	0.86
4:C:5003:CPS:C9	4:C:5003:CPS:C10	2.54	0.85
4:D:5009:CPS:C9	4:D:5009:CPS:C10	2.55	0.85
1:E:215:GLN:HB3	5:E:6005:RXP:H18	1.59	0.85
4:B:5007:CPS:C10	4:B:5007:CPS:C9	2.54	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:5002:CPS:C10	4:B:5002:CPS:C6	2.54	0.84
4:B:5002:CPS:C10	4:B:5002:CPS:C9	2.54	0.84
1:B:138:LEU:HD13	1:B:221:PHE:CD2	2.12	0.84
4:D:5004:CPS:C10	4:D:5004:CPS:C6	2.56	0.84
4:F:5011:CPS:C9	4:F:5011:CPS:C10	2.56	0.84
4:D:5004:CPS:C10	4:D:5004:CPS:C9	2.55	0.84
4:A:5006:CPS:C6	4:A:5006:CPS:C10	2.56	0.83
4:C:5008:CPS:C9	4:C:5008:CPS:C10	2.56	0.83
1:A:165:ARG:HH11	1:A:165:ARG:HB2	1.44	0.83
4:F:5091:CPS:C18	4:F:5091:CPS:C3	2.56	0.83
1:C:245:TYR:HB3	6:C:6183:HOH:O	1.76	0.83
1:D:245:TYR:O	1:D:246:PRO:C	2.04	0.83
1:D:101:MET:O	1:D:112:THR:HG23	1.78	0.83
4:A:5001:CPS:C10	4:A:5001:CPS:C9	2.55	0.82
4:E:5005:CPS:C6	4:E:5005:CPS:C10	2.56	0.82
4:E:5010:CPS:C10	4:E:5010:CPS:C6	2.56	0.82
1:A:236:LEU:HD22	1:A:249:LEU:HD23	1.59	0.82
4:A:5001:CPS:C10	4:A:5001:CPS:C6	2.57	0.82
4:B:5007:CPS:C10	4:B:5007:CPS:C4	2.57	0.82
1:A:165:ARG:HH11	1:A:165:ARG:CB	1.91	0.82
4:E:5010:CPS:C10	4:E:5010:CPS:C9	2.57	0.82
1:F:240:PHE:CE2	4:F:5091:CPS:H29B	2.14	0.82
4:E:5005:CPS:C10	4:E:5005:CPS:C9	2.57	0.82
1:A:114:LEU:HD21	6:A:6118:HOH:O	1.80	0.82
1:B:251:PRO:O	1:B:255:ARG:HG3	1.79	0.81
4:F:5091:CPS:H25	6:F:493:HOH:O	1.78	0.81
1:B:189:THR:CG2	6:B:6013:HOH:O	1.90	0.81
4:D:5004:CPS:C10	4:D:5004:CPS:C4	2.58	0.81
4:C:5003:CPS:C10	4:C:5003:CPS:C6	2.58	0.81
4:E:5010:CPS:C4	4:E:5010:CPS:C10	2.58	0.81
4:D:5009:CPS:C10	4:D:5009:CPS:C6	2.58	0.81
4:B:5007:CPS:C10	4:B:5007:CPS:C6	2.58	0.81
1:F:180:ILE:HG13	6:F:1080:HOH:O	1.81	0.81
4:C:5008:CPS:C4	4:C:5008:CPS:C10	2.58	0.81
1:A:215:GLN:HE22	1:A:244:ARG:H	1.26	0.81
1:F:138:LEU:HD13	1:F:221:PHE:CD2	2.17	0.80
1:F:246:PRO:HB2	6:F:1638:HOH:O	1.82	0.80
4:F:5011:CPS:C10	4:F:5011:CPS:C6	2.59	0.80
4:A:5001:CPS:C10	4:A:5001:CPS:C4	2.60	0.79
1:E:166:TYR:C	1:E:167:TRP:CA	2.51	0.79
4:D:5009:CPS:C4	4:D:5009:CPS:C10	2.59	0.79
5:E:6005:RXP:C36	6:E:6013:HOH:O	2.30	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:5011:CPS:C4	4:F:5011:CPS:C10	2.61	0.78
1:B:245:TYR:O	1:B:247:LEU:N	2.16	0.78
1:F:165:ARG:O	1:F:166:TYR:C	2.19	0.78
4:E:5005:CPS:C4	4:E:5005:CPS:C10	2.60	0.78
1:A:165:ARG:NH1	1:A:165:ARG:HB2	1.97	0.78
1:E:209:GLN:HA	1:E:209:GLN:HE21	1.47	0.77
1:C:114:LEU:HD21	6:C:6273:HOH:O	1.84	0.77
4:B:5002:CPS:C4	4:B:5002:CPS:C10	2.63	0.77
1:B:180:ILE:HD13	5:B:6002:RXP:H7	1.67	0.77
4:A:5006:CPS:C10	4:A:5006:CPS:C4	2.63	0.77
1:B:236:LEU:HG	6:B:6080:HOH:O	1.85	0.76
4:C:5003:CPS:C4	4:C:5003:CPS:C10	2.63	0.76
1:A:115:THR:HG23	1:C:101:MET:CE	2.15	0.76
1:C:113:ASP:OD1	1:C:148:THR:HG21	1.85	0.75
1:D:236:LEU:HD22	1:D:249:LEU:HD12	1.67	0.75
1:A:111:LYS:HG2	1:C:111:LYS:HG2	1.68	0.75
1:E:213:LEU:HD23	6:E:6302:HOH:O	1.85	0.74
1:A:186:PHE:CE2	4:A:5006:CPS:H16	2.23	0.74
1:B:138:LEU:HB3	6:B:6229:HOH:O	1.86	0.74
1:B:128:GLU:HA	6:B:6038:HOH:O	1.87	0.74
4:F:5091:CPS:H29A	6:F:1547:HOH:O	1.59	0.74
1:E:183:HIS:HB3	6:E:6342:HOH:O	1.88	0.73
1:D:257:ILE:CG1	6:D:660:HOH:O	2.37	0.73
1:A:215:GLN:NE2	1:A:244:ARG:H	1.87	0.73
1:F:101:MET:HA	1:F:112:THR:OG1	1.88	0.73
1:B:222:GLY:CA	1:B:237:MET:HE1	2.16	0.73
1:B:213:LEU:HD12	6:B:6277:HOH:O	1.90	0.72
1:E:236:LEU:CD2	1:E:249:LEU:HD23	2.18	0.72
4:F:5091:CPS:C4	4:F:5091:CPS:C10	2.68	0.72
1:C:246:PRO:HD3	6:C:6183:HOH:O	1.89	0.71
1:A:115:THR:HG23	1:C:101:MET:HE2	1.70	0.71
4:F:5091:CPS:C17	4:F:5091:CPS:C19	2.66	0.71
1:A:104:LEU:HG	6:A:6189:HOH:O	1.91	0.71
1:D:215:GLN:HB3	5:D:6004:RXP:H18	1.71	0.70
1:D:214:LEU:HD11	6:D:937:HOH:O	1.91	0.70
1:B:189:THR:HG23	1:B:190:HIS:CD2	2.26	0.70
1:C:236:LEU:HD22	1:C:249:LEU:HD23	1.73	0.70
1:F:125:LEU:O	6:F:750:HOH:O	2.09	0.69
4:F:5091:CPS:C10	4:F:5091:CPS:C6	2.69	0.69
1:F:101:MET:CG	1:F:102:PHE:H	2.06	0.69
4:F:5091:CPS:H261	6:F:1762:HOH:O	1.92	0.69
1:C:245:TYR:O	1:C:247:LEU:N	2.26	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:5091:CPS:H271	6:F:1260:HOH:O	1.93	0.68
1:B:207:ASP:OD2	1:B:209:GLN:HG3	1.94	0.68
1:A:138:LEU:HD13	1:A:221:PHE:CD2	2.29	0.68
1:C:211:THR:HG23	6:C:6251:HOH:O	1.93	0.68
1:B:166:TYR:HB3	1:B:167:TRP:HE3	1.58	0.67
1:F:248:SER:HA	6:F:581:HOH:O	1.95	0.67
1:B:262:GLY:HA3	6:B:6177:HOH:O	1.93	0.67
1:B:235:ALA:HB1	6:B:6151:HOH:O	1.93	0.66
1:B:110:GLU:HG2	6:B:6134:HOH:O	1.95	0.66
1:F:168:HIS:N	1:F:168:HIS:ND1	2.44	0.66
1:C:205:ILE:O	1:C:205:ILE:HD12	1.95	0.65
1:F:112:THR:HG22	6:F:997:HOH:O	1.95	0.65
1:B:165:ARG:HD2	1:B:200:ASP:OD1	1.97	0.65
4:F:5091:CPS:C10	4:F:5091:CPS:C9	2.70	0.65
1:C:102:PHE:CE1	6:C:6013:HOH:O	2.49	0.65
1:D:189:THR:HG22	1:D:189:THR:O	1.96	0.65
1:B:238:SER:HB2	6:B:6149:HOH:O	1.96	0.65
1:A:137:ALA:HA	6:A:6115:HOH:O	1.96	0.64
1:B:215:GLN:HB3	5:B:6002:RXP:H18	1.79	0.64
1:A:228:GLN:HG2	6:A:6229:HOH:O	1.97	0.64
1:F:209:GLN:HA	1:F:209:GLN:HE21	1.63	0.64
1:E:167:TRP:CB	1:E:167:TRP:N	2.58	0.63
1:F:101:MET:HG3	1:F:112:THR:N	2.06	0.63
1:E:131:ARG:HD3	6:E:6198:HOH:O	1.98	0.63
1:A:127:ARG:HB2	6:A:6337:HOH:O	1.97	0.63
1:C:102:PHE:CD1	6:C:6013:HOH:O	2.51	0.63
1:D:148:THR:HG22	6:D:448:HOH:O	1.97	0.63
1:E:265:GLN:CD	1:E:265:GLN:N	2.52	0.62
1:F:101:MET:CG	1:F:102:PHE:N	2.63	0.62
1:C:219:HIS:HA	6:C:6357:HOH:O	1.99	0.62
1:B:259:HIS:O	1:B:259:HIS:ND1	2.33	0.62
1:A:197:PHE:CE1	6:A:6365:HOH:O	2.45	0.62
1:C:215:GLN:HB3	5:C:6003:RXP:H18	1.81	0.61
1:A:137:ALA:O	1:A:140:VAL:HG12	2.00	0.61
1:E:139:GLN:O	1:E:143:GLU:HG3	2.00	0.61
1:A:139:GLN:O	1:A:143:GLU:HG3	2.00	0.61
1:C:247:LEU:HA	6:C:6136:HOH:O	1.99	0.61
1:A:218:ALA:HB2	6:A:6115:HOH:O	2.01	0.61
1:C:236:LEU:HG	6:C:6122:HOH:O	2.00	0.60
1:D:234:LYS:HD3	6:D:1691:HOH:O	2.00	0.60
1:A:127:ARG:HD3	6:A:6017:HOH:O	2.00	0.60
1:E:214:LEU:HD13	1:E:247:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:113:ASP:OD1	1:B:148:THR:HG21	2.00	0.60
1:D:103:VAL:HB	6:D:835:HOH:O	2.00	0.60
1:D:138:LEU:HD13	1:D:221:PHE:CD2	2.37	0.60
4:F:5091:CPS:O1	6:F:493:HOH:O	2.16	0.60
1:A:113:ASP:HB2	6:A:6299:HOH:O	2.02	0.60
1:E:165:ARG:NH2	1:E:166:TYR:HE1	1.99	0.60
1:F:245:TYR:O	1:F:246:PRO:C	2.30	0.60
1:F:245:TYR:O	1:F:247:LEU:N	2.35	0.60
1:B:209:GLN:CD	1:B:210:GLY:N	2.54	0.60
1:A:165:ARG:NH1	1:A:200:ASP:OD2	2.35	0.60
1:E:145:THR:HB	1:E:146:PRO:CD	2.32	0.60
1:D:236:LEU:CD2	1:D:249:LEU:HD12	2.32	0.60
1:C:204:THR:HB	1:C:207:ASP:HB3	1.84	0.59
1:E:219:HIS:CD2	5:E:6005:RXP:H392	2.37	0.59
1:C:113:ASP:HA	1:C:148:THR:CG2	2.26	0.59
1:A:128:GLU:HG2	6:A:6137:HOH:O	2.01	0.59
1:B:149:PHE:HB2	6:B:6229:HOH:O	2.01	0.59
1:B:109:TRP:HZ3	6:B:6180:HOH:O	1.85	0.59
1:F:188:LYS:HB2	6:F:876:HOH:O	2.02	0.59
1:E:228:GLN:NE2	4:E:5005:CPS:O2	2.35	0.58
1:F:101:MET:CG	1:F:112:THR:H	2.11	0.58
1:B:233:ALA:HA	6:B:6203:HOH:O	2.03	0.58
1:E:244:ARG:HD2	6:E:6246:HOH:O	2.02	0.58
1:A:115:THR:HG22	1:C:101:MET:N	2.18	0.58
1:A:115:THR:CG2	1:C:101:MET:N	2.66	0.58
1:E:167:TRP:HA	1:E:167:TRP:N	2.03	0.58
1:B:236:LEU:HD11	1:B:247:LEU:CD1	2.34	0.58
1:A:245:TYR:O	6:A:6051:HOH:O	2.17	0.58
1:A:128:GLU:HG2	6:A:6251:HOH:O	2.03	0.57
1:F:126:VAL:CG2	1:F:129:GLN:HG3	2.34	0.57
1:B:131:ARG:NH1	6:B:6037:HOH:O	2.36	0.57
1:D:227:LEU:N	1:D:227:LEU:HD12	2.20	0.57
1:B:101:MET:HE2	6:D:1978:HOH:O	2.04	0.57
1:F:240:PHE:CE2	4:F:5091:CPS:H28A	2.40	0.57
1:B:255:ARG:HG2	6:B:6255:HOH:O	2.04	0.57
1:F:215:GLN:NE2	6:F:585:HOH:O	1.79	0.57
1:E:138:LEU:HD13	1:E:221:PHE:CD2	2.39	0.57
4:F:5091:CPS:H32	6:F:1237:HOH:O	2.06	0.56
1:F:172:LEU:HB3	1:F:183:HIS:CE1	2.40	0.56
4:F:5091:CPS:C19	4:F:5091:CPS:C6	2.77	0.56
1:A:236:LEU:HD22	1:A:249:LEU:CD2	2.35	0.56
1:B:131:ARG:HD2	6:B:6038:HOH:O	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:118:ILE:HG13	6:D:1833:HOH:O	2.05	0.56
1:A:170:ASP:O	1:A:171:ASN:HB2	2.06	0.56
1:D:172:LEU:HD12	6:D:1632:HOH:O	2.06	0.56
1:D:242:THR:HG23	6:D:842:HOH:O	2.06	0.56
1:E:170:ASP:O	1:E:171:ASN:HB2	2.06	0.56
1:C:137:ALA:O	1:C:140:VAL:HG12	2.06	0.56
1:B:187:PRO:HG3	1:B:194:ASP:OD1	2.06	0.55
1:C:245:TYR:HD2	6:C:6183:HOH:O	1.88	0.55
1:E:245:TYR:O	1:E:247:LEU:N	2.40	0.55
1:A:162:ASP:O	1:A:196:HIS:HA	2.05	0.55
6:A:6260:HOH:O	1:C:191:ARG:HD2	2.07	0.55
1:E:205:ILE:HD11	6:E:6302:HOH:O	2.05	0.55
1:F:101:MET:HG2	1:F:102:PHE:N	2.22	0.55
1:C:246:PRO:CD	6:C:6183:HOH:O	2.50	0.55
1:C:205:ILE:HA	6:C:6107:HOH:O	2.07	0.55
1:F:137:ALA:O	1:F:140:VAL:HG13	2.06	0.55
1:A:165:ARG:N	6:A:6022:HOH:O	2.39	0.55
1:F:167:TRP:CE3	6:F:514:HOH:O	2.53	0.55
1:C:208:ASN:HD22	1:C:208:ASN:C	2.10	0.55
1:C:208:ASN:HD22	1:C:209:GLN:N	2.05	0.55
1:F:240:PHE:HD2	4:F:5091:CPS:C29	2.03	0.55
1:B:245:TYR:O	1:B:246:PRO:C	2.30	0.55
1:E:236:LEU:HD22	1:E:249:LEU:HD23	1.89	0.55
5:E:6005:RXP:H17	6:E:6090:HOH:O	2.06	0.54
1:D:215:GLN:HE22	1:D:243:PHE:HA	1.73	0.54
1:F:143:GLU:HG2	6:F:1686:HOH:O	2.08	0.54
1:B:133:THR:OG1	1:B:205:ILE:HD12	2.07	0.54
1:E:229:HIS:ND1	4:E:5005:CPS:H14	2.23	0.54
1:E:221:PHE:HA	1:E:224:VAL:HG12	1.90	0.54
1:D:108:ARG:HH11	1:D:108:ARG:HG3	1.71	0.54
1:D:257:ILE:HG12	6:D:660:HOH:O	2.06	0.53
1:E:138:LEU:HD13	1:E:221:PHE:CE2	2.43	0.53
1:F:145:THR:HB	1:F:146:PRO:HD2	1.91	0.53
1:B:237:MET:HB2	6:B:6151:HOH:O	2.07	0.53
1:A:111:LYS:HB2	1:C:111:LYS:HE2	1.90	0.53
1:B:249:LEU:HB3	1:B:253:ASP:HB2	1.90	0.53
1:E:111:LYS:H	1:E:111:LYS:HD2	1.74	0.53
1:D:189:THR:CG2	1:D:189:THR:O	2.58	0.53
1:B:101:MET:N	6:B:6043:HOH:O	2.42	0.53
1:D:129:GLN:HG2	6:D:466:HOH:O	2.07	0.52
1:D:124:GLN:H	1:D:124:GLN:NE2	2.07	0.52
1:D:121:PHE:HB3	6:D:774:HOH:O	2.08	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:LYS:CG	1:C:111:LYS:HG2	2.37	0.52
1:F:101:MET:HG3	1:F:102:PHE:H	1.75	0.52
1:D:132:GLN:HG2	6:D:1413:HOH:O	2.10	0.52
1:C:116:TYR:CZ	1:C:151:GLU:HB2	2.44	0.52
1:D:208:ASN:H	1:D:208:ASN:ND2	2.07	0.52
1:F:103:VAL:HB	6:F:997:HOH:O	2.09	0.52
1:F:138:LEU:HD13	1:F:221:PHE:CE2	2.44	0.52
1:E:254:ARG:HD2	6:E:6202:HOH:O	2.10	0.52
1:E:228:GLN:HE21	1:E:228:GLN:HA	1.74	0.52
6:A:6072:HOH:O	1:C:102:PHE:CZ	2.41	0.52
1:E:121:PHE:HB3	6:E:6039:HOH:O	2.09	0.52
1:C:202:THR:HB	6:C:6293:HOH:O	2.10	0.52
1:C:138:LEU:HD13	1:C:221:PHE:CD2	2.45	0.52
1:A:215:GLN:HE22	1:A:244:ARG:N	2.04	0.52
1:F:209:GLN:HA	1:F:209:GLN:NE2	2.23	0.52
1:E:126:VAL:HG12	6:E:6136:HOH:O	2.09	0.52
1:E:165:ARG:NH2	1:E:166:TYR:CE1	2.78	0.52
1:E:264:PRO:HB3	6:E:6356:HOH:O	2.10	0.52
1:E:127:ARG:HD3	6:E:6138:HOH:O	2.10	0.51
1:E:228:GLN:NE2	1:E:228:GLN:HA	2.25	0.51
1:D:247:LEU:HB3	6:D:937:HOH:O	2.11	0.51
1:E:137:ALA:O	1:E:140:VAL:HG12	2.10	0.51
1:B:232:ALA:HB3	1:B:235:ALA:HB2	1.91	0.51
1:D:233:ALA:O	1:D:234:LYS:HB2	2.11	0.51
1:A:122:PRO:HD3	1:A:163:PHE:CE2	2.46	0.51
1:C:236:LEU:HD22	1:C:249:LEU:CD2	2.39	0.51
1:F:139:GLN:O	1:F:143:GLU:HG3	2.11	0.51
1:E:108:ARG:HG3	1:E:108:ARG:HH11	1.75	0.51
1:B:113:ASP:OD1	1:B:148:THR:CG2	2.59	0.51
1:E:254:ARG:HB3	6:E:6202:HOH:O	2.09	0.50
1:F:121:PHE:HB3	1:F:122:PRO:HD2	1.94	0.50
1:B:116:TYR:CZ	1:B:151:GLU:HB2	2.46	0.50
1:A:165:ARG:NH1	1:A:165:ARG:CB	2.63	0.50
1:F:244:ARG:HD3	6:F:607:HOH:O	2.11	0.50
1:A:115:THR:HG23	1:C:101:MET:HE3	1.91	0.50
1:D:122:PRO:HD3	1:D:163:PHE:CE2	2.46	0.50
1:F:261:TYR:O	1:F:262:GLY:O	2.29	0.50
1:C:186:PHE:CE2	4:C:5008:CPS:H16	2.47	0.50
1:A:129:GLN:NE2	6:A:6139:HOH:O	2.44	0.50
1:F:167:TRP:HE3	6:F:514:HOH:O	1.90	0.50
1:B:260:LEU:HD21	6:B:6188:HOH:O	2.11	0.50
1:E:166:TYR:O	1:E:168:HIS:CE1	2.62	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:255:ARG:HB3	6:B:6164:HOH:O	2.12	0.50
1:E:146:PRO:HB3	1:E:265:GLN:OE1	2.12	0.49
1:D:156:ARG:NH1	1:D:192:GLU:OE1	2.45	0.49
1:E:246:PRO:HD2	6:E:6093:HOH:O	2.12	0.49
1:D:145:THR:HG21	6:D:1611:HOH:O	2.12	0.49
1:A:215:GLN:HB3	5:A:6001:RXP:H18	1.94	0.49
1:B:180:ILE:HD12	5:B:6002:RXP:O5	2.13	0.49
1:E:245:TYR:O	1:E:246:PRO:C	2.37	0.49
1:D:112:THR:HG21	6:D:835:HOH:O	2.12	0.49
1:D:146:PRO:HD3	6:D:1854:HOH:O	2.12	0.49
1:A:145:THR:HB	1:A:146:PRO:HD2	1.93	0.49
1:B:189:THR:HG23	1:B:190:HIS:HD2	1.74	0.49
1:E:219:HIS:CE1	1:E:238:SER:O	2.65	0.49
1:F:103:VAL:HG23	1:F:112:THR:HG21	1.95	0.49
1:D:117:ARG:HD2	6:D:625:HOH:O	2.12	0.48
1:A:214:LEU:HD22	6:A:6115:HOH:O	2.13	0.48
4:E:5005:CPS:H18	4:E:5005:CPS:H10A	1.94	0.48
1:B:236:LEU:HD11	1:B:247:LEU:HD11	1.94	0.48
1:C:154:GLU:HB2	6:C:6014:HOH:O	2.13	0.48
5:E:6005:RXP:C37	6:E:6013:HOH:O	2.59	0.47
1:E:130:VAL:HA	6:E:6302:HOH:O	2.13	0.47
1:C:215:GLN:OE1	1:C:242:THR:O	2.33	0.47
1:E:233:ALA:C	1:E:234:LYS:HG2	2.35	0.47
1:E:108:ARG:NH1	6:E:6082:HOH:O	2.39	0.47
1:F:254:ARG:HD2	6:F:1396:HOH:O	2.14	0.47
4:B:5002:CPS:H12	6:B:6300:HOH:O	2.14	0.47
1:E:180:ILE:CG2	6:E:6342:HOH:O	2.62	0.47
1:D:117:ARG:HG3	1:D:118:ILE:N	2.27	0.47
1:F:124:GLN:CD	1:F:124:GLN:H	2.17	0.47
1:F:248:SER:HB2	6:F:587:HOH:O	2.15	0.47
1:D:172:LEU:HB2	6:D:1632:HOH:O	2.14	0.47
1:B:229:HIS:ND1	4:B:5002:CPS:H14	2.29	0.47
1:D:208:ASN:HD22	1:D:208:ASN:N	2.12	0.47
1:E:108:ARG:HG3	1:E:108:ARG:NH1	2.30	0.47
1:A:242:THR:HB	6:A:6165:HOH:O	2.15	0.47
1:A:210:GLY:O	6:A:6043:HOH:O	2.21	0.47
4:F:5011:CPS:C8	4:F:5011:CPS:C10	2.93	0.47
1:B:113:ASP:HA	1:B:148:THR:HG23	1.96	0.47
1:F:111:LYS:HG2	6:F:794:HOH:O	2.15	0.47
1:E:113:ASP:OD2	1:E:148:THR:OG1	2.33	0.47
1:A:191:ARG:HD3	6:C:6161:HOH:O	2.15	0.46
1:B:103:VAL:CG2	1:B:112:THR:CG2	2.93	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:111:LYS:HA	6:D:885:HOH:O	2.15	0.46
1:B:244:ARG:HB2	6:B:6233:HOH:O	2.15	0.46
1:D:101:MET:HA	1:D:112:THR:OG1	2.16	0.46
1:E:130:VAL:O	1:E:134:VAL:HG23	2.15	0.46
1:F:165:ARG:HB2	6:F:1074:HOH:O	2.13	0.46
1:C:230:THR:HB	6:C:6317:HOH:O	2.15	0.46
1:B:236:LEU:HD11	1:B:247:LEU:HD12	1.97	0.46
1:E:231:THR:HG23	6:E:6272:HOH:O	2.14	0.46
1:A:186:PHE:HE2	4:A:5006:CPS:H16	1.79	0.46
1:C:245:TYR:O	1:C:246:PRO:C	2.45	0.46
1:B:116:TYR:HA	1:B:159:ILE:O	2.16	0.46
1:B:139:GLN:HA	1:B:142:SER:OG	2.15	0.46
1:D:126:VAL:HG13	6:D:789:HOH:O	2.14	0.46
1:A:126:VAL:HG21	6:A:6251:HOH:O	2.16	0.46
1:A:256:GLY:HA2	6:A:6333:HOH:O	2.15	0.46
4:E:5005:CPS:C10	4:E:5005:CPS:H18	2.46	0.46
1:A:255:ARG:HD3	1:E:123:TRP:CD2	2.51	0.46
1:F:255:ARG:HB3	6:F:568:HOH:O	2.15	0.46
1:B:223:HIS:CE1	6:B:6144:HOH:O	2.68	0.46
1:F:214:LEU:HD13	1:F:247:LEU:HD12	1.98	0.46
1:B:111:LYS:HB3	6:D:1612:HOH:O	2.15	0.46
1:A:167:TRP:HA	6:A:6026:HOH:O	2.15	0.46
1:C:148:THR:HB	6:C:6346:HOH:O	2.15	0.45
1:E:240:PHE:CD1	1:E:240:PHE:N	2.84	0.45
1:D:208:ASN:H	1:D:208:ASN:HD22	1.64	0.45
1:E:251:PRO:HA	6:E:6202:HOH:O	2.16	0.45
1:F:234:LYS:HA	1:F:244:ARG:CZ	2.47	0.45
1:E:215:GLN:HE22	1:E:243:PHE:HA	1.82	0.45
1:E:127:ARG:HD2	6:E:6209:HOH:O	2.16	0.45
4:B:5002:CPS:H18	4:B:5002:CPS:H10A	1.99	0.45
1:B:138:LEU:HD13	1:B:221:PHE:CE2	2.51	0.45
1:B:205:ILE:HG12	1:B:205:ILE:O	2.16	0.45
1:D:108:ARG:NH1	1:D:108:ARG:HG3	2.30	0.45
1:C:234:LYS:HD3	6:C:6343:HOH:O	2.16	0.45
4:E:5010:CPS:C10	4:E:5010:CPS:C8	2.94	0.45
1:A:197:PHE:HZ	6:A:6365:HOH:O	1.76	0.45
4:C:5008:CPS:H10A	4:C:5008:CPS:H18	1.99	0.45
4:E:5010:CPS:C10	4:E:5010:CPS:C7	2.94	0.45
1:D:120:ARG:HB2	1:D:162:ASP:OD1	2.17	0.45
4:F:5011:CPS:C7	4:F:5011:CPS:C10	2.95	0.44
1:C:184:ALA:HA	1:C:194:ASP:O	2.17	0.44
1:E:238:SER:O	5:E:6005:RXP:H15	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:227:LEU:CD1	1:D:227:LEU:N	2.81	0.44
1:F:257:ILE:HA	1:F:257:ILE:HD13	1.87	0.44
5:E:6005:RXP:H17	6:E:6088:HOH:O	2.17	0.44
5:E:6005:RXP:H26	6:E:6218:HOH:O	2.16	0.44
1:F:180:ILE:HD13	5:F:6006:RXP:H7	1.99	0.44
1:B:246:PRO:HD2	6:B:6086:HOH:O	2.15	0.44
1:B:176:GLY:HA2	1:B:200:ASP:OD2	2.17	0.44
1:F:126:VAL:HG23	1:F:129:GLN:HG3	1.99	0.44
1:C:139:GLN:O	1:C:143:GLU:HG3	2.17	0.44
1:A:180:ILE:HD13	5:A:6001:RXP:H7	1.99	0.44
1:B:180:ILE:CD1	5:B:6002:RXP:H7	2.44	0.44
1:A:247:LEU:HG	6:A:6115:HOH:O	2.16	0.44
1:A:147:LEU:HD21	4:A:5006:CPS:H10B	2.00	0.44
1:C:170:ASP:O	1:C:171:ASN:HB2	2.17	0.44
1:C:148:THR:HG23	6:C:6091:HOH:O	2.16	0.44
1:F:234:LYS:HA	1:F:244:ARG:NH2	2.32	0.44
1:A:187:PRO:HD2	1:A:192:GLU:O	2.18	0.44
1:E:147:LEU:HD21	1:E:261:TYR:CD2	2.52	0.44
4:A:5006:CPS:C8	4:A:5006:CPS:C10	2.96	0.44
1:E:147:LEU:HD21	1:E:261:TYR:CE2	2.53	0.44
1:A:184:ALA:HA	1:A:194:ASP:O	2.18	0.44
1:E:263:ARG:HH11	1:E:263:ARG:HG3	1.83	0.44
1:E:108:ARG:HA	6:E:6310:HOH:O	2.17	0.44
1:C:234:LYS:HE3	6:C:6227:HOH:O	2.18	0.44
1:C:251:PRO:HD3	6:C:6150:HOH:O	2.18	0.44
1:B:147:LEU:HD22	6:B:6264:HOH:O	2.18	0.43
1:B:244:ARG:HD2	6:B:6234:HOH:O	2.18	0.43
1:B:121:PHE:HB3	1:B:122:PRO:HD2	2.00	0.43
1:B:242:THR:HG22	6:B:6295:HOH:O	2.17	0.43
1:E:209:GLN:CA	1:E:209:GLN:HE21	2.25	0.43
1:E:243:PHE:HB2	6:E:6326:HOH:O	2.18	0.43
1:F:111:LYS:HB2	6:F:2103:HOH:O	2.18	0.43
1:A:166:TYR:O	1:A:168:HIS:ND1	2.51	0.43
1:B:213:LEU:HA	6:B:6277:HOH:O	2.18	0.43
1:E:111:LYS:N	1:E:111:LYS:HD2	2.32	0.43
1:D:191:ARG:HG2	1:D:191:ARG:H	1.49	0.43
1:D:242:THR:HG21	6:D:1584:HOH:O	2.19	0.43
1:A:182:ALA:O	5:A:6001:RXP:H211	2.18	0.43
1:E:229:HIS:HD1	4:E:5005:CPS:H14	1.82	0.43
1:D:208:ASN:ND2	1:D:208:ASN:N	2.67	0.43
1:E:120:ARG:HG2	6:E:6166:HOH:O	2.18	0.43
1:C:156:ARG:NH1	1:C:192:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:216:VAL:O	1:B:220:GLU:HG2	2.19	0.43
1:A:138:LEU:HD13	1:A:221:PHE:CG	2.53	0.43
1:F:215:GLN:HG2	6:F:585:HOH:O	2.17	0.43
1:E:263:ARG:HG3	1:E:263:ARG:NH1	2.33	0.43
1:C:229:HIS:ND1	4:C:5003:CPS:H14	2.34	0.43
1:C:113:ASP:OD1	1:C:148:THR:CG2	2.60	0.43
1:D:257:ILE:HB	6:D:660:HOH:O	2.18	0.43
1:D:137:ALA:O	1:D:140:VAL:HG12	2.18	0.43
1:F:216:VAL:O	1:F:220:GLU:HG2	2.19	0.43
4:B:5007:CPS:C10	4:B:5007:CPS:C8	2.97	0.43
1:F:101:MET:O	1:F:102:PHE:HB2	2.18	0.43
1:C:245:TYR:CB	6:C:6183:HOH:O	2.48	0.43
1:A:209:GLN:HB2	6:A:6347:HOH:O	2.18	0.43
1:B:139:GLN:O	1:B:143:GLU:HG3	2.18	0.42
4:B:5007:CPS:H14	4:B:5007:CPS:H19	1.99	0.42
4:F:5011:CPS:C8	4:F:5011:CPS:H10	2.50	0.42
1:B:129:GLN:HG2	1:B:205:ILE:HD13	2.02	0.42
1:C:245:TYR:O	1:C:245:TYR:CG	2.69	0.42
1:F:242:THR:HG22	6:F:613:HOH:O	2.20	0.42
4:A:5001:CPS:H4	5:A:6001:RXP:O5	2.19	0.42
1:C:214:LEU:HB2	6:C:6107:HOH:O	2.18	0.42
1:F:114:LEU:N	1:F:114:LEU:HD23	2.34	0.42
1:C:222:GLY:O	1:C:227:LEU:HD23	2.19	0.42
4:C:5008:CPS:C7	4:C:5008:CPS:C10	2.97	0.42
1:C:165:ARG:O	1:C:174:PHE:HB2	2.19	0.42
1:A:168:HIS:ND1	1:A:168:HIS:N	2.67	0.42
4:A:5001:CPS:H18	4:A:5001:CPS:H10A	2.01	0.42
1:C:208:ASN:ND2	1:C:208:ASN:C	2.73	0.42
1:C:231:THR:O	1:C:231:THR:HG22	2.19	0.42
1:C:215:GLN:HE22	1:C:244:ARG:H	1.67	0.42
1:C:188:LYS:HG2	6:C:6274:HOH:O	2.18	0.42
1:E:163:PHE:CD1	1:E:197:PHE:HB2	2.55	0.42
1:D:101:MET:HB2	6:D:885:HOH:O	2.19	0.42
1:C:191:ARG:HG2	1:C:191:ARG:H	1.66	0.42
1:B:127:ARG:HD2	6:B:6147:HOH:O	2.20	0.42
5:A:6001:RXP:H26	6:A:6035:HOH:O	2.20	0.41
1:A:220:GLU:HB2	6:A:6365:HOH:O	2.20	0.41
1:C:247:LEU:HD12	6:C:6136:HOH:O	2.18	0.41
1:A:111:LYS:CB	1:C:111:LYS:HG2	2.49	0.41
1:F:226:GLY:HA3	1:F:260:LEU:HD21	2.02	0.41
1:E:116:TYR:CZ	1:E:151:GLU:HB2	2.55	0.41
1:C:257:ILE:HA	1:C:257:ILE:HD13	1.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:C:5008:CPS:C8	4:C:5008:CPS:C10	2.99	0.41
1:E:165:ARG:CZ	1:E:166:TYR:HE1	2.33	0.41
1:C:188:LYS:HA	6:C:6274:HOH:O	2.21	0.41
1:E:191:ARG:H	1:E:191:ARG:HG2	1.75	0.41
4:A:5006:CPS:C10	4:A:5006:CPS:C7	2.97	0.41
1:A:111:LYS:HG2	1:C:111:LYS:CG	2.45	0.41
1:D:257:ILE:HG13	6:D:660:HOH:O	2.15	0.41
1:D:145:THR:HB	1:D:146:PRO:HD2	2.02	0.41
1:B:165:ARG:O	1:B:168:HIS:ND1	2.52	0.41
1:A:245:TYR:N	6:A:6051:HOH:O	2.44	0.41
1:B:103:VAL:CG2	1:B:112:THR:HG22	2.50	0.41
1:C:149:PHE:HB2	6:C:6185:HOH:O	2.20	0.41
1:E:176:GLY:HA2	1:E:200:ASP:OD2	2.20	0.41
4:B:5002:CPS:C10	4:B:5002:CPS:H18	2.50	0.41
1:B:185:PHE:O	1:B:187:PRO:HD3	2.21	0.41
1:B:191:ARG:H	1:B:191:ARG:HG2	1.68	0.41
1:E:166:TYR:N	1:E:174:PHE:HB2	2.35	0.41
1:B:257:ILE:HD12	1:B:257:ILE:HA	1.88	0.41
4:B:5007:CPS:C10	4:B:5007:CPS:C7	2.99	0.41
1:F:209:GLN:CA	1:F:209:GLN:HE21	2.27	0.41
4:D:5004:CPS:C10	4:D:5004:CPS:C8	2.99	0.41
4:A:5001:CPS:C10	4:A:5001:CPS:H18	2.51	0.41
1:E:174:PHE:HA	6:E:6291:HOH:O	2.20	0.41
1:C:205:ILE:O	1:C:205:ILE:CD1	2.66	0.41
1:E:121:PHE:HB3	1:E:122:PRO:HD2	2.03	0.41
1:E:225:LEU:HA	1:E:225:LEU:HD23	1.91	0.41
1:A:227:LEU:HD11	1:A:257:ILE:HD13	2.02	0.41
1:F:191:ARG:HA	6:F:520:HOH:O	2.20	0.41
1:E:139:GLN:O	1:E:139:GLN:HG2	2.21	0.41
1:C:204:THR:CB	1:C:207:ASP:HB3	2.51	0.41
1:E:234:LYS:HE3	1:E:244:ARG:NH2	2.36	0.41
1:E:166:TYR:H	1:E:174:PHE:HB2	1.85	0.40
5:F:6006:RXP:H37	6:F:498:HOH:O	2.20	0.40
1:D:198:ASP:HB3	1:D:201:GLU:HG2	2.01	0.40
4:C:5003:CPS:C8	4:C:5003:CPS:C10	2.99	0.40
1:C:215:GLN:HG2	6:C:6109:HOH:O	2.20	0.40
1:F:188:LYS:HE2	6:F:876:HOH:O	2.21	0.40
1:F:126:VAL:HG22	1:F:129:GLN:HG3	2.02	0.40
1:A:101:MET:HG2	1:A:102:PHE:N	2.37	0.40
4:E:5005:CPS:H12	6:E:6108:HOH:O	2.21	0.40
1:F:108:ARG:HG3	1:F:108:ARG:NH1	2.37	0.40
1:E:188:LYS:HB2	6:E:6226:HOH:O	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:240:PHE:CZ	4:F:5091:CPS:H28A	2.55	0.40
6:A:6089:HOH:O	1:E:165:ARG:N	2.54	0.40
1:F:214:LEU:HG	6:F:532:HOH:O	2.21	0.40
1:D:257:ILE:CB	6:D:660:HOH:O	2.67	0.40
4:C:5008:CPS:H18	4:C:5008:CPS:C10	2.51	0.40
1:D:225:LEU:HD13	6:D:1611:HOH:O	2.20	0.40
1:D:116:TYR:CZ	1:D:151:GLU:HB2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:101:MET:CE	6:E:6062:HOH:O[2_665]	1.33	0.87

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/165 (97%)	155 (97%)	5 (3%)	0	100	100
1	B	162/165 (98%)	148 (91%)	12 (7%)	2 (1%)	19	39
1	C	160/165 (97%)	151 (94%)	9 (6%)	0	100	100
1	D	160/165 (97%)	151 (94%)	7 (4%)	2 (1%)	18	35
1	E	163/165 (99%)	152 (93%)	10 (6%)	1 (1%)	33	63
1	F	160/165 (97%)	153 (96%)	7 (4%)	0	100	100
All	All	965/990 (98%)	910 (94%)	50 (5%)	5 (0%)	38	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	LYS
1	B	189	THR
1	D	167	TRP
1	E	167	TRP

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Mol	Chain	Res	Type
1	D	245	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/140 (98%)	132 (96%)	5 (4%)	47	76
1	B	139/140 (99%)	126 (91%)	13 (9%)	13	23
1	C	137/140 (98%)	131 (96%)	6 (4%)	39	68
1	D	137/140 (98%)	125 (91%)	12 (9%)	14	27
1	E	140/140 (100%)	127 (91%)	13 (9%)	13	24
1	F	137/140 (98%)	125 (91%)	12 (9%)	14	27
All	All	827/840 (98%)	766 (93%)	61 (7%)	20	38

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	165	ARG
1	A	187	PRO
1	A	191	ARG
1	A	214	LEU
1	B	104	LEU
1	B	117	ARG
1	B	138	LEU
1	B	148	THR
1	B	209	GLN
1	B	214	LEU
1	B	225	LEU
1	B	227	LEU
1	B	228	GLN
1	B	236	LEU
1	B	245	TYR
1	B	252	ASP
1	B	259	HIS

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Mol	Chain	Res	Type
1	C	101	MET
1	C	138	LEU
1	C	165	ARG
1	C	208	ASN
1	C	214	LEU
1	C	255	ARG
1	D	124	GLN
1	D	126	VAL
1	D	138	LEU
1	D	165	ARG
1	D	170	ASP
1	D	191	ARG
1	D	208	ASN
1	D	214	LEU
1	D	245	TYR
1	D	247	LEU
1	D	249	LEU
1	D	255	ARG
1	E	111	LYS
1	E	126	VAL
1	E	138	LEU
1	E	165	ARG
1	E	209	GLN
1	E	214	LEU
1	E	227	LEU
1	E	230	THR
1	E	234	LYS
1	E	236	LEU
1	E	244	ARG
1	E	245	TYR
1	E	265	GLN
1	F	105	SER
1	F	114	LEU
1	F	117	ARG
1	F	124	GLN
1	F	138	LEU
1	F	165	ARG
1	F	172	LEU
1	F	209	GLN
1	F	214	LEU
1	F	244	ARG
1	F	247	LEU

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Mol	Chain	Res	Type
1	F	249	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	215	GLN
1	A	258	GLN
1	B	129	GLN
1	B	190	HIS
1	B	258	GLN
1	C	129	GLN
1	C	208	ASN
1	C	215	GLN
1	D	124	GLN
1	D	129	GLN
1	D	132	GLN
1	D	208	ASN
1	D	215	GLN
1	D	258	GLN
1	E	129	GLN
1	E	190	HIS
1	E	209	GLN
1	E	215	GLN
1	E	228	GLN
1	E	259	HIS
1	F	258	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 36 ligands modelled in this entry, 18 are monoatomic - leaving 18 for Mogul analysis.

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$
4	CPS	A	5001	-	29,29,45	6.97	18 (62%)	46,47,70	4.19	27 (58%)
4	CPS	A	5006	-	29,29,45	7.05	17 (58%)	46,47,70	4.13	24 (52%)
5	RXP	A	6001	2	54,54,54	4.94	39 (72%)	73,73,73	2.85	30 (41%)
4	CPS	B	5002	-	29,29,45	7.28	17 (58%)	46,47,70	4.06	27 (58%)
4	CPS	B	5007	-	29,29,45	6.81	18 (62%)	46,47,70	4.06	27 (58%)
5	RXP	B	6002	2	54,54,54	5.63	40 (74%)	73,73,73	2.88	25 (34%)
4	CPS	C	5003	-	29,29,45	6.91	15 (51%)	46,47,70	4.19	29 (63%)
4	CPS	C	5008	-	29,29,45	6.85	18 (62%)	46,47,70	4.07	24 (52%)
5	RXP	C	6003	2	54,54,54	4.90	38 (70%)	73,73,73	3.11	30 (41%)
4	CPS	D	5004	-	29,29,45	7.29	17 (58%)	46,47,70	4.08	28 (60%)
4	CPS	D	5009	-	29,29,45	6.92	17 (58%)	46,47,70	4.02	27 (58%)
5	RXP	D	6004	2	54,54,54	5.09	35 (64%)	73,73,73	2.78	31 (42%)
4	CPS	E	5005	-	29,29,45	6.85	16 (55%)	46,47,70	4.26	27 (58%)
4	CPS	E	5010	-	29,29,45	6.84	17 (58%)	46,47,70	4.08	26 (56%)
5	RXP	E	6005	2	54,54,54	4.70	37 (68%)	73,73,73	2.76	31 (42%)
4	CPS	F	5011	-	29,29,45	6.92	18 (62%)	46,47,70	3.98	26 (56%)
4	CPS	F	5091	-	45,45,45	4.59	25 (55%)	70,70,70	3.20	33 (47%)
5	RXP	F	6006	2	54,54,54	4.70	37 (68%)	73,73,73	2.76	31 (42%)

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
4	CPS	A	5001	-	-	0/6/71/90	0/0/4/4
4	CPS	A	5006	-	-	0/6/71/90	0/0/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	RXP	A	6001	2	-	1/46/46/46	0/3/5/5
4	CPS	B	5002	-	-	0/6/71/90	0/0/4/4
4	CPS	B	5007	-	-	0/6/71/90	0/0/4/4
5	RXP	B	6002	2	-	1/46/46/46	0/3/5/5
4	CPS	C	5003	-	-	0/6/71/90	0/0/4/4
4	CPS	C	5008	-	-	0/6/71/90	0/0/4/4
5	RXP	C	6003	2	-	1/46/46/46	0/3/5/5
4	CPS	D	5004	-	-	0/6/71/90	0/0/4/4
4	CPS	D	5009	-	-	0/6/71/90	0/0/4/4
5	RXP	D	6004	2	-	0/46/46/46	0/3/5/5
4	CPS	E	5005	-	-	0/6/71/90	0/0/4/4
4	CPS	E	5010	-	-	0/6/71/90	0/0/4/4
5	RXP	E	6005	2	-	1/46/46/46	0/3/5/5
4	CPS	F	5011	-	-	0/6/71/90	0/0/4/4
4	CPS	F	5091	-	-	0/25/90/90	0/0/4/4
5	RXP	F	6006	2	-	1/46/46/46	0/3/5/5

All (439) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5004	CPS	C23-C22	-30.11	1.43	1.55
4	B	5002	CPS	C23-C22	-30.03	1.43	1.55
4	A	5006	CPS	C23-C22	-28.78	1.43	1.55
4	C	5003	CPS	C23-C22	-27.58	1.44	1.55
4	A	5001	CPS	C23-C22	-27.28	1.44	1.55
4	E	5005	CPS	C23-C22	-26.90	1.44	1.55
4	F	5011	CPS	C23-C22	-26.90	1.44	1.55
4	C	5008	CPS	C23-C22	-26.74	1.44	1.55
4	E	5010	CPS	C23-C22	-26.61	1.44	1.55
4	D	5009	CPS	C23-C22	-26.61	1.44	1.55
4	B	5007	CPS	C23-C22	-26.54	1.44	1.55
4	F	5091	CPS	C10-C5	18.10	1.84	1.54
4	F	5011	CPS	C10-C5	13.47	1.76	1.54
4	E	5005	CPS	C10-C5	13.44	1.76	1.54
4	A	5001	CPS	C10-C5	13.40	1.76	1.54
5	A	6001	RXP	P-O2P	-13.26	1.33	1.55
4	C	5003	CPS	C10-C5	13.26	1.76	1.54
5	C	6003	RXP	P-C22	-13.17	1.74	1.83
4	B	5002	CPS	C10-C5	13.17	1.76	1.54
4	C	5008	CPS	C10-C5	12.88	1.75	1.54
4	D	5009	CPS	O4-C4	-12.84	1.21	1.43
4	A	5006	CPS	C10-C5	12.79	1.75	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5004	CPS	O4-C4	-12.70	1.21	1.43
4	E	5010	CPS	C10-C5	12.62	1.75	1.54
4	D	5004	CPS	C10-C5	12.42	1.75	1.54
4	D	5009	CPS	C10-C5	12.35	1.75	1.54
4	B	5007	CPS	C10-C5	12.31	1.74	1.54
4	A	5001	CPS	O4-C4	-12.04	1.22	1.43
5	D	6004	RXP	P-C22	-12.00	1.75	1.83
4	E	5010	CPS	O4-C4	-11.87	1.22	1.43
5	B	6002	RXP	C37-C32	11.68	1.65	1.38
4	B	5007	CPS	O4-C4	-11.50	1.23	1.43
4	B	5002	CPS	O4-C4	-11.35	1.23	1.43
4	C	5008	CPS	O4-C4	-11.29	1.23	1.43
4	C	5003	CPS	O4-C4	-11.25	1.23	1.43
4	F	5011	CPS	O4-C4	-11.23	1.24	1.43
5	B	6002	RXP	C4-C6	10.90	1.60	1.41
4	E	5005	CPS	O4-C4	-10.76	1.24	1.43
4	F	5091	CPS	C18-C19	10.73	1.75	1.53
4	A	5006	CPS	O4-C4	-10.58	1.25	1.43
5	B	6002	RXP	C36-C37	10.40	1.63	1.39
5	D	6004	RXP	P-O2P	-10.30	1.38	1.55
5	B	6002	RXP	C34-C33	10.15	1.62	1.39
4	F	5091	CPS	O4-C4	-9.58	1.26	1.43
5	B	6002	RXP	C25-C24	9.54	1.60	1.38
5	F	6006	RXP	C36-C37	9.47	1.61	1.39
5	E	6005	RXP	C36-C37	9.46	1.61	1.39
5	D	6004	RXP	C4-C6	9.29	1.57	1.41
5	C	6003	RXP	C37-C32	9.19	1.59	1.38
4	B	5002	CPS	C18-C19	9.03	1.71	1.53
5	D	6004	RXP	C10-C8	8.90	1.57	1.36
5	A	6001	RXP	C36-C37	8.89	1.59	1.39
4	C	5008	CPS	C18-C17	8.82	1.68	1.53
5	F	6006	RXP	P-O2P	-8.75	1.41	1.55
5	E	6005	RXP	P-O2P	-8.73	1.41	1.55
5	B	6002	RXP	C33-C32	8.68	1.58	1.38
5	A	6001	RXP	C4-C6	8.62	1.56	1.41
5	C	6003	RXP	C34-C33	8.61	1.59	1.39
5	D	6004	RXP	C28-C26	8.52	1.58	1.39
5	A	6001	RXP	P-O1P	-8.49	1.31	1.49
5	B	6002	RXP	P-O2P	-8.47	1.41	1.55
4	E	5005	CPS	C18-C19	8.46	1.70	1.53
4	F	5011	CPS	C18-C19	8.43	1.70	1.53
5	B	6002	RXP	C35-C34	8.35	1.62	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5003	CPS	C18-C19	8.32	1.70	1.53
4	E	5010	CPS	C18-C19	8.29	1.70	1.53
5	D	6004	RXP	C34-C33	8.24	1.58	1.39
4	D	5009	CPS	C18-C17	8.24	1.67	1.53
5	A	6001	RXP	C37-C32	8.21	1.57	1.38
4	D	5004	CPS	C18-C19	8.16	1.70	1.53
5	A	6001	RXP	O5-C30	8.13	1.37	1.21
4	B	5007	CPS	C18-C19	8.06	1.70	1.53
5	E	6005	RXP	C10-C8	7.87	1.54	1.36
5	F	6006	RXP	C10-C8	7.86	1.54	1.36
5	D	6004	RXP	C36-C37	7.82	1.57	1.39
5	B	6002	RXP	C28-C26	7.77	1.57	1.39
4	A	5006	CPS	C18-C19	7.69	1.69	1.53
5	C	6003	RXP	C4-C6	7.65	1.54	1.41
4	A	5001	CPS	C18-C19	7.65	1.69	1.53
5	E	6005	RXP	O6-C31	7.59	1.63	1.45
5	E	6005	RXP	C35-C34	7.58	1.59	1.37
5	F	6006	RXP	O6-C31	7.57	1.63	1.45
5	F	6006	RXP	C35-C34	7.55	1.59	1.37
5	C	6003	RXP	C35-C34	7.55	1.59	1.37
5	B	6002	RXP	O5-C30	7.55	1.36	1.21
5	C	6003	RXP	C36-C37	7.46	1.56	1.39
4	E	5005	CPS	C18-C17	7.41	1.66	1.53
5	B	6002	RXP	C29-C28	7.40	1.59	1.37
5	B	6002	RXP	C10-C8	7.39	1.53	1.36
5	D	6004	RXP	C25-C24	7.39	1.55	1.38
4	C	5008	CPS	C5-C9	-7.37	1.42	1.55
5	B	6002	RXP	C29-C27	7.37	1.59	1.37
5	A	6001	RXP	C25-C24	7.33	1.55	1.38
5	F	6006	RXP	C4-C6	7.29	1.53	1.41
4	D	5009	CPS	C18-C19	7.29	1.68	1.53
5	E	6005	RXP	C4-C6	7.26	1.53	1.41
5	A	6001	RXP	C34-C33	7.25	1.55	1.39
5	C	6003	RXP	C10-C8	7.25	1.53	1.36
5	C	6003	RXP	O5-C30	7.22	1.35	1.21
4	C	5008	CPS	C18-C19	7.18	1.68	1.53
4	A	5001	CPS	C5-C9	-7.18	1.43	1.55
5	A	6001	RXP	C33-C32	7.13	1.55	1.38
4	A	5006	CPS	C18-C17	7.08	1.65	1.53
4	B	5007	CPS	C5-C9	-7.04	1.43	1.55
4	A	5006	CPS	C5-C9	-7.02	1.43	1.55
5	F	6006	RXP	C25-C24	7.01	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	6005	RXP	C25-C24	7.00	1.54	1.38
5	F	6006	RXP	C36-C35	6.99	1.58	1.37
5	D	6004	RXP	C26-C24	6.99	1.54	1.38
5	E	6005	RXP	C36-C35	6.98	1.58	1.37
4	D	5004	CPS	C5-C9	-6.97	1.43	1.55
5	C	6003	RXP	C33-C32	6.95	1.54	1.38
4	B	5002	CPS	C5-C9	-6.94	1.43	1.55
4	B	5002	CPS	C18-C17	6.94	1.65	1.53
5	B	6002	RXP	C36-C35	6.93	1.58	1.37
5	F	6006	RXP	C28-C26	6.93	1.55	1.39
4	E	5010	CPS	C5-C9	-6.92	1.43	1.55
5	E	6005	RXP	C28-C26	6.92	1.55	1.39
5	A	6001	RXP	O6-C30	6.89	1.49	1.35
5	D	6004	RXP	C7-C4	6.81	1.56	1.42
5	A	6001	RXP	C10-C9	6.77	1.57	1.37
4	F	5091	CPS	C3-C4	6.76	1.65	1.53
5	E	6005	RXP	C34-C33	6.75	1.54	1.39
5	D	6004	RXP	C37-C32	6.74	1.54	1.38
4	F	5011	CPS	C5-C9	-6.73	1.44	1.55
5	F	6006	RXP	C34-C33	6.72	1.54	1.39
4	D	5009	CPS	C5-C9	-6.72	1.44	1.55
5	D	6004	RXP	C10-C9	6.69	1.57	1.37
4	C	5003	CPS	C3-C4	6.67	1.65	1.53
5	B	6002	RXP	C26-C24	6.65	1.54	1.38
4	F	5091	CPS	C18-C17	6.65	1.64	1.53
5	D	6004	RXP	C35-C34	6.65	1.57	1.37
4	F	5011	CPS	C18-C17	6.61	1.64	1.53
5	E	6005	RXP	C10-C9	6.61	1.57	1.37
5	F	6006	RXP	C10-C9	6.60	1.57	1.37
4	B	5007	CPS	C18-C17	6.57	1.64	1.53
5	F	6006	RXP	C33-C32	6.54	1.53	1.38
4	A	5001	CPS	C3-C4	6.53	1.65	1.53
5	C	6003	RXP	O6-C31	6.52	1.60	1.45
5	A	6001	RXP	C35-C34	6.52	1.56	1.37
5	E	6005	RXP	C33-C32	6.52	1.53	1.38
5	E	6005	RXP	C9-C7	6.49	1.51	1.36
5	A	6001	RXP	C19-C14	6.48	1.53	1.38
5	F	6006	RXP	C9-C7	6.48	1.51	1.36
5	A	6001	RXP	C10-C8	6.44	1.51	1.36
4	E	5005	CPS	C3-C4	6.42	1.65	1.53
5	B	6002	RXP	C19-C14	6.41	1.53	1.38
5	B	6002	RXP	C16-C15	6.41	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5001	CPS	C18-C17	6.39	1.64	1.53
5	A	6001	RXP	C36-C35	6.35	1.56	1.37
5	C	6003	RXP	C9-C7	6.32	1.51	1.36
5	C	6003	RXP	C36-C35	6.31	1.56	1.37
4	A	5006	CPS	C3-C4	6.28	1.64	1.53
5	A	6001	RXP	C9-C7	6.25	1.51	1.36
4	C	5003	CPS	C5-C9	-6.23	1.44	1.55
5	E	6005	RXP	C8-C6	6.23	1.54	1.40
5	F	6006	RXP	C8-C6	6.20	1.54	1.40
4	F	5011	CPS	C3-C4	6.20	1.64	1.53
4	E	5010	CPS	C3-C4	6.18	1.64	1.53
5	C	6003	RXP	C19-C14	6.17	1.53	1.38
5	B	6002	RXP	C10-C9	6.16	1.55	1.37
5	D	6004	RXP	C29-C27	6.12	1.55	1.37
4	F	5091	CPS	C20-C9	6.12	1.66	1.54
5	E	6005	RXP	O6-C30	6.11	1.48	1.35
5	F	6006	RXP	O6-C30	6.11	1.48	1.35
5	B	6002	RXP	C9-C7	6.10	1.50	1.36
4	D	5009	CPS	C8-C9	6.09	1.68	1.54
4	D	5009	CPS	C3-C4	6.07	1.64	1.53
5	E	6005	RXP	C18-C19	6.06	1.53	1.39
4	E	5005	CPS	C5-C9	-6.04	1.45	1.55
5	F	6006	RXP	C18-C19	6.04	1.53	1.39
5	B	6002	RXP	C7-C4	6.01	1.54	1.42
5	C	6003	RXP	C31-C32	6.00	1.64	1.50
4	E	5010	CPS	C18-C17	5.99	1.63	1.53
5	D	6004	RXP	P-O1P	-5.96	1.36	1.49
5	D	6004	RXP	C29-C28	5.95	1.55	1.37
5	B	6002	RXP	C18-C19	5.80	1.52	1.39
5	E	6005	RXP	C37-C32	5.79	1.52	1.38
4	D	5004	CPS	C18-C17	5.76	1.63	1.53
5	D	6004	RXP	C23-C24	-5.75	1.37	1.51
5	F	6006	RXP	C37-C32	5.75	1.52	1.38
5	D	6004	RXP	C36-C35	5.74	1.54	1.37
4	C	5003	CPS	C18-C17	5.72	1.63	1.53
4	B	5007	CPS	C3-C4	5.70	1.63	1.53
5	B	6002	RXP	C30-N4	5.70	1.50	1.34
5	B	6002	RXP	C27-C25	5.66	1.52	1.39
5	D	6004	RXP	C9-C7	5.66	1.49	1.36
4	C	5003	CPS	O3-C17	-5.62	1.30	1.43
4	A	5001	CPS	O3-C17	-5.62	1.30	1.43
5	C	6003	RXP	C18-C19	5.62	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	6005	RXP	C7-C4	5.61	1.53	1.42
5	F	6006	RXP	C7-C4	5.60	1.53	1.42
4	B	5007	CPS	O3-C17	-5.56	1.30	1.43
5	C	6003	RXP	C25-C24	5.55	1.51	1.38
5	D	6004	RXP	C27-C25	5.54	1.51	1.39
5	B	6002	RXP	C5-C3	5.54	1.46	1.37
5	F	6006	RXP	C29-C27	5.42	1.53	1.37
4	F	5091	CPS	O3-C17	-5.41	1.31	1.43
5	E	6005	RXP	C29-C27	5.39	1.53	1.37
5	B	6002	RXP	C8-C6	5.37	1.52	1.40
5	B	6002	RXP	C20-C12	5.36	1.60	1.51
5	D	6004	RXP	C33-C32	5.35	1.51	1.38
5	C	6003	RXP	C29-C28	5.34	1.53	1.37
4	C	5008	CPS	C3-C4	5.33	1.63	1.53
5	D	6004	RXP	C19-C14	5.31	1.51	1.38
4	D	5004	CPS	C3-C4	5.31	1.63	1.53
4	E	5010	CPS	O3-C17	-5.30	1.31	1.43
5	A	6001	RXP	O6-C31	5.27	1.57	1.45
5	A	6001	RXP	C29-C28	5.27	1.53	1.37
5	C	6003	RXP	C10-C9	5.27	1.53	1.37
4	F	5091	CPS	C11-C2	5.20	1.64	1.54
5	D	6004	RXP	O5-C30	5.19	1.31	1.21
5	C	6003	RXP	C28-C26	5.09	1.50	1.39
5	E	6005	RXP	C29-C28	5.08	1.52	1.37
5	F	6006	RXP	C29-C28	5.07	1.52	1.37
4	C	5003	CPS	C8-C9	5.03	1.66	1.54
5	A	6001	RXP	C26-C24	4.95	1.50	1.38
4	B	5002	CPS	C8-C9	4.95	1.66	1.54
4	D	5004	CPS	C8-C9	4.95	1.66	1.54
5	E	6005	RXP	C16-C15	4.95	1.50	1.39
5	F	6006	RXP	C16-C15	4.94	1.50	1.39
5	B	6002	RXP	C17-C16	4.93	1.52	1.37
5	A	6001	RXP	C28-C26	4.91	1.50	1.39
4	F	5011	CPS	C8-C9	4.89	1.66	1.54
5	D	6004	RXP	C8-C6	4.87	1.51	1.40
5	B	6002	RXP	P-C22	-4.85	1.80	1.83
5	D	6004	RXP	C17-C16	4.79	1.51	1.37
5	E	6005	RXP	P-O1P	-4.79	1.38	1.49
5	C	6003	RXP	C30-N4	4.77	1.48	1.34
4	E	5005	CPS	C8-C9	4.76	1.65	1.54
4	B	5002	CPS	O3-C17	-4.76	1.32	1.43
5	F	6006	RXP	P-O1P	-4.76	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5005	CPS	O3-C17	-4.75	1.32	1.43
5	E	6005	RXP	C26-C24	4.73	1.49	1.38
5	F	6006	RXP	C26-C24	4.72	1.49	1.38
4	D	5009	CPS	C8-C7	4.72	1.67	1.54
4	B	5007	CPS	C8-C9	4.67	1.65	1.54
4	D	5004	CPS	O3-C17	-4.67	1.32	1.43
5	C	6003	RXP	O6-C30	4.66	1.45	1.35
5	D	6004	RXP	C16-C15	4.62	1.49	1.39
4	F	5091	CPS	C14-C13	4.60	1.60	1.51
4	A	5006	CPS	C8-C9	4.60	1.65	1.54
4	E	5010	CPS	C8-C9	4.55	1.65	1.54
5	C	6003	RXP	C5-C3	4.51	1.45	1.37
5	C	6003	RXP	C7-C4	4.51	1.51	1.42
5	C	6003	RXP	C29-C27	4.46	1.50	1.37
4	A	5001	CPS	C8-C9	4.46	1.64	1.54
4	F	5091	CPS	O1S-S	4.44	1.55	1.45
4	F	5011	CPS	O2-C13	4.43	1.57	1.43
4	F	5091	CPS	C8-C9	4.42	1.64	1.54
5	E	6005	RXP	C27-C25	4.40	1.49	1.39
4	E	5005	CPS	C8-C7	4.38	1.66	1.54
5	C	6003	RXP	C27-C25	4.37	1.49	1.39
5	F	6006	RXP	C27-C25	4.36	1.49	1.39
4	C	5008	CPS	C5-C4	-4.36	1.47	1.54
5	A	6001	RXP	C5-C3	4.35	1.44	1.37
4	A	5006	CPS	O3-C17	-4.34	1.33	1.43
4	C	5008	CPS	C8-C9	4.33	1.64	1.54
5	D	6004	RXP	C20-C12	4.32	1.59	1.51
5	C	6003	RXP	P-O2P	-4.32	1.48	1.55
4	F	5091	CPS	C2-C15	4.31	1.62	1.55
4	B	5007	CPS	C8-C7	4.31	1.66	1.54
4	B	5002	CPS	C3-C4	4.30	1.61	1.53
4	F	5091	CPS	C14-C15	4.30	1.61	1.53
5	C	6003	RXP	C17-C16	4.30	1.50	1.37
4	F	5091	CPS	C8-C7	4.29	1.66	1.54
4	F	5011	CPS	C14-C15	4.28	1.61	1.53
4	B	5007	CPS	C14-C15	4.27	1.61	1.53
5	E	6005	RXP	C23-C24	-4.27	1.40	1.51
5	F	6006	RXP	C23-C24	-4.26	1.40	1.51
5	B	6002	RXP	O6-C31	4.24	1.55	1.45
5	A	6001	RXP	C18-C19	4.18	1.48	1.39
5	A	6001	RXP	C31-C32	4.13	1.60	1.50
4	A	5006	CPS	C16-C15	-4.11	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5010	CPS	C8-C7	4.09	1.65	1.54
4	F	5091	CPS	C5-C9	-4.09	1.48	1.55
5	C	6003	RXP	C26-C24	4.08	1.48	1.38
4	D	5009	CPS	C16-C15	-4.08	1.46	1.53
4	B	5002	CPS	O2-C13	4.07	1.56	1.43
5	B	6002	RXP	O6-C30	4.06	1.43	1.35
4	C	5003	CPS	C16-C15	-4.03	1.46	1.53
4	D	5009	CPS	O2-C13	4.00	1.56	1.43
5	C	6003	RXP	C20-C12	3.98	1.58	1.51
4	B	5002	CPS	C8-C7	3.88	1.65	1.54
5	A	6001	RXP	C16-C15	3.87	1.48	1.39
5	E	6005	RXP	C19-C14	3.86	1.47	1.38
4	C	5008	CPS	C16-C15	-3.85	1.47	1.53
5	F	6006	RXP	C19-C14	3.83	1.47	1.38
5	B	6002	RXP	C31-C32	3.80	1.59	1.50
5	D	6004	RXP	C5-C3	3.80	1.44	1.37
5	F	6006	RXP	C15-C14	3.78	1.47	1.38
5	E	6005	RXP	C15-C14	3.78	1.47	1.38
4	A	5006	CPS	C8-C7	3.76	1.64	1.54
4	C	5008	CPS	O3-C17	-3.76	1.34	1.43
4	E	5010	CPS	C14-C15	3.73	1.60	1.53
5	C	6003	RXP	C16-C15	3.73	1.47	1.39
4	A	5001	CPS	C16-C15	-3.72	1.47	1.53
5	E	6005	RXP	C18-C17	3.70	1.48	1.37
4	C	5008	CPS	C8-C7	3.69	1.64	1.54
5	F	6006	RXP	C18-C17	3.69	1.48	1.37
4	E	5010	CPS	C5-C4	-3.69	1.48	1.54
4	E	5005	CPS	C11-C2	3.69	1.61	1.54
5	A	6001	RXP	C29-C27	3.69	1.48	1.37
5	C	6003	RXP	C23-C24	-3.67	1.42	1.51
4	D	5009	CPS	C5-C4	-3.66	1.48	1.54
5	A	6001	RXP	P-C21	-3.65	1.76	1.79
5	E	6005	RXP	C21-C20	3.65	1.60	1.54
4	D	5004	CPS	C11-C2	3.64	1.61	1.54
5	F	6006	RXP	P-C22	-3.64	1.81	1.83
5	F	6006	RXP	C21-C20	3.61	1.60	1.54
5	E	6005	RXP	P-C22	-3.60	1.81	1.83
5	D	6004	RXP	O6-C30	3.57	1.42	1.35
4	D	5004	CPS	C8-C7	3.57	1.64	1.54
4	C	5008	CPS	O2-C13	3.57	1.54	1.43
4	D	5009	CPS	O3-C17	-3.56	1.35	1.43
5	F	6006	RXP	C20-C12	3.55	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	6005	RXP	C20-C12	3.54	1.57	1.51
5	B	6002	RXP	P-O1P	-3.53	1.41	1.49
4	F	5011	CPS	C8-C7	3.52	1.64	1.54
4	F	5011	CPS	O3-C17	-3.52	1.35	1.43
4	C	5003	CPS	C8-C7	3.51	1.64	1.54
5	A	6001	RXP	O2-C12	-3.50	1.16	1.23
5	B	6002	RXP	C18-C17	3.50	1.48	1.37
4	D	5004	CPS	C16-C15	-3.49	1.47	1.53
4	D	5004	CPS	O2-C13	3.48	1.54	1.43
4	E	5010	CPS	O2-C13	3.47	1.54	1.43
4	A	5006	CPS	C14-C15	3.45	1.59	1.53
4	F	5011	CPS	C14-C13	3.45	1.58	1.51
4	F	5011	CPS	C16-C15	-3.45	1.47	1.53
4	F	5091	CPS	O2S-S	3.43	1.53	1.45
4	F	5091	CPS	O3S-S	3.43	1.53	1.45
4	B	5007	CPS	C5-C4	-3.40	1.49	1.54
4	D	5004	CPS	C14-C13	3.40	1.58	1.51
4	F	5011	CPS	C2-C19	3.39	1.61	1.56
4	A	5001	CPS	C11-C2	3.39	1.60	1.54
5	A	6001	RXP	C1-C11	3.38	1.58	1.52
4	C	5008	CPS	C14-C15	3.37	1.59	1.53
4	A	5001	CPS	C8-C7	3.37	1.63	1.54
5	A	6001	RXP	C7-C4	3.35	1.49	1.42
4	E	5005	CPS	O2-C13	3.31	1.53	1.43
5	A	6001	RXP	C8-C6	3.30	1.47	1.40
5	A	6001	RXP	C20-C12	3.28	1.57	1.51
4	A	5001	CPS	C14-C15	3.26	1.59	1.53
4	D	5009	CPS	C14-C15	3.26	1.59	1.53
4	B	5007	CPS	C14-C13	3.25	1.58	1.51
4	A	5001	CPS	C14-C13	3.25	1.58	1.51
4	B	5002	CPS	C14-C15	3.26	1.59	1.53
5	A	6001	RXP	C30-N4	3.25	1.43	1.34
4	F	5011	CPS	C5-C4	-3.24	1.49	1.54
4	C	5003	CPS	C11-C2	3.23	1.60	1.54
4	C	5003	CPS	O2-C13	3.23	1.53	1.43
5	C	6003	RXP	C22-N4	-3.22	1.42	1.46
4	A	5006	CPS	C14-C13	3.20	1.58	1.51
5	B	6002	RXP	C5-N3	3.20	1.43	1.37
5	C	6003	RXP	C18-C17	3.14	1.47	1.37
5	F	6006	RXP	C30-N4	3.13	1.43	1.34
5	E	6005	RXP	C30-N4	3.13	1.43	1.34
4	E	5010	CPS	C14-C13	3.13	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5006	CPS	O2-C13	3.12	1.53	1.43
4	F	5091	CPS	C18-C6	3.12	1.60	1.53
5	D	6004	RXP	C30-N4	3.12	1.43	1.34
4	F	5091	CPS	C32-S	3.12	1.83	1.78
5	A	6001	RXP	C27-C25	3.11	1.46	1.39
5	C	6003	RXP	O1-C11	-3.11	1.17	1.23
5	B	6002	RXP	C2-C3	3.09	1.56	1.51
4	B	5002	CPS	C16-C15	-3.08	1.48	1.53
5	A	6001	RXP	P-C22	-3.05	1.81	1.83
5	B	6002	RXP	C15-C14	3.05	1.45	1.38
4	B	5002	CPS	C11-C2	3.05	1.60	1.54
4	B	5007	CPS	C20-C9	3.03	1.60	1.54
4	D	5009	CPS	C11-C2	3.02	1.60	1.54
5	C	6003	RXP	C15-C14	3.00	1.45	1.38
5	D	6004	RXP	C1-C11	2.99	1.58	1.52
4	E	5010	CPS	C16-C15	-2.98	1.48	1.53
5	F	6006	RXP	O5-C30	2.98	1.27	1.21
5	E	6005	RXP	O5-C30	2.97	1.27	1.21
4	D	5009	CPS	C20-C9	2.94	1.60	1.54
4	E	5010	CPS	C11-C2	2.91	1.60	1.54
4	A	5001	CPS	C5-C4	-2.90	1.49	1.54
4	E	5010	CPS	C20-C9	2.89	1.60	1.54
5	A	6001	RXP	C17-C16	2.89	1.46	1.37
4	B	5007	CPS	C16-C15	-2.87	1.48	1.53
4	A	5006	CPS	C11-C2	2.85	1.59	1.54
4	B	5007	CPS	C3-C19	-2.84	1.49	1.53
4	D	5004	CPS	C14-C15	2.83	1.58	1.53
4	E	5005	CPS	C14-C13	2.80	1.57	1.51
4	F	5011	CPS	C11-C2	2.79	1.59	1.54
5	A	6001	RXP	C23-C24	-2.79	1.44	1.51
4	C	5003	CPS	C20-C9	2.79	1.60	1.54
4	D	5004	CPS	C5-C4	-2.78	1.50	1.54
4	E	5005	CPS	C16-C15	-2.78	1.49	1.53
4	C	5008	CPS	C20-C9	2.78	1.60	1.54
4	A	5001	CPS	C20-C9	2.78	1.60	1.54
4	E	5005	CPS	C14-C15	2.77	1.58	1.53
4	B	5007	CPS	O2-C13	2.77	1.52	1.43
5	C	6003	RXP	C8-C6	2.75	1.46	1.40
4	E	5005	CPS	C20-C9	2.74	1.59	1.54
4	F	5091	CPS	C21-C20	2.74	1.60	1.53
5	C	6003	RXP	C21-C20	2.74	1.59	1.54
4	B	5007	CPS	C11-C2	2.73	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	6005	RXP	C17-C16	2.72	1.45	1.37
5	D	6004	RXP	O2-C12	-2.72	1.18	1.23
5	F	6006	RXP	C17-C16	2.71	1.45	1.37
4	B	5002	CPS	C14-C13	2.69	1.57	1.51
4	F	5011	CPS	C20-C9	2.67	1.59	1.54
4	D	5009	CPS	C14-C13	2.67	1.57	1.51
5	B	6002	RXP	C21-C20	2.66	1.58	1.54
5	A	6001	RXP	C15-C14	2.65	1.44	1.38
5	D	6004	RXP	C18-C19	2.60	1.45	1.39
4	C	5008	CPS	C14-C13	2.58	1.56	1.51
4	A	5006	CPS	C20-C9	2.52	1.59	1.54
5	F	6006	RXP	C5-C3	2.50	1.41	1.37
4	F	5091	CPS	C5-C6	-2.50	1.51	1.55
5	D	6004	RXP	O6-C31	2.48	1.51	1.45
4	C	5008	CPS	C11-C2	2.48	1.59	1.54
5	E	6005	RXP	C5-C3	2.46	1.41	1.37
4	A	5001	CPS	O2-C13	2.41	1.51	1.43
5	B	6002	RXP	O1-C11	-2.40	1.19	1.23
5	B	6002	RXP	O2-C12	-2.40	1.18	1.23
4	F	5091	CPS	O2-C13	2.37	1.51	1.43
5	A	6001	RXP	C18-C17	2.31	1.44	1.37
4	D	5004	CPS	C20-C9	2.30	1.59	1.54
4	F	5091	CPS	C1-C2	2.28	1.58	1.54
4	B	5002	CPS	C20-C9	2.23	1.58	1.54
5	F	6006	RXP	C3-C4	-2.22	1.35	1.42
5	E	6005	RXP	C3-C4	-2.20	1.35	1.42
4	B	5002	CPS	C5-C6	-2.20	1.51	1.55
4	A	5006	CPS	C3-C19	-2.18	1.50	1.53
4	C	5008	CPS	C7-C6	-2.17	1.49	1.54
5	D	6004	RXP	C18-C17	2.14	1.44	1.37
4	F	5091	CPS	C29-N2	2.14	1.56	1.50
4	C	5003	CPS	C14-C13	2.14	1.56	1.51
5	F	6006	RXP	C5-N3	-2.13	1.33	1.37
4	A	5001	CPS	C7-C6	-2.11	1.49	1.54
5	B	6002	RXP	C1-N2	2.11	1.50	1.45
5	A	6001	RXP	C39-C14	-2.09	1.45	1.51
5	E	6005	RXP	C5-N3	-2.08	1.33	1.37
4	F	5091	CPS	C2-C19	2.07	1.59	1.56
5	C	6003	RXP	C5-N3	2.02	1.40	1.37

All (503) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5005	CPS	C6-C18-C17	12.17	126.85	111.81
4	C	5008	CPS	C6-C18-C17	11.95	126.58	111.81
4	B	5007	CPS	C6-C18-C17	11.91	126.53	111.81
4	E	5010	CPS	C6-C18-C17	11.82	126.41	111.81
4	A	5001	CPS	C6-C18-C17	11.67	126.23	111.81
4	A	5006	CPS	C6-C18-C17	11.36	125.84	111.81
4	D	5004	CPS	C6-C18-C17	11.32	125.80	111.81
4	D	5009	CPS	C6-C18-C17	11.30	125.77	111.81
4	C	5003	CPS	C6-C18-C17	11.27	125.73	111.81
4	F	5011	CPS	C6-C18-C17	11.24	125.70	111.81
4	B	5002	CPS	C6-C18-C17	11.23	125.69	111.81
5	B	6002	RXP	O6-C31-C32	11.17	137.51	109.38
4	F	5011	CPS	C19-C18-C17	-10.62	100.11	111.97
5	C	6003	RXP	C23-C22-N4	-10.53	102.38	112.02
4	E	5005	CPS	C19-C3-C4	9.85	127.20	114.35
5	D	6004	RXP	C2-C1-C11	9.74	124.09	109.80
4	D	5009	CPS	C19-C18-C17	-9.66	101.18	111.97
4	C	5003	CPS	C19-C18-C17	-9.60	101.25	111.97
4	E	5010	CPS	C19-C18-C17	-9.41	101.47	111.97
4	A	5006	CPS	C19-C18-C17	-9.39	101.48	111.97
4	D	5009	CPS	C19-C3-C4	9.27	126.45	114.35
4	B	5007	CPS	C19-C18-C17	-9.22	101.68	111.97
4	A	5001	CPS	C19-C3-C4	9.16	126.30	114.35
4	C	5008	CPS	C19-C3-C4	9.00	126.09	114.35
4	D	5004	CPS	C19-C18-C17	-8.95	101.98	111.97
4	A	5001	CPS	C19-C18-C17	-8.86	102.08	111.97
4	C	5003	CPS	C19-C3-C4	8.82	125.87	114.35
5	F	6006	RXP	O1P-P-C22	-8.81	98.21	112.22
4	B	5002	CPS	C19-C18-C17	-8.80	102.15	111.97
5	E	6005	RXP	O1P-P-C22	-8.79	98.24	112.22
4	E	5005	CPS	C19-C18-C17	-8.72	102.23	111.97
4	D	5004	CPS	C19-C3-C4	8.72	125.73	114.35
4	A	5006	CPS	C19-C3-C4	8.66	125.65	114.35
4	B	5007	CPS	C19-C3-C4	8.64	125.63	114.35
4	B	5002	CPS	C19-C3-C4	8.64	125.62	114.35
4	E	5010	CPS	C19-C3-C4	8.34	125.24	114.35
5	A	6001	RXP	C22-N4-C30	8.23	142.21	121.57
5	A	6001	RXP	C2-C1-C11	8.20	121.83	109.80
4	C	5003	CPS	C9-C5-C4	8.17	125.21	117.67
4	E	5005	CPS	C2-C19-C18	8.17	120.59	111.90
4	C	5008	CPS	C19-C18-C17	-8.16	102.86	111.97
5	B	6002	RXP	C23-C22-N4	-7.89	104.80	112.02
4	F	5091	CPS	C19-C18-C17	-7.85	103.21	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5009	CPS	C2-C19-C18	7.76	120.15	111.90
4	E	5005	CPS	C9-C5-C4	7.52	124.61	117.67
4	A	5006	CPS	C9-C5-C4	7.52	124.61	117.67
4	E	5005	CPS	C9-C5-C6	7.50	107.73	100.07
4	F	5011	CPS	C19-C3-C4	7.50	124.14	114.35
4	A	5001	CPS	C9-C5-C4	7.50	124.59	117.67
4	B	5002	CPS	C9-C5-C6	7.34	107.57	100.07
5	A	6001	RXP	C13-C38-C39	7.34	131.64	112.85
4	B	5002	CPS	C2-C19-C18	7.31	119.67	111.90
4	C	5008	CPS	C2-C19-C18	7.31	119.67	111.90
5	A	6001	RXP	C23-C22-N4	-7.29	105.35	112.02
4	F	5091	CPS	C6-C18-C17	7.23	120.75	111.81
4	A	5001	CPS	C2-C19-C18	7.18	119.53	111.90
5	B	6002	RXP	O2-C12-C20	-7.09	114.45	121.89
5	C	6003	RXP	O5-C30-N4	-7.01	112.43	124.90
4	A	5006	CPS	C2-C19-C18	7.00	119.34	111.90
4	C	5008	CPS	C9-C5-C6	6.99	107.21	100.07
4	C	5003	CPS	C2-C19-C18	6.98	119.33	111.90
4	F	5011	CPS	C9-C5-C4	6.97	124.10	117.67
5	C	6003	RXP	C21-P-C22	6.90	119.90	106.65
4	F	5091	CPS	C2-C19-C18	6.86	119.19	111.90
4	A	5006	CPS	C9-C5-C6	6.84	107.05	100.07
5	D	6004	RXP	C39-C14-C15	-6.79	103.88	121.23
4	D	5004	CPS	C9-C5-C4	6.78	123.93	117.67
4	A	5001	CPS	C9-C5-C6	6.71	106.92	100.07
5	C	6003	RXP	C2-C1-C11	6.68	119.61	109.80
4	D	5004	CPS	C2-C19-C18	6.68	119.00	111.90
4	A	5001	CPS	C7-C6-C18	-6.67	108.82	118.30
4	F	5091	CPS	C7-C6-C18	-6.58	108.95	118.30
4	D	5009	CPS	C9-C5-C6	6.54	106.76	100.07
4	B	5007	CPS	C2-C19-C18	6.53	118.84	111.90
4	B	5007	CPS	C9-C5-C4	6.49	123.66	117.67
4	F	5011	CPS	C7-C6-C18	-6.49	109.08	118.30
4	F	5011	CPS	C5-C6-C18	6.43	122.09	114.81
4	C	5003	CPS	C7-C6-C18	-6.42	109.17	118.30
4	C	5008	CPS	C7-C6-C18	-6.42	109.18	118.30
5	B	6002	RXP	C20-C12-N2	6.41	126.35	116.19
4	E	5010	CPS	C2-C19-C18	6.35	118.65	111.90
4	B	5007	CPS	C9-C5-C6	6.26	106.46	100.07
5	C	6003	RXP	C22-N4-C30	6.25	137.25	121.57
5	E	6005	RXP	C22-N4-C30	6.25	137.24	121.57
4	E	5005	CPS	C10-C5-C6	-6.24	101.31	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	6006	RXP	C22-N4-C30	6.24	137.21	121.57
4	C	5008	CPS	C10-C5-C6	-6.23	101.33	111.22
5	A	6001	RXP	C39-C14-C15	-6.21	105.36	121.23
4	F	5091	CPS	C3-C19-C18	-6.21	101.88	110.81
4	D	5004	CPS	C7-C6-C18	-6.20	109.49	118.30
4	E	5005	CPS	C7-C6-C18	-6.19	109.50	118.30
4	A	5006	CPS	C3-C19-C18	-6.17	101.93	110.81
4	A	5006	CPS	C7-C6-C18	-6.11	109.61	118.30
4	B	5002	CPS	C9-C5-C4	6.09	123.29	117.67
4	F	5091	CPS	C21-C20-C22	-6.08	100.00	110.37
4	C	5003	CPS	C3-C19-C18	-6.07	102.07	110.81
4	D	5009	CPS	C3-C19-C18	-6.07	102.08	110.81
4	B	5002	CPS	C10-C5-C6	-6.07	101.59	111.22
4	E	5010	CPS	C9-C5-C4	6.06	123.26	117.67
4	E	5010	CPS	C7-C6-C18	-6.03	109.73	118.30
4	F	5011	CPS	C3-C19-C18	-6.02	102.16	110.81
4	C	5008	CPS	C3-C19-C18	-6.02	102.16	110.81
4	E	5010	CPS	C3-C19-C18	-6.00	102.18	110.81
4	B	5007	CPS	C3-C19-C18	-6.00	102.18	110.81
4	E	5005	CPS	C3-C19-C18	-5.99	102.19	110.81
4	C	5003	CPS	C9-C5-C6	5.94	106.14	100.07
4	A	5001	CPS	C3-C19-C18	-5.91	102.30	110.81
4	D	5009	CPS	C9-C5-C4	5.89	123.11	117.67
4	C	5008	CPS	C9-C5-C4	5.88	123.09	117.67
4	B	5007	CPS	C7-C6-C18	-5.87	109.96	118.30
4	E	5010	CPS	C5-C6-C18	5.86	121.45	114.81
4	E	5010	CPS	C15-C16-C17	5.81	120.65	114.46
5	B	6002	RXP	C22-N4-C30	5.80	136.13	121.57
4	D	5004	CPS	C9-C5-C6	5.80	105.99	100.07
5	C	6003	RXP	O6-C31-C32	5.78	123.94	109.38
4	B	5002	CPS	C7-C6-C18	-5.76	110.10	118.30
5	D	6004	RXP	C1-C11-N1	-5.74	105.69	116.78
4	D	5004	CPS	C3-C19-C18	-5.72	102.58	110.81
4	D	5004	CPS	C15-C16-C17	5.71	120.54	114.46
4	F	5091	CPS	C15-C16-C17	5.64	120.47	114.46
4	E	5010	CPS	C9-C5-C6	5.63	105.82	100.07
5	C	6003	RXP	P-C22-N4	-5.63	96.34	109.19
5	C	6003	RXP	C39-C14-C15	-5.62	106.87	121.23
4	A	5006	CPS	C10-C5-C6	-5.58	102.35	111.22
4	B	5007	CPS	C5-C6-C18	5.58	121.13	114.81
4	A	5001	CPS	C10-C5-C6	-5.57	102.38	111.22
4	D	5004	CPS	C5-C6-C18	5.56	121.12	114.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5011	CPS	C2-C19-C18	5.56	117.81	111.90
4	B	5002	CPS	C7-C6-C5	5.51	109.09	103.58
4	A	5001	CPS	C15-C16-C17	5.51	120.33	114.46
4	C	5003	CPS	C5-C6-C18	5.50	121.04	114.81
4	F	5091	CPS	C16-C17-C18	5.49	117.33	111.51
4	B	5002	CPS	C3-C19-C18	-5.46	102.96	110.81
5	C	6003	RXP	C13-C38-C39	5.46	126.81	112.85
4	D	5004	CPS	C10-C5-C6	-5.42	102.61	111.22
5	B	6002	RXP	C39-C14-C15	-5.42	107.38	121.23
4	A	5006	CPS	C15-C16-C17	5.41	120.22	114.46
5	F	6006	RXP	C39-C14-C15	-5.37	107.49	121.23
5	D	6004	RXP	C24-C23-C22	5.37	122.59	113.47
5	E	6005	RXP	C39-C14-C15	-5.35	107.55	121.23
4	D	5009	CPS	C10-C5-C6	-5.34	102.74	111.22
4	C	5003	CPS	C15-C16-C17	5.33	120.14	114.46
4	E	5010	CPS	C10-C5-C6	-5.32	102.77	111.22
4	C	5008	CPS	C15-C16-C17	5.31	120.12	114.46
5	F	6006	RXP	C21-P-C22	5.29	116.81	106.65
5	E	6005	RXP	C21-P-C22	5.27	116.78	106.65
4	B	5002	CPS	C15-C16-C17	5.27	120.08	114.46
4	F	5091	CPS	C15-C14-C13	-5.27	105.21	112.95
4	C	5003	CPS	C10-C5-C6	-5.25	102.89	111.22
4	D	5009	CPS	C7-C6-C18	-5.24	110.85	118.30
4	E	5005	CPS	C15-C16-C17	5.23	120.03	114.46
5	B	6002	RXP	C13-C38-C39	5.20	126.16	112.85
4	B	5007	CPS	C16-C17-C18	5.20	117.02	111.51
5	C	6003	RXP	O1-C11-C1	-5.14	112.73	120.33
4	C	5003	CPS	C7-C6-C5	5.06	108.65	103.58
5	E	6005	RXP	O6-C31-C32	5.06	122.12	109.38
5	F	6006	RXP	O6-C31-C32	5.06	122.12	109.38
5	F	6006	RXP	C23-C22-N4	-5.06	107.39	112.02
5	E	6005	RXP	C23-C22-N4	-5.02	107.43	112.02
4	B	5007	CPS	C15-C16-C17	4.99	119.78	114.46
4	A	5006	CPS	C5-C6-C18	4.98	120.46	114.81
5	D	6004	RXP	C13-C38-C39	4.97	125.57	112.85
4	D	5004	CPS	C7-C6-C5	4.94	108.53	103.58
4	D	5009	CPS	C5-C6-C18	4.94	120.41	114.81
4	C	5008	CPS	C5-C6-C18	4.94	120.41	114.81
4	F	5091	CPS	C6-C5-C4	4.94	111.97	107.40
5	E	6005	RXP	C2-C1-C11	4.84	116.91	109.80
5	A	6001	RXP	C13-C20-C12	4.84	117.63	109.28
5	F	6006	RXP	C2-C1-C11	4.80	116.84	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	6004	RXP	C39-C14-C19	4.78	133.45	121.23
4	F	5091	CPS	C7-C6-C5	4.77	108.35	103.58
4	D	5009	CPS	O4-C4-C5	-4.75	103.32	111.13
4	A	5001	CPS	C7-C6-C5	4.73	108.31	103.58
4	F	5091	CPS	C19-C3-C4	4.69	120.47	114.35
4	A	5001	CPS	C5-C6-C18	4.68	120.12	114.81
4	F	5011	CPS	C10-C5-C6	-4.68	103.79	111.22
4	B	5007	CPS	C10-C5-C6	-4.64	103.85	111.22
5	D	6004	RXP	C13-C20-C12	4.63	117.29	109.28
4	A	5006	CPS	C7-C6-C5	4.58	108.17	103.58
4	E	5005	CPS	C10-C5-C4	-4.57	104.53	109.08
5	D	6004	RXP	O2P-P-C21	4.56	122.93	108.04
4	D	5009	CPS	C7-C6-C5	4.55	108.14	103.58
4	F	5091	CPS	C30-N2-C27	-4.52	97.77	111.72
5	D	6004	RXP	O1-C11-N1	4.52	130.68	123.03
5	E	6005	RXP	C1-C11-N1	-4.52	108.05	116.78
5	F	6006	RXP	C1-C11-N1	-4.51	108.06	116.78
5	F	6006	RXP	C3-C4-C6	-4.50	101.86	107.01
5	C	6003	RXP	O1-C11-N1	4.50	130.64	123.03
5	E	6005	RXP	C3-C4-C6	-4.50	101.88	107.01
5	E	6005	RXP	C13-C38-C39	4.49	124.34	112.85
4	C	5008	CPS	C7-C6-C5	4.48	108.06	103.58
5	F	6006	RXP	C13-C38-C39	4.48	124.30	112.85
5	B	6002	RXP	C13-C20-C12	4.46	116.98	109.28
4	F	5011	CPS	C9-C5-C6	4.45	104.62	100.07
5	F	6006	RXP	P-C21-C20	4.40	127.79	114.22
5	E	6005	RXP	P-C21-C20	4.39	127.75	114.22
4	F	5091	CPS	C9-C5-C4	4.35	121.68	117.67
5	C	6003	RXP	C36-C37-C32	4.34	127.90	120.64
5	A	6001	RXP	C39-C14-C19	4.31	132.26	121.23
5	D	6004	RXP	O1P-P-C22	-4.29	105.40	112.22
4	E	5005	CPS	C7-C6-C5	4.27	107.86	103.58
4	A	5006	CPS	C10-C5-C9	-4.27	104.44	111.22
5	A	6001	RXP	O2P-P-C21	4.26	121.94	108.04
4	C	5003	CPS	C10-C5-C9	-4.26	104.46	111.22
5	F	6006	RXP	O2-C12-C20	-4.25	117.43	121.89
4	C	5008	CPS	O4-C4-C5	-4.25	104.15	111.13
5	E	6005	RXP	O2-C12-C20	-4.24	117.45	121.89
4	F	5011	CPS	C5-C9-C20	4.22	124.58	119.51
4	E	5010	CPS	O4-C4-C5	-4.21	104.22	111.13
5	A	6001	RXP	O5-C30-N4	-4.20	117.42	124.90
4	F	5091	CPS	C21-C20-C9	4.20	120.31	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	6006	RXP	C39-C14-C19	4.18	131.91	121.23
4	A	5006	CPS	C16-C17-C18	4.18	115.93	111.51
5	C	6003	RXP	O6-C30-N4	4.17	120.55	110.57
5	E	6005	RXP	C39-C14-C19	4.17	131.88	121.23
4	C	5008	CPS	C5-C9-C20	4.13	124.47	119.51
4	A	5001	CPS	C16-C17-C18	4.12	115.87	111.51
4	F	5091	CPS	C11-C2-C19	-4.12	105.84	111.17
4	B	5002	CPS	C5-C6-C18	4.11	119.47	114.81
5	D	6004	RXP	C23-C22-N4	-4.11	108.26	112.02
5	C	6003	RXP	O1P-P-C22	-4.10	105.70	112.22
5	B	6002	RXP	C39-C14-C19	4.10	131.71	121.23
5	B	6002	RXP	O1P-P-C21	-4.10	97.33	111.16
5	C	6003	RXP	C13-C20-C12	4.08	116.33	109.28
4	E	5010	CPS	C5-C9-C20	4.07	124.41	119.51
4	D	5009	CPS	C15-C16-C17	4.06	118.79	114.46
4	E	5010	CPS	C16-C17-C18	4.05	115.80	111.51
4	F	5011	CPS	O4-C4-C5	-4.01	104.55	111.13
4	F	5091	CPS	O3-C17-C18	-4.00	100.75	109.23
4	F	5091	CPS	C10-C5-C4	-3.99	105.10	109.08
4	B	5007	CPS	C7-C6-C5	3.95	107.54	103.58
5	E	6005	RXP	C31-O6-C30	3.93	126.00	115.98
5	F	6006	RXP	C31-O6-C30	3.91	125.95	115.98
5	A	6001	RXP	O1-C11-N1	3.91	129.65	123.03
5	D	6004	RXP	O6-C30-N4	-3.91	101.22	110.57
4	F	5011	CPS	C15-C16-C17	3.90	118.61	114.46
4	E	5005	CPS	C5-C6-C18	3.88	119.21	114.81
5	B	6002	RXP	C35-C34-C33	3.85	126.58	120.17
4	A	5006	CPS	C5-C9-C20	3.83	124.12	119.51
4	F	5011	CPS	C7-C6-C5	3.81	107.39	103.58
5	D	6004	RXP	O1P-P-C21	-3.80	98.33	111.16
4	B	5002	CPS	C6-C5-C4	3.80	110.91	107.40
5	A	6001	RXP	O6-C31-C32	3.79	118.92	109.38
4	B	5007	CPS	C10-C5-C4	-3.79	105.30	109.08
4	D	5004	CPS	C10-C5-C4	-3.78	105.31	109.08
4	F	5091	CPS	C31-C30-N2	3.73	124.51	115.39
4	D	5004	CPS	O4-C4-C5	-3.71	105.03	111.13
4	A	5001	CPS	C10-C5-C4	-3.70	105.39	109.08
4	E	5010	CPS	C7-C6-C5	3.70	107.28	103.58
4	B	5002	CPS	C10-C5-C9	-3.69	105.37	111.22
4	E	5005	CPS	C16-C17-C18	3.68	115.41	111.51
4	A	5001	CPS	C15-C14-C13	-3.67	107.56	112.95
4	B	5002	CPS	C21-C20-C9	3.66	119.37	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5091	CPS	C14-C13-C12	3.66	115.21	110.54
4	E	5010	CPS	C10-C5-C4	-3.65	105.45	109.08
5	E	6005	RXP	C38-C39-C14	3.63	127.95	113.77
5	F	6006	RXP	C38-C39-C14	3.61	127.89	113.77
4	E	5005	CPS	C15-C14-C13	-3.61	107.66	112.95
4	B	5002	CPS	C19-C2-C15	-3.58	103.69	108.67
5	C	6003	RXP	C39-C14-C19	3.58	130.38	121.23
5	A	6001	RXP	O1-C11-C1	-3.57	115.06	120.33
4	A	5001	CPS	C10-C5-C9	-3.57	105.56	111.22
4	B	5007	CPS	C5-C9-C20	3.56	123.80	119.51
4	F	5011	CPS	C19-C2-C15	-3.56	103.72	108.67
5	A	6001	RXP	O2P-P-O1P	-3.54	108.39	113.71
4	C	5003	CPS	C16-C17-C18	3.54	115.26	111.51
4	A	5001	CPS	O4-C4-C5	-3.53	105.34	111.13
5	D	6004	RXP	C2-C3-C4	-3.52	119.26	126.56
5	D	6004	RXP	C16-C15-C14	-3.51	114.75	120.64
5	B	6002	RXP	C31-O6-C30	3.48	124.85	115.98
4	E	5010	CPS	C6-C5-C4	3.48	110.62	107.40
4	C	5003	CPS	C15-C14-C13	-3.48	107.85	112.95
5	D	6004	RXP	O6-C30-O5	3.47	131.77	124.19
4	E	5010	CPS	C15-C14-C13	-3.46	107.88	112.95
4	F	5091	CPS	C16-C15-C14	-3.44	107.05	111.14
5	A	6001	RXP	C3-C2-C1	-3.43	109.15	114.55
4	D	5004	CPS	C6-C5-C4	3.42	110.57	107.40
4	C	5008	CPS	C11-C2-C1	3.42	113.99	108.17
4	B	5007	CPS	O4-C4-C5	-3.41	105.52	111.13
5	C	6003	RXP	O1P-P-C21	-3.41	99.66	111.16
5	D	6004	RXP	C21-C20-C12	-3.40	105.02	110.03
4	E	5005	CPS	C10-C5-C9	-3.39	105.84	111.22
4	A	5006	CPS	O4-C4-C5	-3.38	105.57	111.13
4	C	5008	CPS	C19-C2-C15	-3.38	103.97	108.67
4	F	5011	CPS	C10-C5-C9	-3.37	105.87	111.22
5	A	6001	RXP	C18-C19-C14	-3.37	115.00	120.64
4	D	5009	CPS	C21-C20-C9	3.35	118.82	112.96
5	F	6006	RXP	O5-C30-N4	-3.34	118.95	124.90
5	A	6001	RXP	O1P-P-C21	-3.34	99.89	111.16
4	A	5001	CPS	C11-C2-C19	-3.33	106.86	111.17
5	E	6005	RXP	O5-C30-N4	-3.32	118.99	124.90
4	B	5007	CPS	C10-C5-C9	-3.30	105.98	111.22
5	E	6005	RXP	C13-C20-C12	3.30	114.98	109.28
5	F	6006	RXP	C13-C20-C12	3.30	114.98	109.28
5	C	6003	RXP	C31-O6-C30	-3.30	107.59	115.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5010	CPS	C19-C2-C15	-3.29	104.09	108.67
4	B	5007	CPS	C19-C2-C15	-3.28	104.10	108.67
4	B	5002	CPS	C16-C17-C18	3.28	114.98	111.51
4	B	5002	CPS	C10-C5-C4	-3.28	105.81	109.08
4	D	5009	CPS	C15-C14-C13	-3.27	108.15	112.95
4	F	5011	CPS	C21-C20-C9	3.26	118.68	112.96
4	E	5010	CPS	C21-C20-C9	3.26	118.67	112.96
4	B	5007	CPS	O3-C17-C18	-3.25	102.35	109.23
4	C	5003	CPS	O4-C4-C5	-3.24	105.81	111.13
4	D	5004	CPS	C21-C20-C9	3.24	118.63	112.96
4	D	5004	CPS	C15-C14-C13	-3.23	108.20	112.95
4	B	5007	CPS	C21-C20-C9	3.23	118.61	112.96
5	B	6002	RXP	C1-N2-C12	3.23	128.76	121.63
4	D	5009	CPS	C10-C5-C9	-3.22	106.11	111.22
5	A	6001	RXP	C35-C36-C37	-3.22	114.81	120.17
5	D	6004	RXP	C3-C4-C6	-3.21	103.34	107.01
5	D	6004	RXP	C38-C39-C14	3.20	126.29	113.77
4	C	5008	CPS	C21-C20-C9	3.20	118.57	112.96
5	D	6004	RXP	C21-P-C22	3.19	112.78	106.65
4	F	5011	CPS	C6-C5-C4	3.16	110.33	107.40
4	A	5001	CPS	C5-C9-C20	3.15	123.30	119.51
4	D	5004	CPS	C16-C17-C18	3.12	114.82	111.51
4	B	5007	CPS	C15-C14-C13	-3.12	108.37	112.95
4	A	5001	CPS	O3-C17-C18	-3.09	102.68	109.23
4	C	5003	CPS	C8-C9-C20	-3.08	106.36	112.06
4	D	5004	CPS	C11-C2-C19	-3.08	107.18	111.17
4	C	5003	CPS	C21-C20-C9	3.08	118.35	112.96
4	A	5006	CPS	C15-C14-C13	-3.08	108.44	112.95
4	D	5009	CPS	O4-C4-C3	-3.07	102.82	108.99
4	A	5001	CPS	C21-C20-C9	3.06	118.31	112.96
4	C	5008	CPS	C8-C9-C20	-3.05	106.42	112.06
4	E	5005	CPS	C6-C5-C4	3.05	110.22	107.40
4	A	5006	CPS	C8-C9-C20	-3.05	106.42	112.06
5	B	6002	RXP	C21-P-C22	3.05	112.51	106.65
4	D	5004	CPS	C10-C5-C9	-3.04	106.39	111.22
4	A	5006	CPS	C21-C20-C9	3.04	118.28	112.96
4	F	5011	CPS	O3-C17-C18	-3.04	102.80	109.23
5	C	6003	RXP	C35-C36-C37	-3.03	115.12	120.17
5	E	6005	RXP	C5-C3-C4	3.00	110.99	107.29
4	B	5002	CPS	O4-C4-C3	-3.00	102.96	108.99
5	B	6002	RXP	P-C22-C23	2.98	117.67	110.73
4	A	5006	CPS	C11-C2-C1	2.98	113.25	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5008	CPS	C10-C5-C4	-2.98	106.11	109.08
5	F	6006	RXP	C5-C3-C4	2.98	110.96	107.29
4	E	5010	CPS	O3-C17-C18	-2.97	102.94	109.23
4	F	5091	CPS	C10-C5-C6	-2.96	106.51	111.22
5	A	6001	RXP	C13-C20-C21	-2.96	101.72	110.12
5	C	6003	RXP	O2P-P-C22	-2.96	100.93	107.23
4	E	5005	CPS	C21-C20-C9	2.96	118.14	112.96
4	D	5004	CPS	O3-C17-C18	-2.95	102.97	109.23
4	E	5005	CPS	O4-C4-C5	-2.93	106.31	111.13
4	D	5009	CPS	C11-C2-C1	2.93	113.16	108.17
4	F	5091	CPS	C26-C25-N1	-2.92	103.41	112.21
4	D	5004	CPS	C19-C2-C15	-2.92	104.61	108.67
5	E	6005	RXP	C21-C20-C12	-2.91	105.74	110.03
4	E	5010	CPS	C1-C12-C13	2.90	115.18	110.37
4	C	5003	CPS	C11-C2-C19	-2.89	107.43	111.17
4	C	5003	CPS	O3-C17-C18	-2.89	103.10	109.23
4	B	5002	CPS	C8-C9-C20	-2.89	106.72	112.06
5	F	6006	RXP	C21-C20-C12	-2.89	105.78	110.03
4	A	5006	CPS	O3-C17-C18	-2.88	103.13	109.23
5	F	6006	RXP	C9-C7-C4	-2.88	116.69	120.88
5	C	6003	RXP	P-C22-C23	2.87	117.41	110.73
4	C	5003	CPS	C11-C2-C1	2.86	113.04	108.17
4	F	5091	CPS	C25-N1-C24	-2.86	117.02	122.84
4	E	5005	CPS	C8-C9-C20	-2.85	106.79	112.06
4	F	5011	CPS	C8-C9-C20	-2.85	106.80	112.06
5	D	6004	RXP	C31-O6-C30	2.85	123.23	115.98
4	A	5006	CPS	C16-C15-C14	-2.84	107.76	111.14
5	B	6002	RXP	C31-C32-C33	2.83	127.54	120.65
4	D	5004	CPS	C5-C9-C20	2.83	122.91	119.51
5	E	6005	RXP	C9-C7-C4	-2.82	116.77	120.88
4	C	5003	CPS	C16-C15-C14	-2.82	107.79	111.14
5	F	6006	RXP	C31-C32-C33	2.82	127.50	120.65
5	F	6006	RXP	O1P-P-C21	-2.81	101.68	111.16
5	E	6005	RXP	C31-C32-C33	2.81	127.48	120.65
5	E	6005	RXP	O1P-P-C21	-2.80	101.71	111.16
4	F	5091	CPS	C31-C32-S	2.79	116.88	113.20
4	E	5005	CPS	O3-C17-C18	-2.79	103.32	109.23
5	B	6002	RXP	C3-C5-N3	2.79	112.66	107.94
4	B	5002	CPS	C15-C14-C13	-2.79	108.86	112.95
4	A	5001	CPS	C8-C9-C20	-2.78	106.92	112.06
4	C	5003	CPS	C19-C2-C15	-2.78	104.80	108.67
4	C	5003	CPS	C14-C15-C2	2.78	115.68	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5002	CPS	C16-C15-C14	-2.78	107.84	111.14
4	C	5008	CPS	C16-C17-C18	2.77	114.44	111.51
5	E	6005	RXP	O6-C30-N4	2.76	117.18	110.57
5	A	6001	RXP	C20-C12-N2	2.76	120.56	116.19
5	B	6002	RXP	O1P-P-C22	-2.75	107.85	112.22
5	F	6006	RXP	O6-C30-N4	2.74	117.14	110.57
4	F	5091	CPS	C19-C2-C15	-2.74	104.86	108.67
5	C	6003	RXP	O2-C12-C20	-2.73	119.03	121.89
5	B	6002	RXP	C23-C24-C26	-2.73	115.55	120.90
5	D	6004	RXP	C26-C24-C25	2.73	122.76	118.16
4	A	5006	CPS	C19-C2-C15	-2.73	104.88	108.67
4	D	5009	CPS	C5-C9-C20	2.72	122.78	119.51
4	E	5005	CPS	C19-C2-C15	-2.72	104.89	108.67
4	F	5011	CPS	C15-C14-C13	-2.72	108.96	112.95
4	F	5011	CPS	C10-C5-C4	-2.71	106.37	109.08
4	C	5003	CPS	O4-C4-C3	-2.71	103.53	108.99
5	C	6003	RXP	C37-C32-C33	-2.70	113.61	118.16
4	C	5008	CPS	C6-C5-C4	2.70	109.89	107.40
4	E	5005	CPS	C5-C9-C20	2.69	122.75	119.51
4	B	5002	CPS	O3-C17-C18	-2.69	103.54	109.23
4	B	5007	CPS	C6-C5-C4	2.67	109.87	107.40
4	F	5011	CPS	C16-C17-C18	2.67	114.33	111.51
4	F	5011	CPS	C11-C2-C1	2.66	112.70	108.17
4	D	5009	CPS	C10-C5-C4	-2.66	106.43	109.08
4	D	5004	CPS	C11-C2-C1	2.65	112.68	108.17
5	A	6001	RXP	C21-P-C22	2.64	111.73	106.65
4	A	5001	CPS	C19-C2-C15	-2.64	105.00	108.67
4	D	5009	CPS	C6-C5-C4	2.63	109.83	107.40
4	C	5008	CPS	C10-C5-C9	-2.63	107.04	111.22
5	D	6004	RXP	C19-C14-C15	2.63	122.59	118.16
4	F	5091	CPS	C23-C24-N1	-2.62	111.74	116.50
5	A	6001	RXP	C1-N2-C12	2.61	127.41	121.63
5	C	6003	RXP	C11-C1-N2	-2.61	105.10	111.28
4	E	5010	CPS	C10-C5-C9	-2.61	107.08	111.22
5	A	6001	RXP	C3-C4-C6	-2.59	104.05	107.01
4	C	5008	CPS	C15-C14-C13	-2.59	109.15	112.95
4	B	5002	CPS	C1-C12-C13	2.59	114.65	110.37
5	B	6002	RXP	O2P-P-C21	2.58	116.48	108.04
5	F	6006	RXP	C24-C23-C22	2.59	117.86	113.47
5	D	6004	RXP	C1-N2-C12	2.58	127.34	121.63
5	E	6005	RXP	C24-C23-C22	2.57	117.83	113.47
4	C	5003	CPS	C5-C9-C20	2.56	122.59	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5010	CPS	C11-C2-C1	2.56	112.53	108.17
4	A	5001	CPS	C6-C5-C4	2.56	109.77	107.40
4	D	5004	CPS	O4-C4-C3	-2.55	103.86	108.99
4	D	5009	CPS	C19-C2-C15	-2.55	105.13	108.67
4	E	5005	CPS	C11-C2-C1	2.54	112.50	108.17
4	A	5001	CPS	C11-C2-C1	2.54	112.49	108.17
5	E	6005	RXP	O1-C11-N1	2.52	127.30	123.03
5	A	6001	RXP	C29-C27-C25	-2.52	115.98	120.17
5	C	6003	RXP	C19-C14-C15	2.51	122.39	118.16
5	A	6001	RXP	C19-C14-C15	2.50	122.38	118.16
4	A	5006	CPS	O4-C4-C3	-2.51	103.95	108.99
5	F	6006	RXP	O1-C11-N1	2.50	127.26	123.03
4	F	5091	CPS	C9-C5-C6	2.49	102.61	100.07
4	D	5004	CPS	C1-C12-C13	2.48	114.48	110.37
4	C	5003	CPS	C10-C5-C4	-2.48	106.61	109.08
5	D	6004	RXP	C11-C1-N2	-2.47	105.43	111.28
4	D	5004	CPS	C8-C9-C20	-2.47	107.50	112.06
4	C	5003	CPS	C1-C12-C13	2.46	114.45	110.37
4	B	5007	CPS	C1-C12-C13	2.46	114.44	110.37
5	F	6006	RXP	C34-C33-C32	2.46	124.74	120.64
4	E	5005	CPS	C16-C15-C14	-2.45	108.22	111.14
5	F	6006	RXP	C10-C9-C7	2.45	124.06	120.47
5	A	6001	RXP	O2-C12-N2	-2.45	118.21	122.93
5	E	6005	RXP	C10-C9-C7	2.45	124.05	120.47
5	D	6004	RXP	P-C21-C20	2.44	121.76	114.22
5	E	6005	RXP	C34-C33-C32	2.44	124.72	120.64
4	B	5002	CPS	C11-C2-C19	-2.44	108.01	111.17
4	E	5005	CPS	C1-C12-C13	2.42	114.37	110.37
5	B	6002	RXP	C38-C39-C14	2.39	123.13	113.77
4	F	5091	CPS	O1S-S-O3S	2.39	117.04	112.44
4	A	5001	CPS	C1-C12-C13	2.38	114.32	110.37
4	C	5008	CPS	C16-C15-C14	-2.38	108.31	111.14
4	D	5009	CPS	C16-C15-C14	-2.37	108.32	111.14
4	F	5011	CPS	C1-C12-C13	2.37	114.30	110.37
5	D	6004	RXP	C3-C5-N3	2.36	111.94	107.94
4	F	5091	CPS	C22-C20-C9	2.36	115.55	110.25
4	B	5002	CPS	O4-C4-C5	-2.35	107.27	111.13
5	E	6005	RXP	C2-C3-C4	-2.35	121.69	126.56
5	F	6006	RXP	C2-C3-C4	-2.34	121.69	126.56
4	B	5007	CPS	C11-C2-C1	2.34	112.16	108.17
4	D	5009	CPS	C16-C17-C18	2.33	113.97	111.51
4	B	5002	CPS	C11-C2-C1	2.30	112.08	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	6003	RXP	C21-C20-C12	-2.29	106.65	110.03
5	A	6001	RXP	C9-C7-C4	-2.29	117.55	120.88
4	A	5001	CPS	C16-C15-C14	-2.28	108.42	111.14
4	D	5004	CPS	C16-C15-C14	-2.28	108.43	111.14
4	B	5007	CPS	C8-C9-C20	-2.27	107.87	112.06
5	B	6002	RXP	O6-C30-O5	-2.25	119.27	124.19
4	E	5010	CPS	C8-C9-C20	-2.24	107.91	112.06
4	F	5091	CPS	O2S-S-C32	-2.24	100.21	105.99
5	A	6001	RXP	C36-C37-C32	2.23	124.37	120.64
5	D	6004	RXP	O1-C11-C1	2.23	123.63	120.33
5	C	6003	RXP	C7-C4-C3	2.22	138.26	133.71
4	B	5007	CPS	O4-C4-C3	-2.21	104.55	108.99
5	E	6005	RXP	C31-C32-C37	-2.20	115.30	120.65
5	F	6006	RXP	C31-C32-C37	-2.19	115.33	120.65
5	F	6006	RXP	C35-C36-C37	-2.19	116.53	120.17
5	E	6005	RXP	C35-C36-C37	-2.18	116.54	120.17
5	F	6006	RXP	O2P-P-C21	2.18	115.14	108.04
5	E	6005	RXP	O2P-P-C21	2.17	115.12	108.04
4	F	5091	CPS	C1-C2-C19	2.17	114.93	111.45
5	D	6004	RXP	C2-C3-C5	2.16	131.82	128.12
4	F	5091	CPS	C28-N2-C30	2.16	115.07	109.38
5	B	6002	RXP	C31-C32-C37	-2.16	115.40	120.65
4	B	5007	CPS	C16-C15-C14	-2.15	108.58	111.14
5	C	6003	RXP	C18-C19-C14	-2.13	117.06	120.64
4	E	5005	CPS	C14-C15-C2	2.13	114.98	112.67
5	C	6003	RXP	C2-C1-N2	2.12	115.24	110.80
5	A	6001	RXP	C8-C6-C4	2.12	124.23	120.96
5	B	6002	RXP	C36-C35-C34	-2.10	115.60	119.97
5	D	6004	RXP	C23-C24-C26	-2.09	116.79	120.90
4	C	5003	CPS	C6-C5-C4	2.09	109.33	107.40
4	D	5009	CPS	C14-C15-C2	2.09	114.93	112.67
4	D	5009	CPS	C1-C12-C13	2.06	113.78	110.37
4	D	5009	CPS	C8-C9-C20	-2.06	108.26	112.06
4	E	5010	CPS	C11-C2-C19	-2.05	108.51	111.17
5	B	6002	RXP	P-C21-C20	2.05	120.53	114.22
5	D	6004	RXP	C27-C25-C24	-2.04	117.22	120.64
5	A	6001	RXP	C2-C3-C4	-2.03	122.34	126.56
5	A	6001	RXP	C5-C3-C4	2.03	109.79	107.29
5	C	6003	RXP	O2P-P-C21	2.02	114.65	108.04
4	F	5011	CPS	C3-C4-C5	-2.02	109.14	111.21

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	6003	RXP	O5-C30-N4-C22
5	F	6006	RXP	O5-C30-N4-C22
5	E	6005	RXP	O5-C30-N4-C22
5	A	6001	RXP	O5-C30-N4-C22
5	B	6002	RXP	O5-C30-N4-C22

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	162/165 (98%)	-0.55	1 (0%) 86 89	15, 26, 38, 50	0
1	B	164/165 (99%)	-0.22	5 (3%) 48 45	20, 36, 53, 60	0
1	C	162/165 (98%)	-0.45	2 (1%) 75 77	19, 30, 44, 53	0
1	D	162/165 (98%)	-0.42	2 (1%) 75 77	16, 29, 45, 55	0
1	E	165/165 (100%)	-0.41	2 (1%) 75 77	14, 31, 48, 56	0
1	F	162/165 (98%)	-0.42	4 (2%) 54 52	17, 31, 43, 56	0
All	All	977/990 (98%)	-0.41	16 (1%) 67 69	14, 30, 47, 60	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	ALA	6.7
1	C	245	TYR	4.3
1	E	233	ALA	4.3
1	F	233	ALA	3.9
1	F	245	TYR	3.7
1	D	233	ALA	3.3
1	C	233	ALA	3.2
1	B	188	LYS	3.0
1	E	265	GLN	2.7
1	A	101	MET	2.6
1	F	189	THR	2.6
1	B	255	ARG	2.3
1	D	101	MET	2.3
1	B	171	ASN	2.2
1	B	231	THR	2.1
1	F	188	LYS	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	RXP	E	6005	50/50	0.30	8.01	32,41,62,62	0
4	CPS	E	5005	26/42	0.27	5.32	46,48,49,50	4
4	CPS	F	5091	42/42	0.33	4.70	17,17,17,17	0
5	RXP	C	6003	50/50	0.21	4.02	25,34,53,54	0
5	RXP	A	6001	50/50	0.20	2.89	22,29,50,51	0
4	CPS	B	5002	26/42	0.26	2.42	50,51,52,53	4
5	RXP	B	6002	50/50	0.25	2.40	36,44,63,64	0
5	RXP	D	6004	50/50	0.18	2.20	21,27,42,43	0
5	RXP	F	6006	50/50	0.18	2.18	20,25,52,53	0
4	CPS	C	5008	26/42	0.20	1.37	48,49,50,50	4
4	CPS	D	5004	26/42	0.20	1.19	35,37,38,39	4
4	CPS	F	5011	26/42	0.22	0.95	53,54,55,55	4
4	CPS	D	5009	26/42	0.19	0.89	58,59,59,60	4
4	CPS	A	5006	26/42	0.18	0.66	49,50,51,51	4
4	CPS	C	5003	26/42	0.17	0.45	34,36,38,38	4
4	CPS	A	5001	26/42	0.15	0.33	34,36,37,39	4
3	CA	D	5512	1/1	0.11	-0.05	15,15,15,15	0
4	CPS	E	5010	26/42	0.12	-0.38	30,32,34,34	4
4	CPS	B	5007	26/42	0.12	-0.53	33,34,35,37	4
3	CA	F	5518	1/1	0.07	-1.74	18,18,18,18	0
3	CA	B	5506	1/1	0.05	-2.09	26,26,26,26	0
2	ZN	A	5501	1/1	0.07	-2.46	24,24,24,24	0
2	ZN	C	5507	1/1	0.08	-2.49	23,23,23,23	0
2	ZN	A	5502	1/1	0.07	-2.53	19,19,19,19	0
2	ZN	D	5511	1/1	0.08	-2.54	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	D	5510	1/1	0.08	-2.74	22,22,22,22	0
3	CA	A	5503	1/1	0.04	-2.86	18,18,18,18	0
2	ZN	E	5513	1/1	0.07	-3.39	24,24,24,24	0
3	CA	E	5515	1/1	0.06	-3.85	28,28,28,28	0
2	ZN	B	5505	1/1	0.06	-3.86	26,26,26,26	0
2	ZN	F	5517	1/1	0.08	-4.11	23,23,23,23	0
2	ZN	F	5516	1/1	0.08	-4.50	26,26,26,26	0
3	CA	C	5509	1/1	0.05	-4.55	24,24,24,24	0
2	ZN	B	5504	1/1	0.07	-5.16	25,25,25,25	0
2	ZN	C	5508	1/1	0.04	-7.81	16,16,16,16	0
2	ZN	E	5514	1/1	0.04	-13.73	21,21,21,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.