



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:59 am BST

PDB ID : 2NXX
Title : Crystal Structure of the Ligand-Binding Domains of the *T.castaneum* (Coleoptera) Heterodimer EcrUSP Bound to Ponasterone A
Authors : Iwema, T.; Billas, I.; Moras, D.
Deposited on : 2006-11-20
Resolution : 2.75 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

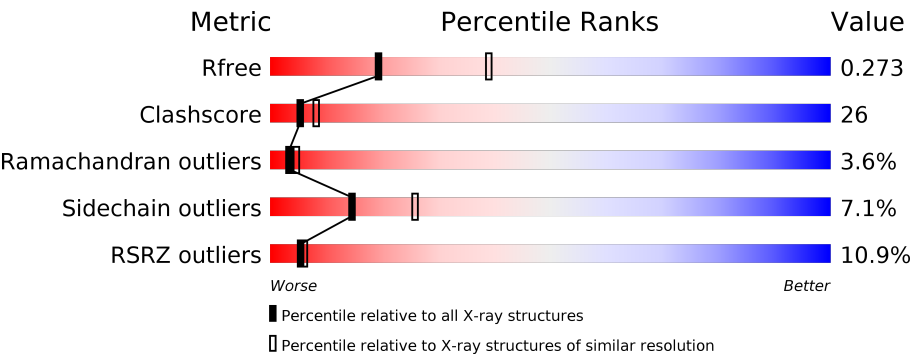
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

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 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 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	235	
1	B	235	
1	C	235	
1	D	235	
2	E	248	
2	F	248	

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Mol	Chain	Length	Quality of chain
2	G	248	<div><div></div><div>6%</div><div>59%</div><div>28%</div><div>6%</div><div>6%</div></div>
2	H	248	<div><div></div><div>5%</div><div>56%</div><div>31%</div><div>6%</div><div>6%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15241 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.

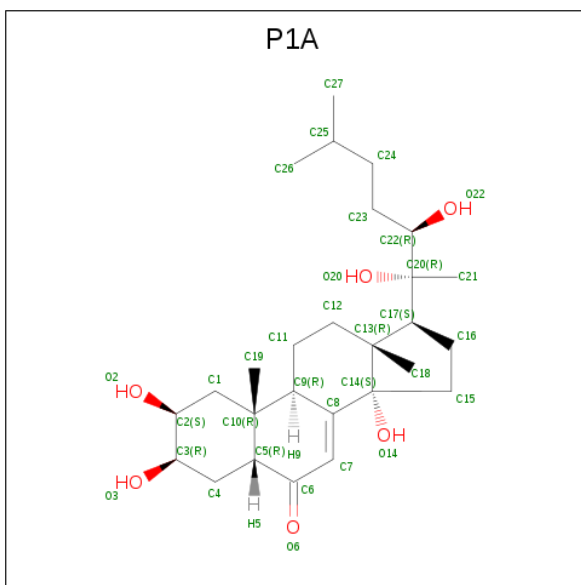
- Molecule 1 is a protein called Ultraspiracle (USP, NR2B4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1780	1137	308	323	12			
1	B	228	Total	C	N	O	S	0	0	0
			1802	1150	312	328	12			
1	C	225	Total	C	N	O	S	0	0	0
			1785	1140	309	324	12			
1	D	227	Total	C	N	O	S	0	0	0
			1797	1147	311	327	12			

- Molecule 2 is a protein called Ecdysone Receptor (EcR, NRH1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	234	Total	C	N	O	S	0	0	0
			1922	1226	327	358	11			
2	F	233	Total	C	N	O	S	0	0	0
			1917	1223	326	357	11			
2	G	233	Total	C	N	O	S	0	0	0
			1914	1220	326	357	11			
2	H	234	Total	C	N	O	S	0	0	0
			1925	1229	327	358	11			

- Molecule 3 is 2,3,14,20,22-PENTAHYDROXYCHOLEST-7-EN-6-ONE (three-letter code: P1A) (formula: C₂₇H₄₄O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 33 27 6	0	0
3	F	1	Total C O 33 27 6	0	0
3	G	1	Total C O 33 27 6	0	0
3	H	1	Total C O 33 27 6	0	0

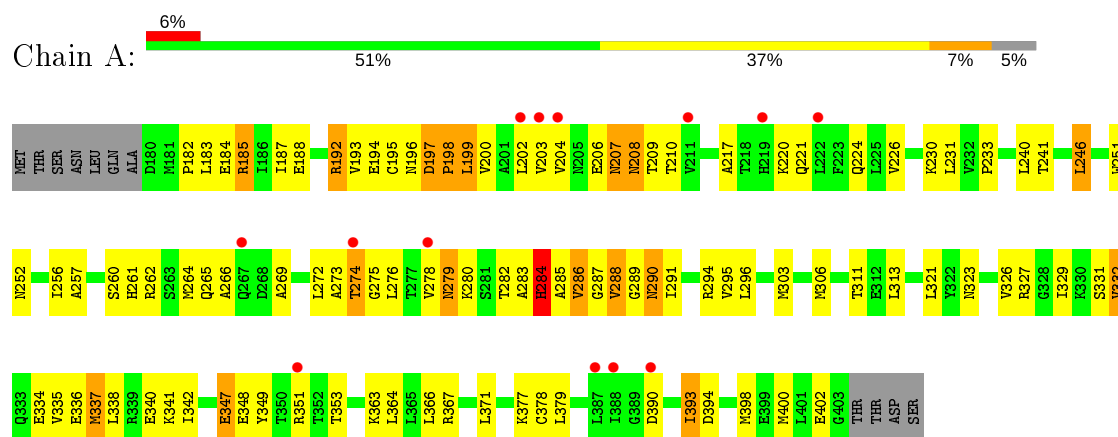
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	51	Total O 51 51	0	0
4	E	53	Total O 53 53	0	0
4	B	23	Total O 23 23	0	0
4	F	41	Total O 41 41	0	0
4	C	16	Total O 16 16	0	0
4	G	30	Total O 30 30	0	0
4	D	26	Total O 26 26	0	0
4	H	27	Total O 27 27	0	0

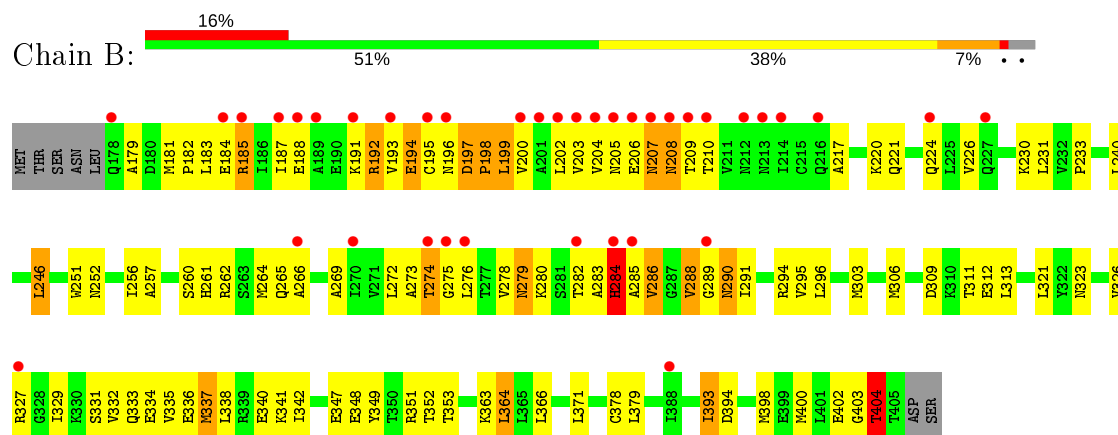
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

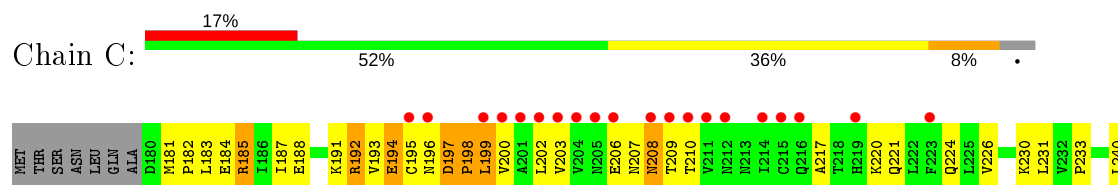
• Molecule 1: Ultraspiracle (USP, NR2B4)

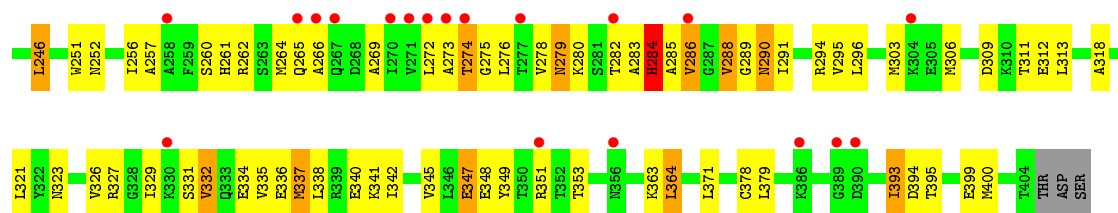


• Molecule 1: Ultraspiracle (USP, NR2B4)

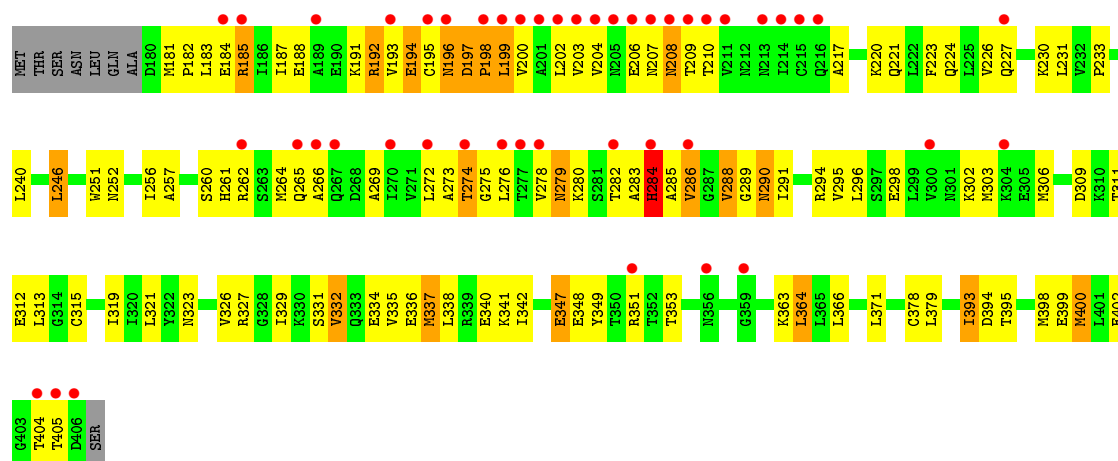


• Molecule 1: Ultraspiracle (USP, NR2B4)

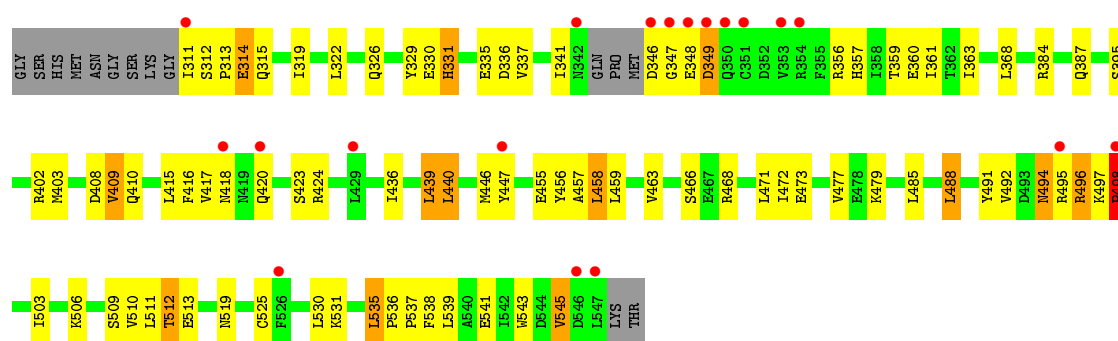




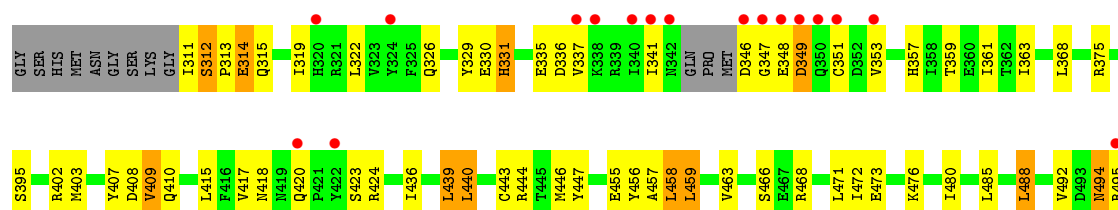
• Molecule 1: Ultraspiracle (USP, NR2B4)

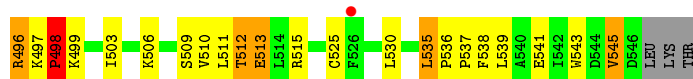


• Molecule 2: Ecdysone Receptor (EcR, NRH1)

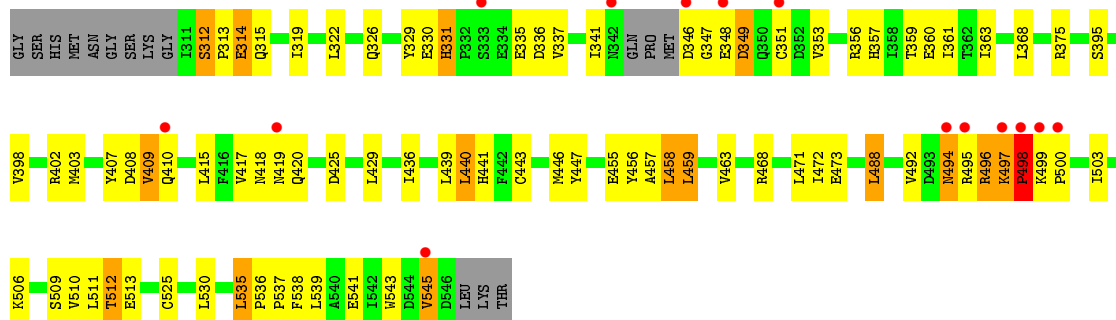


• Molecule 2: Ecdysone Receptor (EcR, NRH1)

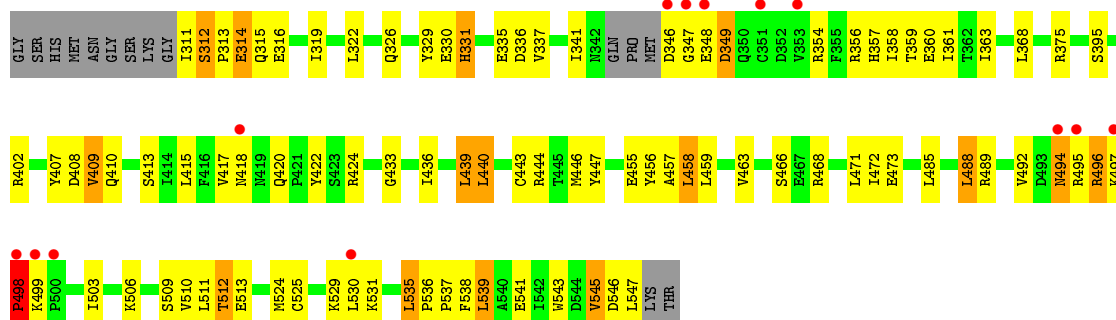




• Molecule 2: Ecdysone Receptor (EcR, NRH1)



• Molecule 2: Ecdysone Receptor (EcR, NRH1)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.54Å 89.63Å 160.25Å 90.00° 91.97° 90.00°	Depositor
Resolution (Å)	50.00 – 2.75 47.90 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.75) 97.6 (47.90-2.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.281 0.241 , 0.273	Depositor DCC
R_{free} test set	2958 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15241	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P1A

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	0.36	0/1810	0.59	0/2450
1	B	0.41	2/1832 (0.1%)	0.76	6/2481 (0.2%)
1	C	0.35	0/1815	0.58	0/2457
1	D	0.36	0/1827	0.60	0/2474
2	E	0.42	0/1957	0.75	4/2641 (0.2%)
2	F	0.41	0/1952	0.74	4/2634 (0.2%)
2	G	0.40	0/1949	0.74	4/2630 (0.2%)
2	H	0.41	0/1960	0.76	4/2645 (0.2%)
All	All	0.39	2/15102 (0.0%)	0.70	22/20412 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	404	THR	C-O	6.22	1.35	1.23
1	B	404	THR	CA-C	-5.58	1.38	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	497	LYS	C-N-CD	-21.45	73.41	120.60
2	G	497	LYS	C-N-CD	-21.40	73.52	120.60
2	E	497	LYS	C-N-CD	-21.39	73.55	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	497	LYS	C-N-CD	-21.20	73.96	120.60
1	B	404	THR	CA-C-N	-14.42	85.47	117.20
2	E	497	LYS	C-N-CA	10.43	165.82	122.00
2	G	497	LYS	C-N-CA	10.21	164.90	122.00
2	H	497	LYS	C-N-CA	9.98	163.92	122.00
2	F	497	LYS	C-N-CA	9.84	163.31	122.00
1	B	403	GLY	N-CA-C	9.18	136.04	113.10
1	B	404	THR	C-N-CA	9.09	144.43	121.70
1	B	404	THR	O-C-N	7.37	134.49	122.70
2	H	498	PRO	CA-N-CD	-6.00	103.11	111.50
2	F	498	PRO	CA-N-CD	-5.96	103.15	111.50
1	B	404	THR	N-CA-C	5.86	126.81	111.00
2	G	498	PRO	CA-N-CD	-5.84	103.32	111.50
2	E	497	LYS	N-CA-C	5.72	126.43	111.00
1	B	404	THR	CA-C-O	5.64	131.94	120.10
2	F	497	LYS	N-CA-C	5.59	126.09	111.00
2	E	498	PRO	CA-N-CD	-5.49	103.82	111.50
2	H	497	LYS	N-CA-C	5.40	125.57	111.00
2	G	497	LYS	N-CA-C	5.16	124.93	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	404	THR	Mainchain

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	1780	0	1837	112	0
1	B	1802	0	1852	145	0
1	C	1785	0	1839	108	0
1	D	1797	0	1848	148	0
2	E	1922	0	1927	78	0
2	F	1917	0	1925	71	0
2	G	1914	0	1916	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1925	0	1936	87	0
3	E	33	0	44	4	0
3	F	33	0	44	3	0
3	G	33	0	44	2	0
3	H	33	0	44	2	0
4	A	51	0	0	8	0
4	B	23	0	0	3	0
4	C	16	0	0	1	0
4	D	26	0	0	3	0
4	E	53	0	0	6	0
4	F	41	0	0	3	0
4	G	30	0	0	4	0
4	H	27	0	0	3	0
All	All	15241	0	15256	795	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 26.

All (795) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:VAL:HG12	1:B:289:GLY:H	1.10	1.15
2:F:311:ILE:HG22	2:F:312:SER:H	1.07	1.14
1:D:288:VAL:HG12	1:D:289:GLY:H	1.08	1.12
1:A:288:VAL:HG12	1:A:289:GLY:H	1.09	1.08
1:B:353:THR:HG22	2:G:419:ASN:HB3	1.31	1.08
1:C:288:VAL:HG12	1:C:289:GLY:H	1.09	1.08
1:B:179:ALA:HB3	1:B:341:LYS:HE3	1.37	1.02
1:B:351:ARG:HH22	2:G:410:GLN:HG3	1.26	0.98
1:B:351:ARG:NH2	2:G:410:GLN:HG3	1.79	0.97
2:F:311:ILE:HG22	2:F:312:SER:N	1.80	0.95
1:B:197:ASP:HB2	1:B:198:PRO:CD	1.97	0.94
1:D:197:ASP:HB2	1:D:198:PRO:CD	1.98	0.94
1:A:197:ASP:HB2	1:A:198:PRO:CD	1.96	0.94
1:C:197:ASP:HB2	1:C:198:PRO:CD	1.97	0.93
2:E:525:CYS:HB3	2:E:545:VAL:HG11	1.50	0.93
2:E:496:ARG:O	2:E:498:PRO:HD2	1.67	0.93
1:D:279:ASN:H	1:D:282:THR:HG23	1.33	0.93
1:A:221:GLN:HE22	1:A:262:ARG:HH22	1.17	0.92
2:F:496:ARG:O	2:F:498:PRO:HD2	1.69	0.92
2:G:496:ARG:O	2:G:498:PRO:HD2	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:311:ILE:CG2	2:F:312:SER:H	1.80	0.92
1:B:279:ASN:H	1:B:282:THR:HG23	1.34	0.92
1:A:279:ASN:H	1:A:282:THR:HG23	1.35	0.92
2:H:496:ARG:O	2:H:498:PRO:HD2	1.69	0.92
2:F:525:CYS:HB3	2:F:545:VAL:HG11	1.53	0.91
2:H:311:ILE:HG22	2:H:312:SER:H	1.33	0.91
1:C:279:ASN:H	1:C:282:THR:HG23	1.34	0.90
1:B:221:GLN:HE22	1:B:262:ARG:HH22	1.19	0.90
2:H:311:ILE:HG22	2:H:312:SER:N	1.86	0.90
1:D:230:LYS:HD3	1:D:404:THR:O	1.70	0.90
2:G:525:CYS:HB3	2:G:545:VAL:HG11	1.55	0.89
2:H:311:ILE:CG2	2:H:312:SER:H	1.86	0.89
2:E:311:ILE:HG22	2:E:312:SER:H	1.36	0.89
2:H:525:CYS:HB3	2:H:545:VAL:HG11	1.51	0.89
1:A:288:VAL:HG12	1:A:289:GLY:N	1.89	0.88
1:D:288:VAL:HG12	1:D:289:GLY:N	1.88	0.88
2:E:495:ARG:O	2:E:496:ARG:HG2	1.74	0.87
1:A:197:ASP:HB2	1:A:198:PRO:HD3	1.56	0.87
2:G:495:ARG:O	2:G:496:ARG:HG2	1.75	0.87
2:H:495:ARG:O	2:H:496:ARG:HG2	1.74	0.87
1:B:197:ASP:HB2	1:B:198:PRO:HD3	1.56	0.86
1:D:260:SER:HB3	1:D:303:MET:HE1	1.56	0.86
1:C:197:ASP:HB2	1:C:198:PRO:HD3	1.56	0.86
2:F:495:ARG:O	2:F:496:ARG:HG2	1.74	0.86
1:B:353:THR:CG2	2:G:419:ASN:HB3	2.06	0.86
1:C:288:VAL:HG12	1:C:289:GLY:N	1.89	0.86
1:B:260:SER:HB3	1:B:303:MET:HE1	1.56	0.86
1:D:197:ASP:HB2	1:D:198:PRO:HD3	1.57	0.86
1:B:192:ARG:HB2	1:B:192:ARG:HH11	1.41	0.85
1:B:288:VAL:HG12	1:B:289:GLY:N	1.90	0.85
2:H:408:ASP:HB2	2:H:415:LEU:HD21	1.58	0.85
1:D:192:ARG:HH11	1:D:192:ARG:HB2	1.42	0.85
1:C:260:SER:HB3	1:C:303:MET:HE1	1.57	0.85
1:C:192:ARG:HB2	1:C:192:ARG:HH11	1.42	0.84
1:C:221:GLN:HE22	1:C:262:ARG:HH22	1.22	0.84
1:D:221:GLN:HE22	1:D:262:ARG:HH22	1.20	0.84
2:E:408:ASP:HB2	2:E:415:LEU:HD21	1.60	0.83
2:F:408:ASP:HB2	2:F:415:LEU:HD21	1.60	0.83
1:B:207:ASN:HB3	1:D:265:GLN:HA	1.61	0.83
1:B:203:VAL:HG13	1:D:196:ASN:HD21	1.41	0.82
2:G:408:ASP:HB2	2:G:415:LEU:HD21	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:HB2	1:A:192:ARG:HH11	1.42	0.82
1:A:260:SER:HB3	1:A:303:MET:HE1	1.61	0.82
1:D:230:LYS:HE2	1:D:405:THR:HA	1.61	0.81
2:E:311:ILE:HG22	2:E:312:SER:N	1.90	0.81
1:A:367:ARG:HD3	4:A:453:HOH:O	1.81	0.80
1:A:202:LEU:HD13	1:A:276:LEU:HD21	1.65	0.79
2:E:535:LEU:HD22	2:E:536:PRO:HD2	1.65	0.79
2:H:545:VAL:HG12	2:H:545:VAL:O	1.81	0.79
1:C:284:HIS:CD2	1:C:284:HIS:H	2.00	0.79
2:F:418:ASN:ND2	2:F:420:GLN:HB2	1.97	0.79
2:E:418:ASN:ND2	2:E:420:GLN:HB2	1.98	0.79
2:E:311:ILE:CG2	2:E:312:SER:H	1.96	0.79
1:D:202:LEU:HD13	1:D:276:LEU:HD21	1.64	0.78
1:D:284:HIS:H	1:D:284:HIS:CD2	1.99	0.78
2:G:418:ASN:ND2	2:G:420:GLN:HB2	1.97	0.78
1:A:284:HIS:CD2	1:A:284:HIS:H	2.01	0.78
1:B:288:VAL:CG1	1:B:289:GLY:H	1.96	0.77
1:C:202:LEU:HD13	1:C:276:LEU:HD21	1.65	0.77
2:H:547:LEU:O	2:H:547:LEU:HD23	1.83	0.77
1:B:353:THR:HG22	2:G:419:ASN:CB	2.12	0.77
2:F:545:VAL:HG12	2:F:545:VAL:O	1.85	0.77
1:D:288:VAL:CG1	1:D:289:GLY:H	1.94	0.76
1:B:202:LEU:HD13	1:B:276:LEU:HD21	1.67	0.76
1:B:284:HIS:H	1:B:284:HIS:CD2	2.01	0.76
2:H:418:ASN:ND2	2:H:420:GLN:HB2	2.00	0.76
1:A:221:GLN:NE2	1:A:262:ARG:HH22	1.82	0.76
2:E:545:VAL:O	2:E:545:VAL:HG12	1.84	0.76
2:H:535:LEU:HD22	2:H:536:PRO:HD2	1.68	0.76
1:B:203:VAL:HG13	1:D:196:ASN:ND2	2.00	0.75
1:D:221:GLN:NE2	1:D:262:ARG:HH22	1.84	0.75
1:B:221:GLN:NE2	1:B:262:ARG:HH22	1.82	0.75
2:G:545:VAL:O	2:G:545:VAL:HG12	1.86	0.75
1:B:207:ASN:HB3	1:D:265:GLN:CA	2.17	0.75
4:D:415:HOH:O	2:H:512:THR:HG21	1.87	0.74
1:D:185:ARG:HE	1:D:185:ARG:HA	1.53	0.74
2:G:535:LEU:HD22	2:G:536:PRO:HD2	1.70	0.73
1:C:221:GLN:NE2	1:C:262:ARG:HH22	1.85	0.73
1:D:230:LYS:HZ3	1:D:405:THR:N	1.87	0.73
1:D:261:HIS:CG	1:D:313:LEU:HD22	2.23	0.73
1:B:205:ASN:HB3	1:D:265:GLN:CB	2.19	0.73
1:B:185:ARG:HE	1:B:185:ARG:HA	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ARG:HE	1:C:185:ARG:HA	1.54	0.72
1:B:278:VAL:HG13	1:B:282:THR:O	1.89	0.72
2:F:513:GLU:HG3	4:F:552:HOH:O	1.87	0.72
1:A:185:ARG:HE	1:A:185:ARG:HA	1.54	0.72
2:F:488:LEU:O	2:F:492:VAL:HG23	1.90	0.72
2:F:535:LEU:HD22	2:F:536:PRO:HD2	1.69	0.72
1:C:284:HIS:HD2	1:C:284:HIS:H	1.37	0.71
1:D:284:HIS:H	1:D:284:HIS:HD2	1.36	0.71
1:B:351:ARG:HH22	2:G:410:GLN:CG	2.01	0.71
1:D:278:VAL:HG13	1:D:282:THR:O	1.90	0.71
1:A:288:VAL:CG1	1:A:289:GLY:H	1.95	0.71
1:B:207:ASN:CB	1:D:265:GLN:HA	2.21	0.71
1:B:203:VAL:HB	1:B:210:THR:HG22	1.74	0.70
1:B:398:MET:HE3	4:B:424:HOH:O	1.91	0.70
2:H:348:GLU:HG3	2:H:349:ASP:H	1.57	0.70
1:C:203:VAL:HB	1:C:210:THR:HG22	1.74	0.70
1:B:205:ASN:ND2	1:D:265:GLN:HE21	1.90	0.70
1:B:205:ASN:HB3	1:D:265:GLN:HB2	1.74	0.69
2:E:488:LEU:O	2:E:492:VAL:HG23	1.91	0.69
1:A:284:HIS:HD2	1:A:284:HIS:H	1.38	0.69
1:B:284:HIS:H	1:B:284:HIS:HD2	1.37	0.69
2:G:488:LEU:O	2:G:492:VAL:HG23	1.91	0.69
1:B:181:MET:N	1:B:182:PRO:HD3	2.07	0.69
1:C:278:VAL:HG13	1:C:282:THR:O	1.92	0.69
1:A:203:VAL:HB	1:A:210:THR:HG22	1.75	0.69
1:C:261:HIS:CG	1:C:313:LEU:HD22	2.27	0.69
2:F:348:GLU:HG3	2:F:349:ASP:H	1.57	0.69
1:A:278:VAL:HG13	1:A:282:THR:O	1.93	0.68
1:B:184:GLU:O	1:B:187:ILE:HG13	1.93	0.68
2:H:488:LEU:O	2:H:492:VAL:HG23	1.93	0.68
2:G:492:VAL:O	2:G:496:ARG:HB2	1.93	0.68
1:A:261:HIS:CG	1:A:313:LEU:HD22	2.28	0.68
2:E:409:VAL:HG23	4:E:598:HOH:O	1.92	0.68
1:D:184:GLU:O	1:D:187:ILE:HG13	1.92	0.68
2:G:348:GLU:HG3	2:G:349:ASP:H	1.58	0.68
2:F:363:ILE:HG23	2:F:538:PHE:CD2	2.29	0.68
1:B:205:ASN:ND2	1:D:265:GLN:NE2	2.42	0.68
1:D:323:ASN:HB3	1:D:326:VAL:HG23	1.76	0.68
2:G:395:SER:HB2	2:G:543:TRP:HE1	1.59	0.68
2:H:492:VAL:O	2:H:496:ARG:HB2	1.94	0.68
1:C:323:ASN:HB3	1:C:326:VAL:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:VAL:HB	1:D:210:THR:HG22	1.76	0.67
2:E:348:GLU:HG3	2:E:349:ASP:H	1.58	0.67
1:C:288:VAL:CG1	1:C:289:GLY:H	1.95	0.67
2:H:337:VAL:HG21	2:H:417:VAL:HG11	1.77	0.67
2:H:446:MET:HE1	2:H:510:VAL:HG22	1.77	0.67
1:C:184:GLU:O	1:C:187:ILE:HG13	1.95	0.67
1:C:182:PRO:HB2	1:C:185:ARG:HB2	1.77	0.67
2:E:395:SER:HB2	2:E:543:TRP:HE1	1.59	0.67
2:E:492:VAL:O	2:E:496:ARG:HB2	1.93	0.67
2:G:337:VAL:HG21	2:G:417:VAL:HG11	1.76	0.67
1:A:184:GLU:O	1:A:187:ILE:HG13	1.95	0.67
1:B:261:HIS:CG	1:B:313:LEU:HD22	2.30	0.67
1:B:288:VAL:O	4:B:423:HOH:O	2.13	0.66
2:H:492:VAL:HG13	2:H:496:ARG:HG3	1.77	0.66
2:F:395:SER:HB2	2:F:543:TRP:HE1	1.60	0.66
2:F:337:VAL:HG21	2:F:417:VAL:HG11	1.77	0.66
1:D:230:LYS:CE	1:D:405:THR:HA	2.26	0.66
2:H:446:MET:HE1	2:H:510:VAL:CG2	2.25	0.66
2:F:492:VAL:O	2:F:496:ARG:HB2	1.95	0.66
1:B:349:TYR:O	1:B:353:THR:HG23	1.96	0.66
1:B:323:ASN:HB3	1:B:326:VAL:HG23	1.78	0.65
2:H:311:ILE:HG21	2:H:316:GLU:HG3	1.78	0.65
1:D:226:VAL:O	1:D:230:LYS:HG3	1.95	0.65
2:E:492:VAL:HG13	2:E:496:ARG:HG3	1.78	0.65
1:B:207:ASN:HB3	1:D:265:GLN:HB3	1.78	0.65
2:G:492:VAL:HG13	2:G:496:ARG:HG3	1.78	0.65
2:F:446:MET:HE1	2:F:510:VAL:HG22	1.79	0.65
1:A:226:VAL:O	1:A:230:LYS:HG3	1.96	0.65
2:H:354:ARG:NH2	4:H:572:HOH:O	2.30	0.65
2:E:337:VAL:HG21	2:E:417:VAL:HG11	1.79	0.64
1:B:207:ASN:HB3	1:D:265:GLN:CB	2.27	0.64
1:D:182:PRO:HB2	1:D:185:ARG:HB2	1.79	0.64
2:E:311:ILE:CG2	2:E:312:SER:N	2.55	0.64
2:H:313:PRO:O	2:H:314:GLU:HB2	1.98	0.64
2:E:313:PRO:O	2:E:314:GLU:HB2	1.98	0.64
1:B:226:VAL:O	1:B:230:LYS:HG3	1.97	0.64
1:C:226:VAL:O	1:C:230:LYS:HG3	1.98	0.64
2:F:492:VAL:HG13	2:F:496:ARG:HG3	1.79	0.64
2:E:446:MET:HE1	2:E:510:VAL:HG22	1.77	0.64
1:C:187:ILE:HD12	1:C:188:GLU:N	2.13	0.64
1:C:337:MET:SD	1:C:341:LYS:HE2	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ASN:H	1:B:282:THR:CG2	2.11	0.63
1:D:298:GLU:HG2	4:D:431:HOH:O	1.97	0.63
1:B:183:LEU:O	1:B:187:ILE:HG23	1.98	0.63
1:D:337:MET:SD	1:D:341:LYS:HE2	2.38	0.63
1:B:187:ILE:HD12	1:B:188:GLU:N	2.14	0.63
2:H:395:SER:HB2	2:H:543:TRP:HE1	1.62	0.63
1:A:323:ASN:HB3	1:A:326:VAL:HG23	1.79	0.63
1:B:269:ALA:HB1	1:B:278:VAL:O	1.99	0.63
1:D:284:HIS:N	1:D:284:HIS:CD2	2.67	0.63
1:A:279:ASN:H	1:A:282:THR:CG2	2.11	0.63
2:E:446:MET:HE1	2:E:510:VAL:CG2	2.28	0.63
2:H:363:ILE:HG23	2:H:538:PHE:CD2	2.33	0.63
1:C:286:VAL:HG12	1:C:286:VAL:O	1.99	0.63
1:A:337:MET:SD	1:A:341:LYS:HE2	2.39	0.62
1:C:378:CYS:O	1:C:379:LEU:HB2	1.98	0.62
2:F:446:MET:HE1	2:F:510:VAL:CG2	2.29	0.62
1:A:366:LEU:HD11	2:E:485:LEU:HD11	1.81	0.62
1:D:187:ILE:HD12	1:D:188:GLU:N	2.13	0.62
1:D:269:ALA:HB1	1:D:278:VAL:O	1.99	0.62
1:C:284:HIS:N	1:C:284:HIS:CD2	2.68	0.62
1:C:197:ASP:CB	1:C:198:PRO:CD	2.77	0.62
2:G:363:ILE:HG23	2:G:538:PHE:CD2	2.34	0.62
2:E:363:ILE:HG23	2:E:538:PHE:CD2	2.34	0.62
1:C:269:ALA:HB1	1:C:278:VAL:O	2.00	0.62
1:D:378:CYS:O	1:D:379:LEU:HB2	1.99	0.62
2:F:496:ARG:O	2:F:498:PRO:CD	2.46	0.62
2:H:311:ILE:CG2	2:H:312:SER:N	2.47	0.62
1:D:286:VAL:HG12	1:D:286:VAL:O	2.00	0.62
2:F:313:PRO:O	2:F:314:GLU:HB2	1.99	0.61
2:H:547:LEU:O	2:H:547:LEU:CD2	2.48	0.61
1:A:269:ALA:HB1	1:A:278:VAL:O	2.00	0.61
1:A:284:HIS:N	1:A:284:HIS:CD2	2.68	0.61
1:B:220:LYS:O	1:B:224:GLN:HG3	2.00	0.61
1:D:183:LEU:O	1:D:187:ILE:HG23	1.99	0.61
2:F:423:SER:HB2	4:F:583:HOH:O	1.99	0.61
1:D:207:ASN:OD1	1:D:209:THR:HB	2.00	0.61
1:A:286:VAL:O	1:A:286:VAL:HG12	2.00	0.61
1:C:195:CYS:HB3	4:C:412:HOH:O	1.99	0.61
1:B:333:GLN:HG2	4:B:427:HOH:O	1.99	0.61
1:C:220:LYS:O	1:C:224:GLN:HG3	2.01	0.61
2:G:313:PRO:O	2:G:314:GLU:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ILE:HD12	1:A:188:GLU:N	2.15	0.61
2:G:446:MET:HE1	2:G:510:VAL:HG22	1.83	0.61
2:H:496:ARG:O	2:H:498:PRO:CD	2.46	0.61
1:D:272:LEU:HD11	1:D:286:VAL:HG11	1.83	0.61
2:E:496:ARG:O	2:E:498:PRO:CD	2.45	0.61
1:A:261:HIS:O	1:A:264:MET:HG3	2.00	0.61
1:B:272:LEU:HD11	1:B:286:VAL:HG11	1.83	0.61
2:E:402:ARG:NH1	4:E:580:HOH:O	2.27	0.61
2:G:496:ARG:O	2:G:498:PRO:CD	2.46	0.61
1:B:207:ASN:OD1	1:B:209:THR:HB	2.01	0.61
1:B:284:HIS:CD2	1:B:284:HIS:N	2.68	0.61
1:B:286:VAL:O	1:B:286:VAL:HG12	2.01	0.61
1:C:192:ARG:NH1	1:C:192:ARG:HB2	2.15	0.61
1:D:197:ASP:CB	1:D:198:PRO:CD	2.78	0.60
1:D:261:HIS:O	1:D:264:MET:HG3	2.01	0.60
1:A:378:CYS:O	1:A:379:LEU:HB2	2.00	0.60
1:A:207:ASN:OD1	1:A:209:THR:HB	2.01	0.60
1:D:192:ARG:NH1	1:D:192:ARG:HB2	2.16	0.60
1:D:366:LEU:HD11	2:H:485:LEU:HD11	1.84	0.60
2:E:423:SER:HB2	4:E:595:HOH:O	2.01	0.60
1:A:377:LYS:NZ	4:A:443:HOH:O	2.31	0.60
1:D:327:ARG:HB3	1:D:327:ARG:HH11	1.67	0.60
2:H:509:SER:O	2:H:512:THR:HG23	2.02	0.60
1:C:193:VAL:CG1	1:C:224:GLN:HB3	2.32	0.60
1:C:272:LEU:HD11	1:C:286:VAL:HG11	1.84	0.60
1:D:349:TYR:O	1:D:353:THR:HG23	2.02	0.60
1:A:287:GLY:HA3	4:A:427:HOH:O	2.00	0.60
1:C:207:ASN:OD1	1:C:209:THR:HB	2.01	0.60
1:B:193:VAL:CG1	1:B:224:GLN:HB3	2.32	0.59
1:B:378:CYS:O	1:B:379:LEU:HB2	2.01	0.59
1:C:285:ALA:O	1:C:286:VAL:HB	2.02	0.59
1:B:207:ASN:CA	1:D:265:GLN:HA	2.32	0.59
1:D:302:LYS:HE3	4:D:428:HOH:O	2.01	0.59
2:G:509:SER:O	2:G:512:THR:HG23	2.02	0.59
1:B:348:GLU:O	1:B:351:ARG:HG2	2.01	0.59
1:C:348:GLU:O	1:C:351:ARG:HG2	2.02	0.59
2:E:311:ILE:HD11	2:E:491:TYR:HA	1.83	0.59
1:A:183:LEU:O	1:A:187:ILE:HG23	2.01	0.59
1:D:348:GLU:O	1:D:351:ARG:HG2	2.02	0.59
1:A:285:ALA:O	1:A:286:VAL:HB	2.02	0.59
1:B:337:MET:SD	1:B:341:LYS:HE2	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ASP:CB	1:C:198:PRO:HD3	2.32	0.59
1:D:220:LYS:O	1:D:224:GLN:HG3	2.02	0.59
1:B:261:HIS:O	1:B:264:MET:HG3	2.03	0.59
1:C:327:ARG:HH11	1:C:327:ARG:HB3	1.67	0.59
1:D:193:VAL:CG1	1:D:224:GLN:HB3	2.33	0.59
1:D:279:ASN:H	1:D:282:THR:CG2	2.09	0.59
2:E:322:LEU:HD12	2:E:458:LEU:HD13	1.85	0.59
2:G:446:MET:HE1	2:G:510:VAL:CG2	2.33	0.59
1:A:272:LEU:HD11	1:A:286:VAL:HG11	1.84	0.58
1:A:336:GLU:O	1:A:340:GLU:HG3	2.04	0.58
1:B:353:THR:CB	2:G:419:ASN:HB3	2.33	0.58
1:C:183:LEU:O	1:C:187:ILE:HG23	2.02	0.58
1:B:197:ASP:CB	1:B:198:PRO:CD	2.77	0.58
1:A:220:LYS:O	1:A:224:GLN:HG3	2.02	0.58
1:C:261:HIS:O	1:C:264:MET:HG3	2.02	0.58
1:C:279:ASN:H	1:C:282:THR:CG2	2.11	0.58
1:A:327:ARG:HH11	1:A:327:ARG:HB3	1.68	0.58
2:H:311:ILE:HG21	2:H:316:GLU:CG	2.34	0.58
1:A:348:GLU:O	1:A:351:ARG:HG2	2.03	0.58
1:B:285:ALA:O	1:B:286:VAL:HB	2.02	0.58
1:B:207:ASN:HA	1:D:265:GLN:HA	1.85	0.58
1:B:197:ASP:CB	1:B:198:PRO:HD3	2.32	0.57
1:A:197:ASP:CB	1:A:198:PRO:HD3	2.32	0.57
1:D:398:MET:O	1:D:402:GLU:HG3	2.03	0.57
2:F:402:ARG:NH1	4:F:580:HOH:O	2.26	0.57
1:A:349:TYR:O	1:A:353:THR:HG23	2.04	0.57
1:B:205:ASN:CG	1:D:265:GLN:HE21	2.08	0.57
1:A:198:PRO:HD2	1:A:275:GLY:HA3	1.87	0.57
1:B:205:ASN:HB3	1:D:265:GLN:HG3	1.86	0.57
1:A:193:VAL:CG1	1:A:224:GLN:HB3	2.33	0.57
1:D:230:LYS:HD3	1:D:404:THR:C	2.24	0.57
2:E:479:LYS:HE2	4:E:576:HOH:O	2.05	0.57
1:D:400:MET:C	1:D:402:GLU:H	2.08	0.57
1:B:203:VAL:HB	1:B:210:THR:CG2	2.35	0.57
1:A:340:GLU:OE2	2:E:506:LYS:HD2	2.04	0.57
2:E:512:THR:HG21	4:E:579:HOH:O	2.04	0.57
1:D:285:ALA:O	1:D:286:VAL:HB	2.04	0.56
2:E:416:PHE:CZ	3:E:5:P1A:H152	2.40	0.56
1:B:193:VAL:HG13	1:B:224:GLN:HB3	1.88	0.56
1:C:198:PRO:HD2	1:C:275:GLY:HA3	1.86	0.56
1:D:185:ARG:HB3	1:D:233:PRO:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ALA:HB2	1:A:371:LEU:HD21	1.87	0.56
2:F:311:ILE:CG2	2:F:312:SER:N	2.49	0.56
1:C:336:GLU:O	1:C:340:GLU:HG3	2.06	0.56
2:G:329:TYR:O	2:G:402:ARG:NH2	2.34	0.56
1:C:349:TYR:O	1:C:353:THR:HG23	2.05	0.56
1:D:230:LYS:HZ3	1:D:405:THR:CA	2.19	0.56
2:H:546:ASP:O	2:H:547:LEU:HB3	2.04	0.56
1:A:203:VAL:HB	1:A:210:THR:CG2	2.35	0.56
1:B:366:LEU:HD11	2:F:485:LEU:HD11	1.88	0.56
2:G:322:LEU:HD12	2:G:458:LEU:HD13	1.86	0.56
1:C:193:VAL:HG13	1:C:224:GLN:HB3	1.87	0.55
1:B:353:THR:HB	2:G:419:ASN:CG	2.26	0.55
1:A:197:ASP:CB	1:A:198:PRO:CD	2.76	0.55
1:B:336:GLU:O	1:B:340:GLU:HG3	2.06	0.55
2:H:525:CYS:HB3	2:H:545:VAL:CG1	2.31	0.55
1:A:192:ARG:HB2	1:A:192:ARG:NH1	2.16	0.55
1:C:203:VAL:HB	1:C:210:THR:CG2	2.35	0.55
2:F:322:LEU:HD12	2:F:458:LEU:HD13	1.87	0.55
1:D:260:SER:HB3	1:D:303:MET:CE	2.34	0.55
1:B:185:ARG:HB3	1:B:233:PRO:HG3	1.89	0.55
1:D:203:VAL:HB	1:D:210:THR:CG2	2.36	0.55
2:H:311:ILE:CG2	2:H:316:GLU:HG3	2.37	0.55
2:H:322:LEU:HD12	2:H:458:LEU:HD13	1.87	0.55
1:B:257:ALA:HB2	1:B:371:LEU:HD21	1.88	0.55
2:F:495:ARG:O	2:F:496:ARG:CG	2.53	0.55
1:B:327:ARG:HH11	1:B:327:ARG:HB3	1.71	0.55
1:D:207:ASN:OD1	1:D:210:THR:HG23	2.07	0.55
1:A:207:ASN:O	1:A:209:THR:N	2.40	0.54
1:B:193:VAL:HG12	1:B:193:VAL:O	2.07	0.54
1:C:185:ARG:HB3	1:C:233:PRO:HG3	1.89	0.54
1:C:257:ALA:HB2	1:C:371:LEU:HD21	1.89	0.54
1:D:197:ASP:CB	1:D:198:PRO:HD3	2.33	0.54
2:F:509:SER:O	2:F:512:THR:HG23	2.07	0.54
2:G:418:ASN:HD21	2:G:420:GLN:HB2	1.73	0.54
1:B:192:ARG:HB2	1:B:192:ARG:NH1	2.15	0.54
1:D:198:PRO:HD2	1:D:275:GLY:HA3	1.89	0.54
1:B:198:PRO:HD2	1:B:275:GLY:HA3	1.88	0.54
1:A:185:ARG:HB3	1:A:233:PRO:HG3	1.89	0.54
1:D:187:ILE:HG22	1:D:311:THR:HG23	1.90	0.54
1:C:340:GLU:OE2	2:G:506:LYS:HD2	2.08	0.54
1:A:193:VAL:O	1:A:193:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:VAL:O	1:C:193:VAL:HG12	2.08	0.54
2:F:348:GLU:HG3	2:F:349:ASP:N	2.24	0.53
2:E:348:GLU:HG3	2:E:349:ASP:N	2.24	0.53
1:B:205:ASN:HB3	1:D:265:GLN:CG	2.37	0.53
1:D:257:ALA:HB2	1:D:371:LEU:HD21	1.89	0.53
1:D:193:VAL:HG13	1:D:224:GLN:HB3	1.89	0.53
1:B:193:VAL:HG13	1:B:224:GLN:CD	2.28	0.53
2:E:525:CYS:HB3	2:E:545:VAL:CG1	2.30	0.53
2:F:359:THR:HB	2:F:536:PRO:HG2	1.91	0.53
1:D:193:VAL:HG13	1:D:224:GLN:CD	2.29	0.53
2:G:402:ARG:NH1	4:G:557:HOH:O	2.41	0.53
2:H:545:VAL:CG1	2:H:545:VAL:O	2.54	0.53
1:B:207:ASN:OD1	1:B:210:THR:HG23	2.08	0.53
1:D:207:ASN:O	1:D:209:THR:N	2.41	0.53
1:D:230:LYS:NZ	1:D:405:THR:N	2.56	0.53
2:E:329:TYR:O	2:E:402:ARG:NH2	2.38	0.53
2:E:509:SER:O	2:E:512:THR:HG23	2.08	0.53
2:G:348:GLU:HG3	2:G:349:ASP:N	2.24	0.53
1:A:193:VAL:HG13	1:A:224:GLN:CD	2.29	0.53
1:C:207:ASN:O	1:C:209:THR:N	2.41	0.53
1:D:338:LEU:O	1:D:342:ILE:HG13	2.09	0.53
1:A:195:CYS:SG	1:A:273:ALA:O	2.67	0.52
1:A:207:ASN:OD1	1:A:210:THR:HG23	2.09	0.52
1:B:187:ILE:HG22	1:B:311:THR:HG23	1.91	0.52
1:A:193:VAL:HG13	1:A:224:GLN:HB3	1.89	0.52
1:A:241:THR:HG23	4:A:447:HOH:O	2.08	0.52
1:B:207:ASN:O	1:B:209:THR:N	2.42	0.52
1:B:279:ASN:N	1:B:282:THR:HG23	2.15	0.52
1:C:207:ASN:OD1	1:C:210:THR:HG23	2.09	0.52
2:E:418:ASN:HD21	2:E:420:GLN:HB2	1.74	0.52
1:B:221:GLN:HE22	1:B:262:ARG:NH2	1.98	0.52
1:D:193:VAL:HG12	1:D:193:VAL:O	2.09	0.52
2:E:408:ASP:OD2	2:E:410:GLN:HB2	2.10	0.52
2:H:409:VAL:HG21	2:H:447:TYR:CZ	2.45	0.52
1:C:187:ILE:HD12	1:C:187:ILE:C	2.30	0.52
1:C:338:LEU:O	1:C:342:ILE:HG13	2.10	0.52
1:D:336:GLU:O	1:D:340:GLU:HG3	2.10	0.52
2:E:494:ASN:C	2:E:494:ASN:HD22	2.13	0.52
2:H:436:ILE:HG13	2:H:440:LEU:HD22	1.92	0.52
1:A:379:LEU:HA	4:A:445:HOH:O	2.10	0.52
1:B:187:ILE:HD12	1:B:187:ILE:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:ASN:N	1:D:282:THR:HG23	2.15	0.52
1:D:246:LEU:HD13	1:D:329:ILE:CD1	2.40	0.52
2:E:495:ARG:O	2:E:496:ARG:CG	2.52	0.52
1:B:351:ARG:CZ	2:G:410:GLN:HG3	2.40	0.52
1:A:221:GLN:HE22	1:A:262:ARG:NH2	1.97	0.52
2:F:494:ASN:C	2:F:494:ASN:HD22	2.13	0.52
2:G:494:ASN:HD22	2:G:494:ASN:C	2.13	0.52
1:B:181:MET:H	1:B:182:PRO:HD3	1.72	0.51
2:G:403:MET:HB2	3:G:5:P1A:H121	1.91	0.51
2:H:348:GLU:HG3	2:H:349:ASP:N	2.23	0.51
1:A:187:ILE:HG22	1:A:311:THR:HG23	1.91	0.51
1:A:187:ILE:HD12	1:A:187:ILE:C	2.31	0.51
1:A:306:MET:HE2	1:A:363:LYS:HE2	1.93	0.51
1:C:187:ILE:HG22	1:C:311:THR:HG23	1.92	0.51
2:F:357:HIS:O	2:F:361:ILE:HG13	2.11	0.51
2:H:312:SER:HB3	2:H:315:GLN:OE1	2.11	0.51
2:H:359:THR:HB	2:H:536:PRO:HG2	1.93	0.51
1:D:187:ILE:C	1:D:187:ILE:HD12	2.31	0.50
2:E:409:VAL:HG21	2:E:447:TYR:CZ	2.46	0.50
2:F:409:VAL:HG21	2:F:447:TYR:CZ	2.46	0.50
2:G:409:VAL:HG21	2:G:447:TYR:CZ	2.46	0.50
2:H:494:ASN:HD22	2:H:494:ASN:C	2.14	0.50
1:C:181:MET:CE	1:C:233:PRO:HB2	2.41	0.50
1:C:193:VAL:HG13	1:C:224:GLN:CD	2.31	0.50
1:B:203:VAL:CG1	1:D:196:ASN:HD21	2.18	0.50
2:E:436:ILE:HG13	2:E:440:LEU:HD22	1.93	0.50
1:B:260:SER:HB3	1:B:303:MET:CE	2.36	0.50
1:D:181:MET:CE	1:D:233:PRO:HB2	2.42	0.50
2:G:525:CYS:HB3	2:G:545:VAL:CG1	2.35	0.50
2:E:535:LEU:HD22	2:E:536:PRO:CD	2.39	0.50
2:G:463:VAL:HG22	2:G:511:LEU:HD22	1.93	0.50
2:H:495:ARG:O	2:H:496:ARG:CG	2.52	0.50
1:B:195:CYS:SG	1:B:273:ALA:O	2.70	0.49
2:F:418:ASN:HD21	2:F:420:GLN:HB2	1.74	0.49
2:F:403:MET:HB2	3:F:5:P1A:H121	1.94	0.49
1:C:285:ALA:O	1:C:286:VAL:CB	2.60	0.49
1:C:279:ASN:OD1	1:C:280:LYS:N	2.45	0.49
1:A:279:ASN:N	1:A:282:THR:HG23	2.16	0.49
1:B:393:ILE:HG22	1:B:394:ASP:N	2.28	0.49
1:D:291:ILE:O	1:D:295:VAL:HG23	2.12	0.49
2:F:329:TYR:O	2:F:402:ARG:NH2	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:359:THR:HB	2:E:536:PRO:HG2	1.93	0.49
1:C:195:CYS:SG	1:C:273:ALA:O	2.71	0.49
1:D:195:CYS:SG	1:D:273:ALA:O	2.70	0.49
1:D:246:LEU:HD13	1:D:329:ILE:HD13	1.94	0.49
2:E:463:VAL:HG22	2:E:511:LEU:HD22	1.94	0.49
2:G:436:ILE:HG13	2:G:440:LEU:HD22	1.93	0.49
1:D:252:ASN:O	1:D:256:ILE:HG13	2.12	0.49
2:F:463:VAL:HG22	2:F:511:LEU:HD22	1.94	0.49
2:E:330:GLU:OE2	2:E:331:HIS:HB3	2.13	0.49
2:H:330:GLU:OE2	2:H:331:HIS:HB3	2.11	0.49
1:B:285:ALA:O	1:B:286:VAL:CB	2.61	0.48
2:G:359:THR:HB	2:G:536:PRO:HG2	1.94	0.48
1:A:246:LEU:HD13	1:A:329:ILE:CD1	2.43	0.48
1:C:252:ASN:O	1:C:256:ILE:HG13	2.13	0.48
1:C:246:LEU:HD13	1:C:329:ILE:CD1	2.42	0.48
2:E:357:HIS:O	2:E:361:ILE:HG13	2.13	0.48
2:F:408:ASP:OD2	2:F:410:GLN:HB2	2.12	0.48
2:G:330:GLU:OE2	2:G:331:HIS:HB3	2.13	0.48
1:B:338:LEU:O	1:B:342:ILE:HG13	2.13	0.48
1:C:279:ASN:N	1:C:282:THR:HG23	2.15	0.48
2:F:330:GLU:OE2	2:F:331:HIS:HB3	2.14	0.48
1:B:265:GLN:HG2	1:B:266:ALA:N	2.28	0.48
1:D:279:ASN:OD1	1:D:280:LYS:N	2.46	0.48
1:D:290:ASN:N	1:D:290:ASN:OD1	2.47	0.48
2:G:455:GLU:O	2:G:459:LEU:HB2	2.14	0.48
2:H:537:PRO:O	2:H:541:GLU:HG2	2.14	0.48
1:D:393:ILE:HG22	1:D:394:ASP:N	2.28	0.48
2:G:335:GLU:HG3	2:G:336:ASP:N	2.29	0.48
2:H:329:TYR:O	2:H:402:ARG:NH2	2.43	0.48
2:H:408:ASP:OD2	2:H:410:GLN:HB2	2.13	0.48
2:H:463:VAL:HG22	2:H:511:LEU:HD22	1.96	0.48
1:A:279:ASN:OD1	1:A:280:LYS:N	2.46	0.48
1:B:265:GLN:HG2	1:B:266:ALA:H	1.79	0.48
1:D:306:MET:HE2	1:D:363:LYS:HE2	1.95	0.48
2:E:424:ARG:HG3	4:E:595:HOH:O	2.12	0.48
1:A:398:MET:O	1:A:402:GLU:HG3	2.14	0.48
2:F:455:GLU:O	2:F:459:LEU:HB2	2.13	0.48
1:B:353:THR:HA	2:G:419:ASN:HB3	1.95	0.48
2:G:495:ARG:O	2:G:496:ARG:CG	2.52	0.48
1:B:246:LEU:HG	1:B:321:LEU:O	2.14	0.48
1:D:223:PHE:HE1	1:D:404:THR:HG1	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:545:VAL:O	2:E:545:VAL:CG1	2.56	0.48
2:F:436:ILE:HG13	2:F:440:LEU:HD22	1.95	0.48
1:B:252:ASN:O	1:B:256:ILE:HG13	2.14	0.48
1:C:378:CYS:O	1:C:379:LEU:CB	2.61	0.48
1:D:312:GLU:HG2	1:D:364:LEU:HD21	1.96	0.48
2:H:395:SER:CB	2:H:543:TRP:HE1	2.27	0.48
1:D:230:LYS:HE2	1:D:405:THR:CA	2.39	0.47
2:E:335:GLU:HG3	2:E:336:ASP:N	2.29	0.47
2:G:357:HIS:O	2:G:361:ILE:HG13	2.14	0.47
2:G:408:ASP:OD2	2:G:410:GLN:HB2	2.13	0.47
1:A:182:PRO:HB2	1:A:185:ARG:HB2	1.95	0.47
1:A:285:ALA:O	1:A:286:VAL:CB	2.61	0.47
1:D:192:ARG:HG2	1:D:231:LEU:HD11	1.96	0.47
1:C:246:LEU:HD13	1:C:329:ILE:HD13	1.95	0.47
2:F:335:GLU:HG3	2:F:336:ASP:N	2.29	0.47
1:C:278:VAL:HG11	1:C:283:ALA:HA	1.96	0.47
1:C:393:ILE:HG22	1:C:394:ASP:N	2.29	0.47
2:G:398:VAL:HG11	4:G:557:HOH:O	2.14	0.47
2:G:537:PRO:O	2:G:541:GLU:HG2	2.14	0.47
1:D:265:GLN:HG2	1:D:266:ALA:H	1.80	0.47
2:H:346:ASP:O	2:H:348:GLU:N	2.47	0.47
1:A:278:VAL:CG1	1:A:283:ALA:HA	2.45	0.47
1:D:246:LEU:HG	1:D:321:LEU:O	2.14	0.47
2:G:395:SER:CB	2:G:543:TRP:HE1	2.26	0.47
1:A:265:GLN:HG2	1:A:266:ALA:N	2.30	0.47
1:D:278:VAL:CG1	1:D:283:ALA:HA	2.45	0.47
1:D:278:VAL:HG11	1:D:283:ALA:HA	1.97	0.47
2:G:346:ASP:O	2:G:348:GLU:N	2.48	0.47
1:A:278:VAL:HG12	1:A:279:ASN:N	2.30	0.47
1:B:278:VAL:HG11	1:B:283:ALA:HA	1.97	0.47
2:E:455:GLU:O	2:E:459:LEU:HB2	2.15	0.47
2:F:346:ASP:O	2:F:348:GLU:N	2.48	0.47
1:A:290:ASN:OD1	1:A:290:ASN:N	2.48	0.47
1:A:378:CYS:O	1:A:379:LEU:CB	2.62	0.47
1:B:279:ASN:OD1	1:B:280:LYS:N	2.47	0.47
1:C:290:ASN:N	1:C:290:ASN:OD1	2.47	0.47
2:E:346:ASP:O	2:E:348:GLU:N	2.48	0.47
2:F:525:CYS:HB3	2:F:545:VAL:CG1	2.35	0.47
1:B:278:VAL:CG1	1:B:283:ALA:HA	2.45	0.46
1:C:331:SER:O	1:C:335:VAL:HG23	2.16	0.46
1:A:278:VAL:HG11	1:A:283:ALA:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ARG:HG2	1:C:231:LEU:HD11	1.96	0.46
1:D:349:TYR:CZ	1:D:353:THR:HG21	2.50	0.46
1:D:378:CYS:O	1:D:379:LEU:CB	2.62	0.46
2:H:455:GLU:O	2:H:459:LEU:HB2	2.14	0.46
1:B:246:LEU:HD13	1:B:329:ILE:CD1	2.45	0.46
1:B:378:CYS:O	1:B:379:LEU:CB	2.62	0.46
1:C:278:VAL:CG1	1:C:283:ALA:HA	2.45	0.46
2:F:341:ILE:O	2:F:341:ILE:HG23	2.16	0.46
2:G:496:ARG:HD2	2:G:503:ILE:HG12	1.97	0.46
1:B:349:TYR:CZ	1:B:353:THR:HG21	2.50	0.46
1:C:203:VAL:O	1:C:210:THR:HG21	2.15	0.46
1:D:265:GLN:HG2	1:D:266:ALA:N	2.29	0.46
2:E:537:PRO:O	2:E:541:GLU:HG2	2.16	0.46
2:G:535:LEU:HD22	2:G:536:PRO:CD	2.44	0.46
1:C:185:ARG:HB3	1:C:233:PRO:CG	2.45	0.46
2:H:335:GLU:HG3	2:H:336:ASP:N	2.30	0.46
1:A:393:ILE:HG22	1:A:394:ASP:N	2.29	0.46
1:B:204:VAL:HG22	1:D:196:ASN:OD1	2.15	0.46
1:B:290:ASN:OD1	1:B:290:ASN:N	2.47	0.46
1:B:291:ILE:O	1:B:295:VAL:HG23	2.16	0.46
1:B:246:LEU:HD13	1:B:329:ILE:HD13	1.97	0.46
1:D:285:ALA:O	1:D:286:VAL:CB	2.63	0.46
2:F:417:VAL:HG23	3:F:5:P1A:O6	2.16	0.46
2:F:537:PRO:O	2:F:541:GLU:HG2	2.16	0.46
2:G:341:ILE:HG23	2:G:341:ILE:O	2.16	0.46
1:B:353:THR:HB	2:G:419:ASN:ND2	2.31	0.46
1:C:260:SER:HB3	1:C:303:MET:CE	2.39	0.46
1:A:331:SER:O	1:A:335:VAL:HG23	2.16	0.46
1:B:206:GLU:C	1:B:208:ASN:H	2.19	0.46
1:B:192:ARG:HG2	1:B:231:LEU:HD11	1.98	0.46
2:E:341:ILE:O	2:E:341:ILE:HG23	2.16	0.46
2:G:468:ARG:H	2:G:471:LEU:HD22	1.81	0.46
2:G:545:VAL:O	2:G:545:VAL:CG1	2.58	0.46
1:C:206:GLU:C	1:C:208:ASN:H	2.19	0.46
2:H:341:ILE:HG23	2:H:341:ILE:O	2.16	0.46
2:H:417:VAL:HG23	3:H:5:P1A:O6	2.15	0.46
1:D:193:VAL:HG11	1:D:224:GLN:HB3	1.98	0.45
2:F:496:ARG:HD2	2:F:503:ILE:HG12	1.98	0.45
2:G:326:GLN:HE22	2:G:456:TYR:HB3	1.80	0.45
1:C:306:MET:HE2	1:C:363:LYS:HE2	1.97	0.45
1:D:221:GLN:HE22	1:D:262:ARG:NH2	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:395:SER:CB	2:E:543:TRP:HE1	2.27	0.45
2:E:417:VAL:HG23	3:E:5:P1A:O6	2.16	0.45
2:G:417:VAL:HG23	3:G:5:P1A:O6	2.16	0.45
1:A:198:PRO:O	1:A:199:LEU:HB2	2.16	0.45
1:A:291:ILE:O	1:A:295:VAL:HG23	2.15	0.45
1:A:338:LEU:O	1:A:342:ILE:HG13	2.17	0.45
1:C:181:MET:HB3	1:C:345:VAL:HG21	1.99	0.45
1:C:207:ASN:C	1:C:209:THR:N	2.70	0.45
1:C:265:GLN:HG2	1:C:266:ALA:N	2.31	0.45
1:D:331:SER:O	1:D:335:VAL:HG23	2.17	0.45
2:E:403:MET:HB2	3:E:5:P1A:H121	1.99	0.45
1:A:203:VAL:O	1:A:210:THR:HG21	2.16	0.45
1:A:206:GLU:C	1:A:208:ASN:H	2.19	0.45
1:B:398:MET:O	1:B:402:GLU:HG2	2.16	0.45
1:C:291:ILE:O	1:C:295:VAL:HG23	2.16	0.45
1:D:207:ASN:C	1:D:209:THR:N	2.70	0.45
1:A:246:LEU:HD13	1:A:329:ILE:HD13	1.98	0.45
1:C:193:VAL:HG11	1:C:224:GLN:HB3	1.99	0.45
1:C:265:GLN:HG2	1:C:266:ALA:H	1.82	0.45
1:A:192:ARG:HG2	1:A:231:LEU:HD11	1.97	0.45
1:C:278:VAL:HG12	1:C:279:ASN:N	2.31	0.45
1:B:207:ASN:HD22	1:D:265:GLN:HB3	1.82	0.45
1:D:327:ARG:NH1	1:D:327:ARG:CB	2.80	0.45
2:G:499:LYS:O	2:G:503:ILE:HD13	2.17	0.45
1:C:331:SER:HB3	1:C:334:GLU:HB3	1.99	0.45
1:D:278:VAL:HG12	1:D:279:ASN:N	2.32	0.45
2:H:424:ARG:HH21	2:H:444:ARG:NH2	2.15	0.45
2:E:315:GLN:O	2:E:319:ILE:HG13	2.16	0.45
1:A:390:ASP:HB2	4:A:420:HOH:O	2.17	0.44
1:C:349:TYR:CZ	1:C:353:THR:HG21	2.52	0.44
1:D:206:GLU:C	1:D:208:ASN:H	2.19	0.44
2:E:496:ARG:HD2	2:E:503:ILE:HG12	1.99	0.44
2:F:322:LEU:HB3	2:F:457:ALA:HB1	1.98	0.44
2:F:545:VAL:CG1	2:F:545:VAL:O	2.57	0.44
2:H:322:LEU:HB3	2:H:457:ALA:HB1	1.98	0.44
1:A:265:GLN:HG2	1:A:266:ALA:H	1.81	0.44
1:A:327:ARG:CB	1:A:327:ARG:NH1	2.80	0.44
1:B:203:VAL:O	1:B:210:THR:HG21	2.17	0.44
1:B:278:VAL:HG12	1:B:279:ASN:N	2.31	0.44
1:B:329:ILE:CG2	1:B:332:VAL:HG22	2.47	0.44
1:B:312:GLU:HG2	1:B:364:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ARG:NH1	1:C:327:ARG:CB	2.81	0.44
2:H:418:ASN:HD21	2:H:420:GLN:HB2	1.76	0.44
1:B:185:ARG:HB3	1:B:233:PRO:CG	2.48	0.44
1:B:207:ASN:C	1:B:209:THR:N	2.70	0.44
1:D:185:ARG:HB3	1:D:233:PRO:CG	2.47	0.44
1:D:230:LYS:HZ3	1:D:405:THR:CB	2.31	0.44
2:G:494:ASN:C	2:G:494:ASN:ND2	2.71	0.44
2:F:468:ARG:H	2:F:471:LEU:HD22	1.83	0.44
2:F:488:LEU:HD22	2:F:492:VAL:CG2	2.48	0.44
1:A:207:ASN:C	1:A:209:THR:N	2.70	0.44
1:A:185:ARG:HB3	1:A:233:PRO:CG	2.47	0.44
2:G:322:LEU:HB3	2:G:457:ALA:HB1	2.00	0.44
1:C:273:ALA:C	1:C:275:GLY:N	2.71	0.44
1:C:246:LEU:HG	1:C:321:LEU:O	2.17	0.44
1:D:327:ARG:NH1	1:D:327:ARG:HB3	2.33	0.44
2:G:417:VAL:HG13	4:G:577:HOH:O	2.17	0.44
1:A:349:TYR:CZ	1:A:353:THR:HG21	2.52	0.44
2:F:494:ASN:C	2:F:494:ASN:ND2	2.70	0.44
2:E:494:ASN:ND2	2:E:494:ASN:C	2.71	0.44
1:A:193:VAL:HG11	1:A:224:GLN:HB3	1.99	0.44
1:B:198:PRO:O	1:B:199:LEU:HB2	2.18	0.44
1:B:353:THR:O	2:G:419:ASN:OD1	2.35	0.44
1:C:273:ALA:C	1:C:275:GLY:H	2.21	0.44
1:C:312:GLU:HG2	1:C:364:LEU:HD21	1.99	0.44
1:D:331:SER:HB3	1:D:334:GLU:HB3	2.00	0.44
1:B:193:VAL:HG13	1:B:224:GLN:NE2	2.33	0.43
2:G:459:LEU:HA	2:G:459:LEU:HD12	1.83	0.43
2:G:488:LEU:HD22	2:G:492:VAL:CG2	2.48	0.43
1:C:221:GLN:HE22	1:C:262:ARG:NH2	2.02	0.43
1:D:261:HIS:CB	1:D:313:LEU:HD22	2.48	0.43
2:E:326:GLN:HE22	2:E:456:TYR:HB3	1.83	0.43
2:H:315:GLN:O	2:H:319:ILE:HG13	2.18	0.43
1:C:274:THR:HG22	1:C:276:LEU:HB2	2.00	0.43
1:C:329:ILE:CG2	1:C:332:VAL:HG22	2.47	0.43
1:A:246:LEU:HG	1:A:321:LEU:O	2.18	0.43
1:B:202:LEU:HA	1:B:276:LEU:HD11	2.00	0.43
1:B:193:VAL:HG11	1:B:224:GLN:HB3	1.99	0.43
1:D:202:LEU:HA	1:D:276:LEU:HD11	2.00	0.43
2:G:530:LEU:HA	2:G:530:LEU:HD23	1.85	0.43
2:H:494:ASN:C	2:H:494:ASN:ND2	2.71	0.43
1:B:217:ALA:HB2	1:B:274:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:THR:CG2	1:C:276:LEU:HB2	2.49	0.43
1:D:203:VAL:O	1:D:210:THR:HG21	2.18	0.43
2:F:530:LEU:HA	2:F:530:LEU:HD23	1.86	0.43
2:H:433:GLY:O	4:H:564:HOH:O	2.21	0.43
1:B:274:THR:HG22	1:B:276:LEU:HB2	2.01	0.43
1:D:198:PRO:O	1:D:199:LEU:HB2	2.19	0.43
3:F:5:P1A:H191	3:F:5:P1A:H111	1.94	0.43
2:H:446:MET:HE1	2:H:510:VAL:HG21	1.99	0.43
1:B:198:PRO:CG	1:B:200:VAL:HG23	2.49	0.43
1:B:398:MET:O	1:B:402:GLU:CG	2.66	0.43
1:C:327:ARG:NH1	1:C:327:ARG:HB3	2.33	0.43
2:F:439:LEU:HA	2:F:439:LEU:HD12	1.85	0.43
2:H:375:ARG:HG3	2:H:375:ARG:HH11	1.84	0.43
1:C:198:PRO:O	1:C:199:LEU:HB2	2.18	0.43
1:D:315:CYS:O	1:D:319:ILE:HG13	2.19	0.43
2:H:496:ARG:HD2	2:H:503:ILE:HG12	2.01	0.43
2:F:395:SER:CB	2:F:543:TRP:HE1	2.29	0.43
4:A:443:HOH:O	2:E:519:ASN:ND2	2.51	0.43
1:A:260:SER:HB3	1:A:303:MET:CE	2.39	0.42
1:A:329:ILE:CG2	1:A:332:VAL:HG22	2.49	0.42
2:F:315:GLN:O	2:F:319:ILE:HG13	2.18	0.42
2:F:326:GLN:HE22	2:F:456:TYR:HB3	1.83	0.42
2:F:466:SER:O	2:F:468:ARG:HG2	2.19	0.42
2:F:543:TRP:HB2	2:F:545:VAL:HG23	2.00	0.42
2:H:468:ARG:H	2:H:471:LEU:HD22	1.83	0.42
1:A:274:THR:HG22	1:A:276:LEU:HB2	2.00	0.42
1:D:204:VAL:O	1:D:204:VAL:HG23	2.19	0.42
1:D:404:THR:HG22	1:D:404:THR:O	2.20	0.42
2:H:356:ARG:O	2:H:360:GLU:HG3	2.19	0.42
1:A:252:ASN:O	1:A:256:ILE:HG13	2.19	0.42
1:D:193:VAL:HG13	1:D:224:GLN:NE2	2.34	0.42
1:D:273:ALA:C	1:D:275:GLY:H	2.23	0.42
2:E:312:SER:HA	2:E:313:PRO:HD3	1.92	0.42
2:H:313:PRO:O	2:H:314:GLU:CB	2.66	0.42
1:A:331:SER:HB3	1:A:334:GLU:HB3	2.01	0.42
2:H:357:HIS:O	2:H:361:ILE:HG13	2.19	0.42
1:D:274:THR:CG2	1:D:276:LEU:HB2	2.49	0.42
2:E:466:SER:O	2:E:468:ARG:HG2	2.19	0.42
2:H:471:LEU:HA	2:H:471:LEU:HD12	1.91	0.42
1:A:347:GLU:HG3	1:A:348:GLU:N	2.34	0.42
1:B:274:THR:CG2	1:B:276:LEU:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:PRO:CG	1:C:200:VAL:HG23	2.50	0.42
2:F:375:ARG:HG3	2:F:375:ARG:HH11	1.84	0.42
2:G:375:ARG:HG3	2:G:375:ARG:HH11	1.85	0.42
1:B:278:VAL:CG1	1:B:279:ASN:N	2.83	0.42
1:D:273:ALA:C	1:D:275:GLY:N	2.73	0.42
2:G:356:ARG:O	2:G:360:GLU:HG3	2.19	0.42
2:H:466:SER:O	2:H:468:ARG:HG2	2.20	0.42
1:A:202:LEU:HA	1:A:276:LEU:HD11	2.00	0.42
1:C:309:ASP:OD2	1:C:309:ASP:C	2.59	0.42
1:D:198:PRO:CG	1:D:200:VAL:HG23	2.49	0.42
2:E:356:ARG:O	2:E:360:GLU:HG3	2.20	0.42
2:E:471:LEU:HD21	2:E:477:VAL:HG21	2.01	0.42
2:F:418:ASN:C	2:F:420:GLN:H	2.22	0.42
1:A:197:ASP:HB2	1:A:198:PRO:HD2	1.92	0.42
1:A:274:THR:CG2	1:A:276:LEU:HB2	2.49	0.42
1:A:278:VAL:CG1	1:A:279:ASN:N	2.82	0.42
1:C:202:LEU:HA	1:C:276:LEU:HD11	2.01	0.42
1:D:217:ALA:HB2	1:D:274:THR:HB	2.02	0.42
1:D:274:THR:HG22	1:D:276:LEU:HB2	2.01	0.42
1:D:329:ILE:CG2	1:D:332:VAL:HG22	2.50	0.42
1:B:352:THR:HB	2:G:415:LEU:HD11	2.02	0.42
2:H:358:ILE:HG23	3:H:5:P1A:H162	2.02	0.42
2:H:326:GLN:HE22	2:H:456:TYR:HB3	1.85	0.41
2:H:499:LYS:O	2:H:503:ILE:HD13	2.19	0.41
2:H:535:LEU:CD1	2:H:539:LEU:HB3	2.50	0.41
1:B:327:ARG:CB	1:B:327:ARG:NH1	2.83	0.41
2:E:530:LEU:C	2:E:531:LYS:O	2.58	0.41
2:G:315:GLN:O	2:G:319:ILE:HG13	2.20	0.41
1:B:331:SER:O	1:B:335:VAL:HG23	2.19	0.41
1:C:261:HIS:CB	1:C:313:LEU:HD22	2.50	0.41
1:D:347:GLU:HG3	1:D:348:GLU:N	2.35	0.41
2:E:418:ASN:C	2:E:420:GLN:H	2.24	0.41
2:G:463:VAL:HG22	2:G:511:LEU:CD2	2.51	0.41
2:H:543:TRP:HB2	2:H:545:VAL:HG23	2.01	0.41
1:B:331:SER:HB3	1:B:334:GLU:HB3	2.01	0.41
1:D:400:MET:C	1:D:402:GLU:N	2.73	0.41
2:G:441:HIS:HD2	4:G:563:HOH:O	2.02	0.41
2:H:472:ILE:HG22	2:H:473:GLU:HG3	2.03	0.41
1:B:273:ALA:C	1:B:275:GLY:N	2.74	0.41
1:B:306:MET:HE2	1:B:363:LYS:HE2	2.02	0.41
1:D:191:LYS:HA	1:D:194:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:ASP:C	1:D:309:ASP:OD2	2.58	0.41
2:G:425:ASP:O	2:G:429:LEU:HG	2.21	0.41
2:H:488:LEU:HD22	2:H:492:VAL:CG2	2.50	0.41
2:H:489:ARG:HA	2:H:489:ARG:HD2	1.89	0.41
2:H:524:MET:HE1	4:H:555:HOH:O	2.19	0.41
1:A:198:PRO:CG	1:A:200:VAL:HG23	2.50	0.41
1:A:367:ARG:NH1	4:A:453:HOH:O	2.16	0.41
1:C:193:VAL:HG13	1:C:224:GLN:NE2	2.36	0.41
2:E:463:VAL:HG22	2:E:511:LEU:CD2	2.51	0.41
2:F:407:TYR:CG	2:F:443:CYS:HB3	2.55	0.41
2:F:472:ILE:HG22	2:F:473:GLU:HG3	2.02	0.41
2:G:313:PRO:O	2:G:314:GLU:CB	2.69	0.41
1:A:273:ALA:C	1:A:275:GLY:N	2.74	0.41
1:B:204:VAL:HG23	1:B:204:VAL:O	2.21	0.41
1:C:191:LYS:HA	1:C:194:GLU:HB2	2.03	0.41
1:C:217:ALA:HB2	1:C:274:THR:HB	2.02	0.41
1:D:274:THR:CG2	1:D:274:THR:O	2.68	0.41
2:E:468:ARG:H	2:E:471:LEU:HD22	1.85	0.41
2:E:543:TRP:HB2	2:E:545:VAL:HG23	2.03	0.41
2:G:312:SER:HA	2:G:313:PRO:HD3	1.96	0.41
1:B:353:THR:CA	2:G:419:ASN:HB3	2.51	0.41
1:A:327:ARG:NH1	1:A:327:ARG:HB3	2.34	0.41
1:C:278:VAL:CG1	1:C:279:ASN:N	2.83	0.41
1:D:260:SER:C	1:D:303:MET:HE3	2.41	0.41
2:E:313:PRO:O	2:E:314:GLU:CB	2.67	0.41
2:E:322:LEU:HB3	2:E:457:ALA:HB1	2.01	0.41
2:E:530:LEU:HA	2:E:530:LEU:HD23	1.88	0.41
2:F:476:LYS:O	2:F:480:ILE:HG13	2.20	0.41
2:H:311:ILE:HG23	2:H:312:SER:H	1.80	0.41
2:H:439:LEU:HD12	2:H:439:LEU:HA	1.85	0.41
1:A:193:VAL:HG13	1:A:224:GLN:NE2	2.36	0.41
1:A:327:ARG:CB	1:A:327:ARG:HH11	2.33	0.41
1:B:273:ALA:C	1:B:275:GLY:H	2.25	0.41
1:A:204:VAL:O	1:A:204:VAL:HG23	2.21	0.41
1:C:207:ASN:C	1:C:209:THR:H	2.24	0.41
2:G:418:ASN:C	2:G:420:GLN:H	2.24	0.41
2:H:529:LYS:O	2:H:531:LYS:O	2.39	0.41
1:D:340:GLU:OE2	2:H:506:LYS:HD2	2.21	0.41
1:B:340:GLU:OE2	2:F:506:LYS:HD2	2.21	0.41
2:H:530:LEU:HA	2:H:530:LEU:HD23	1.88	0.41
1:A:283:ALA:O	1:A:284:HIS:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ARG:HG3	1:B:352:THR:N	2.35	0.40
1:B:353:THR:CB	2:G:419:ASN:CB	2.99	0.40
1:C:318:ALA:HB1	1:C:342:ILE:HD13	2.03	0.40
1:D:334:GLU:O	1:D:338:LEU:HG	2.21	0.40
2:E:439:LEU:HD12	2:E:439:LEU:HA	1.84	0.40
2:E:446:MET:HE1	2:E:510:VAL:HG21	2.03	0.40
2:G:472:ILE:HG22	2:G:473:GLU:HG3	2.03	0.40
2:H:413:SER:HB3	2:H:422:TYR:O	2.21	0.40
2:H:418:ASN:C	2:H:420:GLN:H	2.24	0.40
2:H:535:LEU:HD22	2:H:536:PRO:CD	2.43	0.40
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.89	0.40
1:B:191:LYS:HA	1:B:194:GLU:HB2	2.04	0.40
1:C:347:GLU:HG3	1:C:348:GLU:N	2.35	0.40
1:C:395:THR:O	1:C:399:GLU:HG2	2.21	0.40
1:D:327:ARG:HH11	1:D:327:ARG:CB	2.33	0.40
1:D:395:THR:O	1:D:399:GLU:HG2	2.21	0.40
2:F:351:CYS:C	2:F:353:VAL:H	2.25	0.40
2:F:499:LYS:O	2:F:503:ILE:HD13	2.21	0.40
2:F:515:ARG:HA	2:F:515:ARG:HD3	1.86	0.40
2:H:407:TYR:CG	2:H:443:CYS:HB3	2.55	0.40
1:A:217:ALA:HB2	1:A:274:THR:HB	2.02	0.40
1:A:273:ALA:C	1:A:275:GLY:H	2.25	0.40
1:B:193:VAL:O	1:B:193:VAL:CG1	2.70	0.40
1:B:309:ASP:C	1:B:309:ASP:OD2	2.58	0.40
1:B:351:ARG:HG3	1:B:352:THR:HG23	2.03	0.40
1:D:207:ASN:C	1:D:209:THR:H	2.25	0.40
2:E:472:ILE:HG22	2:E:473:GLU:HG3	2.03	0.40
3:E:5:P1A:H111	3:E:5:P1A:H191	1.95	0.40
2:G:407:TYR:CG	2:G:443:CYS:HB3	2.56	0.40
1:D:279:ASN:N	1:D:282:THR:CG2	2.82	0.40
2:F:424:ARG:HH21	2:F:444:ARG:NH2	2.18	0.40
2:G:543:TRP:HB2	2:G:545:VAL:HG23	2.02	0.40
1:D:227:GLN:HA	1:D:404:THR:CG2	2.51	0.40
2:E:384:ARG:HD2	2:E:387:GLN:NE2	2.37	0.40
2:G:351:CYS:C	2:G:353:VAL:H	2.24	0.40
2:G:497:LYS:HG2	2:G:500:PRO:HG3	2.04	0.40
2:H:408:ASP:HB2	2:H:415:LEU:CD2	2.42	0.40

There are no symmetry-related clashes.

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	222/235 (94%)	190 (86%)	20 (9%)	12 (5%)	2	2
1	B	226/235 (96%)	189 (84%)	25 (11%)	12 (5%)	2	2
1	C	223/235 (95%)	190 (85%)	22 (10%)	11 (5%)	2	2
1	D	225/235 (96%)	188 (84%)	26 (12%)	11 (5%)	2	2
2	E	230/248 (93%)	210 (91%)	15 (6%)	5 (2%)	6	11
2	F	229/248 (92%)	209 (91%)	15 (7%)	5 (2%)	6	11
2	G	229/248 (92%)	210 (92%)	14 (6%)	5 (2%)	6	11
2	H	230/248 (93%)	209 (91%)	16 (7%)	5 (2%)	6	11
All	All	1814/1932 (94%)	1595 (88%)	153 (8%)	66 (4%)	3	5

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	ASP
1	A	198	PRO
1	A	199	LEU
1	A	208	ASN
2	E	347	GLY
2	E	496	ARG
2	E	498	PRO
1	B	197	ASP
1	B	198	PRO
1	B	199	LEU
1	B	208	ASN
1	B	404	THR
2	F	347	GLY
2	F	496	ARG
2	F	498	PRO
1	C	197	ASP
1	C	198	PRO

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Mol	Chain	Res	Type
1	C	199	LEU
1	C	208	ASN
2	G	347	GLY
2	G	496	ARG
2	G	498	PRO
1	D	197	ASP
1	D	198	PRO
1	D	199	LEU
1	D	208	ASN
2	H	347	GLY
2	H	496	ARG
2	H	498	PRO
1	A	286	VAL
1	A	288	VAL
2	E	314	GLU
1	B	286	VAL
1	B	288	VAL
2	F	314	GLU
1	C	286	VAL
1	C	288	VAL
2	G	314	GLU
1	D	286	VAL
1	D	288	VAL
2	H	314	GLU
1	A	194	GLU
1	A	196	ASN
1	B	194	GLU
1	B	196	ASN
1	C	194	GLU
1	D	194	GLU
1	D	196	ASN
2	E	545	VAL
1	B	251	TRP
1	C	196	ASN
1	C	251	TRP
1	D	251	TRP
1	A	251	TRP
1	A	284	HIS
1	B	284	HIS
1	C	284	HIS
2	G	545	VAL
1	D	284	HIS

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Mol	Chain	Res	Type
1	A	207	ASN
1	B	207	ASN
2	F	545	VAL
2	H	545	VAL
1	C	332	VAL
1	D	332	VAL
1	A	332	VAL

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	198/208 (95%)	183 (92%)	15 (8%)	13	23
1	B	199/208 (96%)	184 (92%)	15 (8%)	13	23
1	C	198/208 (95%)	183 (92%)	15 (8%)	13	23
1	D	199/208 (96%)	184 (92%)	15 (8%)	13	23
2	E	213/225 (95%)	200 (94%)	13 (6%)	18	33
2	F	213/225 (95%)	198 (93%)	15 (7%)	15	26
2	G	212/225 (94%)	197 (93%)	15 (7%)	14	26
2	H	214/225 (95%)	200 (94%)	14 (6%)	17	30
All	All	1646/1732 (95%)	1529 (93%)	117 (7%)	14	26

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	ARG
1	A	192	ARG
1	A	240	LEU
1	A	246	LEU
1	A	274	THR
1	A	279	ASN
1	A	284	HIS
1	A	290	ASN

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Mol	Chain	Res	Type
1	A	294	ARG
1	A	296	LEU
1	A	337	MET
1	A	347	GLU
1	A	364	LEU
1	A	393	ILE
1	A	400	MET
2	E	331	HIS
2	E	349	ASP
2	E	368	LEU
2	E	409	VAL
2	E	439	LEU
2	E	440	LEU
2	E	458	LEU
2	E	488	LEU
2	E	494	ASN
2	E	512	THR
2	E	513	GLU
2	E	535	LEU
2	E	539	LEU
1	B	185	ARG
1	B	192	ARG
1	B	240	LEU
1	B	246	LEU
1	B	274	THR
1	B	279	ASN
1	B	284	HIS
1	B	290	ASN
1	B	294	ARG
1	B	296	LEU
1	B	337	MET
1	B	347	GLU
1	B	364	LEU
1	B	393	ILE
1	B	400	MET
2	F	312	SER
2	F	331	HIS
2	F	349	ASP
2	F	368	LEU
2	F	409	VAL
2	F	439	LEU
2	F	440	LEU

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Mol	Chain	Res	Type
2	F	458	LEU
2	F	459	LEU
2	F	488	LEU
2	F	494	ASN
2	F	512	THR
2	F	513	GLU
2	F	535	LEU
2	F	539	LEU
1	C	185	ARG
1	C	192	ARG
1	C	240	LEU
1	C	246	LEU
1	C	274	THR
1	C	279	ASN
1	C	284	HIS
1	C	290	ASN
1	C	294	ARG
1	C	296	LEU
1	C	337	MET
1	C	347	GLU
1	C	364	LEU
1	C	393	ILE
1	C	400	MET
2	G	312	SER
2	G	331	HIS
2	G	349	ASP
2	G	368	LEU
2	G	409	VAL
2	G	439	LEU
2	G	440	LEU
2	G	458	LEU
2	G	459	LEU
2	G	488	LEU
2	G	494	ASN
2	G	512	THR
2	G	513	GLU
2	G	535	LEU
2	G	539	LEU
1	D	185	ARG
1	D	192	ARG
1	D	240	LEU
1	D	246	LEU

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Mol	Chain	Res	Type
1	D	274	THR
1	D	279	ASN
1	D	284	HIS
1	D	290	ASN
1	D	294	ARG
1	D	296	LEU
1	D	337	MET
1	D	347	GLU
1	D	364	LEU
1	D	393	ILE
1	D	400	MET
2	H	312	SER
2	H	331	HIS
2	H	349	ASP
2	H	368	LEU
2	H	409	VAL
2	H	439	LEU
2	H	440	LEU
2	H	458	LEU
2	H	488	LEU
2	H	494	ASN
2	H	512	THR
2	H	513	GLU
2	H	535	LEU
2	H	539	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	212	ASN
1	A	227	GLN
1	A	267	GLN
1	A	279	ASN
1	A	284	HIS
2	E	326	GLN
2	E	342	ASN
2	E	367	GLN
2	E	387	GLN
2	E	494	ASN
2	E	519	ASN
1	B	205	ASN

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Mol	Chain	Res	Type
1	B	212	ASN
1	B	227	GLN
1	B	234	HIS
1	B	267	GLN
1	B	279	ASN
1	B	284	HIS
2	F	326	GLN
2	F	342	ASN
2	F	367	GLN
2	F	387	GLN
2	F	494	ASN
1	C	205	ASN
1	C	212	ASN
1	C	221	GLN
1	C	227	GLN
1	C	267	GLN
1	C	279	ASN
1	C	284	HIS
2	G	326	GLN
2	G	342	ASN
2	G	367	GLN
2	G	387	GLN
2	G	441	HIS
2	G	494	ASN
1	D	205	ASN
1	D	212	ASN
1	D	221	GLN
1	D	227	GLN
1	D	267	GLN
1	D	279	ASN
1	D	284	HIS
2	H	326	GLN
2	H	342	ASN
2	H	367	GLN
2	H	387	GLN
2	H	494	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	P1A	F	5	-	36,36,36	2.60	16 (44%)	59,60,60	1.58	12 (20%)
3	P1A	E	5	-	36,36,36	2.72	17 (47%)	59,60,60	1.62	13 (22%)
3	P1A	H	5	-	36,36,36	2.84	17 (47%)	59,60,60	1.61	15 (25%)
3	P1A	G	5	-	36,36,36	2.75	16 (44%)	59,60,60	1.61	12 (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
3	P1A	F	5	-	-	0/17/87/87	0/4/4/4
3	P1A	E	5	-	-	0/17/87/87	0/4/4/4
3	P1A	H	5	-	-	2/17/87/87	0/4/4/4
3	P1A	G	5	-	-	2/17/87/87	0/4/4/4

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	5	P1A	C10-C9	6.81	1.67	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	5	P1A	C10-C9	6.69	1.67	1.56
3	E	5	P1A	C10-C9	6.62	1.67	1.56
3	F	5	P1A	C10-C9	6.39	1.66	1.56
3	G	5	P1A	C23-C22	5.64	1.60	1.52
3	E	5	P1A	C3-C2	5.27	1.60	1.52
3	H	5	P1A	C3-C2	5.27	1.60	1.52
3	H	5	P1A	C9-C8	5.26	1.62	1.52
3	F	5	P1A	C9-C8	4.99	1.61	1.52
3	G	5	P1A	C7-C8	4.92	1.40	1.34
3	H	5	P1A	C4-C3	4.89	1.61	1.52
3	F	5	P1A	C23-C22	4.87	1.59	1.52
3	F	5	P1A	C3-C2	4.70	1.59	1.52
3	E	5	P1A	C9-C8	4.69	1.61	1.52
3	G	5	P1A	C9-C8	4.59	1.61	1.52
3	H	5	P1A	C5-C6	4.45	1.57	1.51
3	E	5	P1A	C4-C3	4.45	1.60	1.52
3	E	5	P1A	C23-C22	4.36	1.58	1.52
3	H	5	P1A	C23-C22	4.26	1.58	1.52
3	G	5	P1A	C3-C2	4.15	1.58	1.52
3	G	5	P1A	C4-C3	4.11	1.59	1.52
3	F	5	P1A	C5-C6	4.05	1.57	1.51
3	E	5	P1A	C7-C8	4.01	1.39	1.34
3	G	5	P1A	C14-C13	4.00	1.63	1.56
3	H	5	P1A	C14-C13	3.99	1.63	1.56
3	H	5	P1A	C4-C5	3.92	1.61	1.54
3	G	5	P1A	O14-C14	3.91	1.49	1.43
3	G	5	P1A	C5-C6	3.91	1.56	1.51
3	H	5	P1A	C7-C8	3.89	1.39	1.34
3	E	5	P1A	C5-C6	3.84	1.56	1.51
3	F	5	P1A	C7-C8	3.79	1.39	1.34
3	F	5	P1A	C4-C3	3.79	1.59	1.52
3	E	5	P1A	C14-C13	3.70	1.62	1.56
3	E	5	P1A	C4-C5	3.50	1.61	1.54
3	H	5	P1A	O14-C14	3.47	1.49	1.43
3	F	5	P1A	C4-C5	3.46	1.61	1.54
3	H	5	P1A	C20-C17	3.42	1.61	1.55
3	E	5	P1A	C11-C9	3.33	1.59	1.53
3	E	5	P1A	C20-C17	3.24	1.60	1.55
3	G	5	P1A	C4-C5	3.12	1.60	1.54
3	F	5	P1A	C14-C13	3.11	1.62	1.56
3	H	5	P1A	C10-C5	3.01	1.61	1.56
3	H	5	P1A	C11-C9	2.97	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	5	P1A	C16-C17	2.95	1.60	1.54
3	E	5	P1A	O14-C14	2.89	1.48	1.43
3	F	5	P1A	C18-C13	2.87	1.59	1.54
3	F	5	P1A	C11-C9	2.84	1.58	1.53
3	G	5	P1A	C21-C20	2.79	1.57	1.52
3	G	5	P1A	C10-C5	2.77	1.60	1.56
3	F	5	P1A	C20-C17	2.75	1.60	1.55
3	E	5	P1A	C16-C17	2.74	1.59	1.54
3	E	5	P1A	C12-C13	2.73	1.59	1.54
3	E	5	P1A	C10-C5	2.69	1.60	1.56
3	F	5	P1A	C12-C13	2.65	1.59	1.54
3	G	5	P1A	C18-C13	2.65	1.59	1.54
3	E	5	P1A	C21-C20	2.64	1.57	1.52
3	E	5	P1A	C18-C13	2.56	1.59	1.54
3	G	5	P1A	C11-C9	2.54	1.58	1.53
3	H	5	P1A	C18-C13	2.52	1.59	1.54
3	G	5	P1A	C20-C17	2.39	1.59	1.55
3	H	5	P1A	C21-C20	2.38	1.57	1.52
3	F	5	P1A	C10-C5	2.35	1.60	1.56
3	F	5	P1A	C21-C20	2.35	1.57	1.52
3	H	5	P1A	C12-C13	2.29	1.58	1.54
3	F	5	P1A	O14-C14	2.28	1.47	1.43
3	G	5	P1A	C12-C13	2.18	1.58	1.54

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	5	P1A	O14-C14-C15	-4.57	99.86	110.34
3	E	5	P1A	O14-C14-C15	-4.32	100.42	110.34
3	G	5	P1A	O14-C14-C15	-4.14	100.85	110.34
3	E	5	P1A	C13-C14-C8	4.13	117.21	112.27
3	F	5	P1A	O14-C14-C15	-3.99	101.18	110.34
3	G	5	P1A	C24-C23-C22	-3.46	108.33	112.82
3	G	5	P1A	C13-C14-C8	3.44	116.39	112.27
3	F	5	P1A	C24-C23-C22	-3.40	108.41	112.82
3	F	5	P1A	C11-C9-C10	-3.40	107.81	113.96
3	H	5	P1A	C24-C23-C22	-3.29	108.56	112.82
3	F	5	P1A	C13-C14-C8	3.25	116.15	112.27
3	G	5	P1A	C12-C11-C9	3.21	120.66	112.60
3	G	5	P1A	C11-C9-C10	-3.11	108.33	113.96
3	E	5	P1A	C11-C9-C10	-3.05	108.43	113.96
3	G	5	P1A	C11-C12-C13	3.04	118.06	112.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	P1A	C24-C23-C22	-3.03	108.89	112.82
3	F	5	P1A	C11-C12-C13	2.94	117.90	112.84
3	H	5	P1A	C17-C20-C22	2.88	112.15	109.59
3	H	5	P1A	C13-C14-C8	2.87	115.70	112.27
3	E	5	P1A	C21-C20-C22	2.82	111.95	110.28
3	E	5	P1A	C10-C9-C8	-2.80	108.21	112.59
3	G	5	P1A	C10-C9-C8	-2.79	108.23	112.59
3	F	5	P1A	C17-C20-C22	2.77	112.05	109.59
3	H	5	P1A	C11-C9-C10	-2.74	108.99	113.96
3	G	5	P1A	C18-C13-C14	2.72	112.38	109.14
3	H	5	P1A	C10-C9-C8	-2.69	108.39	112.59
3	E	5	P1A	C15-C14-C13	2.64	105.67	103.20
3	H	5	P1A	C12-C13-C14	-2.61	104.01	107.86
3	G	5	P1A	C4-C5-C10	-2.58	109.26	112.80
3	E	5	P1A	C5-C6-C7	2.57	121.05	116.71
3	F	5	P1A	C5-C6-C7	2.49	120.92	116.71
3	E	5	P1A	C12-C11-C9	2.48	118.84	112.60
3	G	5	P1A	C23-C24-C25	2.46	121.05	114.61
3	F	5	P1A	C10-C9-C8	-2.46	108.76	112.59
3	F	5	P1A	C12-C11-C9	2.45	118.75	112.60
3	G	5	P1A	C5-C6-C7	2.44	120.83	116.71
3	H	5	P1A	C12-C11-C9	2.44	118.72	112.60
3	H	5	P1A	C15-C14-C13	2.42	105.46	103.20
3	H	5	P1A	C5-C6-C7	2.37	120.71	116.71
3	H	5	P1A	C11-C12-C13	2.35	116.88	112.84
3	F	5	P1A	C4-C5-C10	-2.33	109.60	112.80
3	H	5	P1A	C18-C13-C14	2.30	111.88	109.14
3	H	5	P1A	C4-C5-C10	-2.25	109.72	112.80
3	E	5	P1A	C12-C13-C14	-2.24	104.56	107.86
3	E	5	P1A	C18-C13-C14	2.23	111.80	109.14
3	E	5	P1A	C5-C4-C3	-2.16	108.88	111.90
3	F	5	P1A	C10-C1-C2	-2.15	110.57	114.09
3	F	5	P1A	C23-C24-C25	2.13	120.19	114.61
3	H	5	P1A	C5-C4-C3	-2.08	108.99	111.90
3	H	5	P1A	C10-C1-C2	-2.06	110.71	114.09
3	E	5	P1A	C11-C12-C13	2.01	116.29	112.84
3	G	5	P1A	C12-C13-C14	-2.00	104.91	107.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	5	P1A	C23-C24-C25-C27
3	G	5	P1A	C23-C24-C25-C26
3	H	5	P1A	C23-C24-C25-C27
3	H	5	P1A	C23-C24-C25-C26

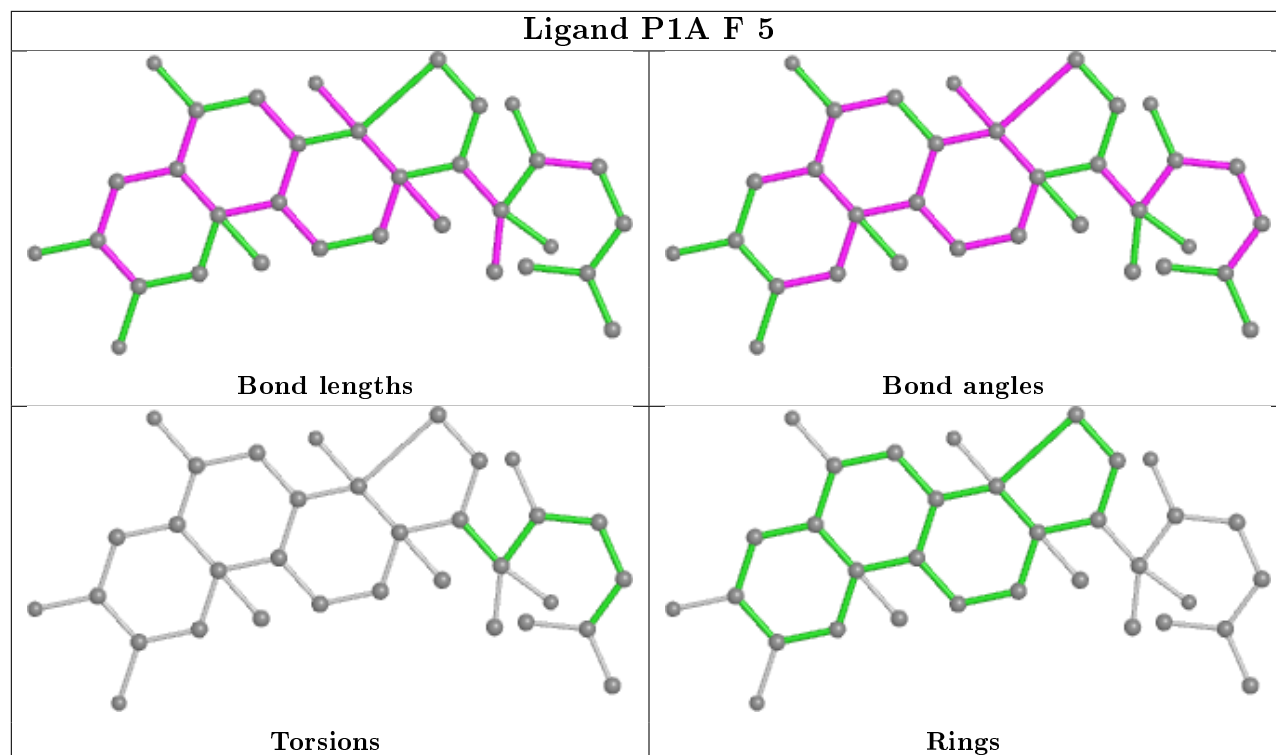
There are no ring outliers.

4 monomers are involved in 11 short contacts:

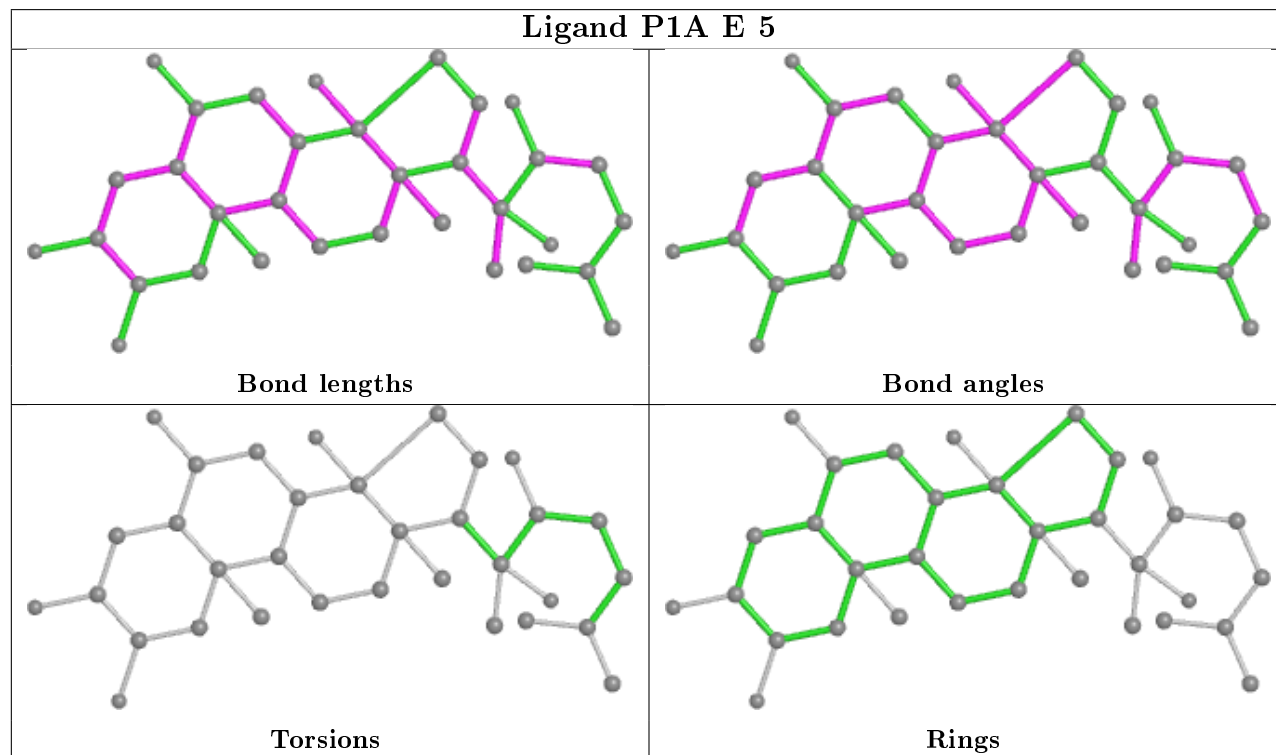
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	5	P1A	3	0
3	E	5	P1A	4	0
3	H	5	P1A	2	0
3	G	5	P1A	2	0

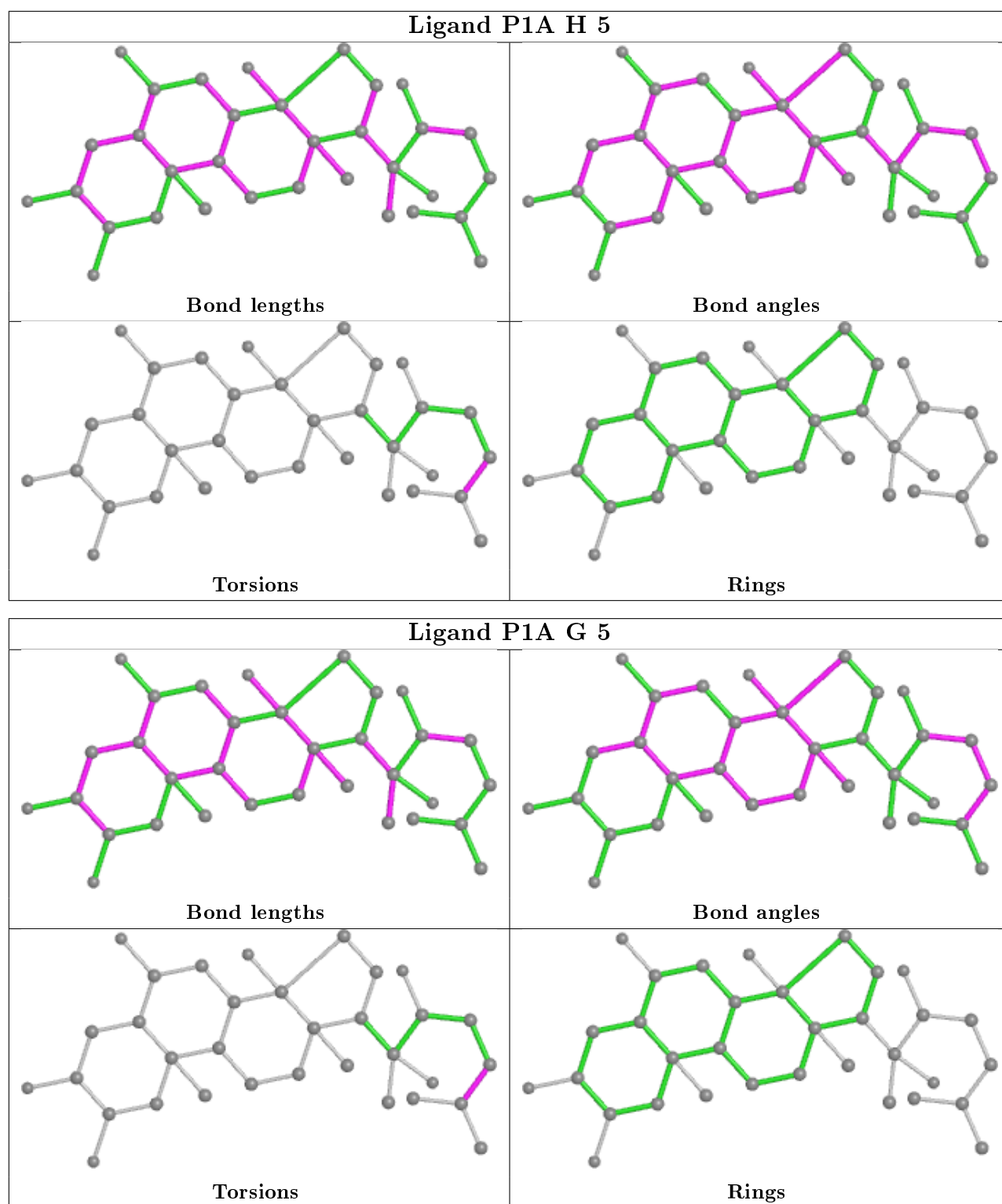
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand P1A F 5



Ligand P1A E 5





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	224/235 (95%)	0.60	13 (5%) 23 28	29, 71, 119, 158	0
1	B	228/235 (97%)	0.76	38 (16%) 1 1	30, 74, 119, 159	0
1	C	225/235 (95%)	0.81	39 (17%) 1 1	32, 74, 119, 158	0
1	D	227/235 (96%)	1.06	46 (20%) 1 1	32, 74, 124, 158	0
2	E	234/248 (94%)	0.46	19 (8%) 12 14	24, 53, 108, 158	0
2	F	233/248 (93%)	0.40	18 (7%) 13 16	25, 55, 105, 158	0
2	G	233/248 (93%)	0.30	14 (6%) 21 26	28, 54, 105, 157	0
2	H	234/248 (94%)	0.35	13 (5%) 24 29	27, 54, 106, 157	0
All	All	1838/1932 (95%)	0.59	200 (10%) 5 6	24, 62, 118, 159	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	419	ASN	12.3
1	B	205	ASN	8.9
1	D	203	VAL	8.6
1	D	204	VAL	6.8
1	B	204	VAL	6.3
1	D	202	LEU	6.0
2	H	418	ASN	6.0
2	E	348	GLU	5.8
1	D	205	ASN	5.8
1	D	199	LEU	5.7
2	F	350	GLN	5.5
2	H	346	ASP	5.5
1	D	209	THR	5.4
2	E	342	ASN	5.4
1	B	203	VAL	5.3
2	H	347	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	213	ASN	5.1
1	B	207	ASN	4.9
1	C	267	GLN	4.8
1	D	270	ILE	4.8
1	C	356	ASN	4.8
1	D	208	ASN	4.8
1	D	282	THR	4.7
1	D	184	GLU	4.7
2	G	346	ASP	4.6
1	B	214	ILE	4.6
2	F	346	ASP	4.6
1	C	203	VAL	4.5
2	H	499	LYS	4.5
2	E	346	ASP	4.5
1	D	274	THR	4.4
1	D	265	GLN	4.4
1	C	202	LEU	4.3
1	B	216	GLN	4.3
1	D	196	ASN	4.3
2	H	348	GLU	4.3
1	C	208	ASN	4.2
2	E	429	LEU	4.2
1	D	406	ASP	4.2
1	D	211	VAL	4.1
1	D	276	LEU	4.0
2	H	498	PRO	4.0
1	B	210	THR	4.0
1	C	216	GLN	4.0
2	F	349	ASP	3.9
1	C	389	GLY	3.9
2	G	498	PRO	3.8
1	C	270	ILE	3.8
2	H	497	LYS	3.7
2	F	342	ASN	3.7
1	C	273	ALA	3.7
2	E	351	CYS	3.7
1	B	284	HIS	3.6
1	D	206	GLU	3.6
1	C	390	ASP	3.6
1	C	204	VAL	3.6
2	G	342	ASN	3.6
2	E	350	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
2	G	497	LYS	3.5
2	F	348	GLU	3.5
1	B	209	THR	3.5
1	C	274	THR	3.4
2	E	420	GLN	3.4
1	D	213	ASN	3.4
1	D	267	GLN	3.4
1	A	388	ILE	3.4
1	C	214	ILE	3.4
2	G	495	ARG	3.3
2	F	324	TYR	3.3
2	E	349	ASP	3.3
2	G	348	GLU	3.3
1	C	271	VAL	3.2
2	G	500	PRO	3.2
2	H	500	PRO	3.2
1	C	206	GLU	3.2
2	G	499	LYS	3.1
2	F	353	VAL	3.1
1	D	284	HIS	3.1
1	D	207	ASN	3.1
1	D	262	ARG	3.1
1	C	209	THR	3.1
1	C	200	VAL	3.1
1	D	286	VAL	3.1
1	B	227	GLN	3.1
1	A	267	GLN	3.0
1	D	359	GLY	3.0
1	A	204	VAL	3.0
1	D	195	CYS	2.9
1	B	188	GLU	2.9
2	E	354	ARG	2.9
2	F	351	CYS	2.9
1	D	201	ALA	2.9
1	B	276	LEU	2.9
1	D	277	THR	2.8
2	F	347	GLY	2.8
1	C	266	ALA	2.8
1	D	216	GLN	2.8
2	F	338	LYS	2.8
1	D	200	VAL	2.7
1	D	300	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	286	VAL	2.7
1	C	272	LEU	2.7
1	C	201	ALA	2.7
2	E	353	VAL	2.7
1	C	210	THR	2.7
2	F	422	TYR	2.7
2	F	320	HIS	2.6
1	B	270	ILE	2.6
1	D	214	ILE	2.6
1	B	224	GLN	2.6
1	C	212	ASN	2.6
2	H	494	ASN	2.6
1	A	390	ASP	2.6
1	C	330	LYS	2.6
1	B	208	ASN	2.6
1	B	184	GLU	2.6
1	A	274	THR	2.6
1	D	405	THR	2.6
1	C	196	ASN	2.6
1	B	178	GLN	2.6
2	E	495	ARG	2.6
1	C	277	THR	2.5
1	C	211	VAL	2.5
1	C	265	GLN	2.5
2	F	341	ILE	2.5
1	C	205	ASN	2.5
1	D	304	LYS	2.5
2	F	337	VAL	2.5
1	D	193	VAL	2.5
1	C	215	CYS	2.5
2	H	351	CYS	2.5
1	B	189	ALA	2.4
2	G	410	GLN	2.4
1	B	195	CYS	2.4
1	C	219	HIS	2.4
2	E	547	LEU	2.4
1	B	274	THR	2.4
1	D	198	PRO	2.4
2	E	498	PRO	2.4
1	B	185	ARG	2.3
1	B	206	GLU	2.3
1	B	285	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	199	LEU	2.3
1	D	210	THR	2.3
2	G	351	CYS	2.3
1	D	266	ALA	2.3
1	D	404	THR	2.3
2	G	545	VAL	2.3
1	C	282	THR	2.3
1	C	304	LYS	2.3
1	D	278	VAL	2.3
1	A	351	ARG	2.3
1	D	215	CYS	2.3
2	H	530	LEU	2.3
2	H	495	ARG	2.3
1	D	272	LEU	2.3
2	F	420	GLN	2.3
2	E	447	TYR	2.3
1	B	200	VAL	2.3
1	C	386	LYS	2.2
1	C	223	PHE	2.2
2	E	418	ASN	2.2
1	B	201	ALA	2.2
2	E	347	GLY	2.2
2	F	340	ILE	2.2
2	G	494	ASN	2.2
1	B	388	ILE	2.2
1	B	196	ASN	2.2
2	G	333	SER	2.2
1	A	202	LEU	2.2
1	C	258	ALA	2.2
1	A	278	VAL	2.2
2	F	526	PHE	2.2
2	E	526	PHE	2.2
1	B	266	ALA	2.1
1	D	351	ARG	2.1
2	H	353	VAL	2.1
2	E	546	ASP	2.1
1	B	212	ASN	2.1
2	E	311	ILE	2.1
1	B	289	GLY	2.1
1	D	189	ALA	2.1
1	B	187	ILE	2.1
1	B	191	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	351	ARG	2.1
1	D	356	ASN	2.1
1	B	327	ARG	2.1
1	A	219	HIS	2.1
1	A	387	LEU	2.1
1	A	211	VAL	2.1
1	C	195	CYS	2.1
1	B	202	LEU	2.0
1	A	203	VAL	2.0
1	B	282	THR	2.0
1	D	227	GLN	2.0
1	D	185	ARG	2.0
1	A	222	LEU	2.0
2	F	495	ARG	2.0
1	B	275	GLY	2.0
1	B	193	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

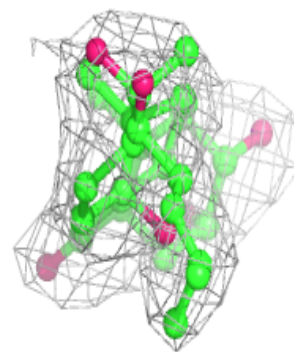
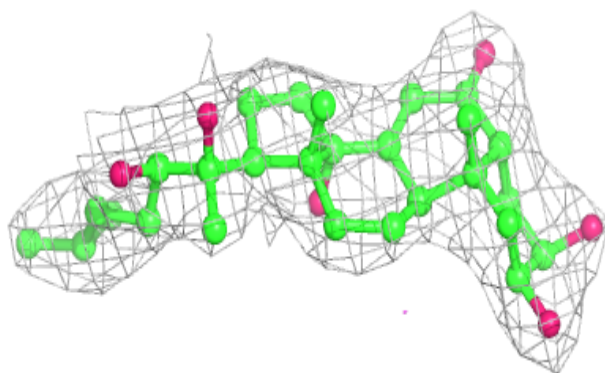
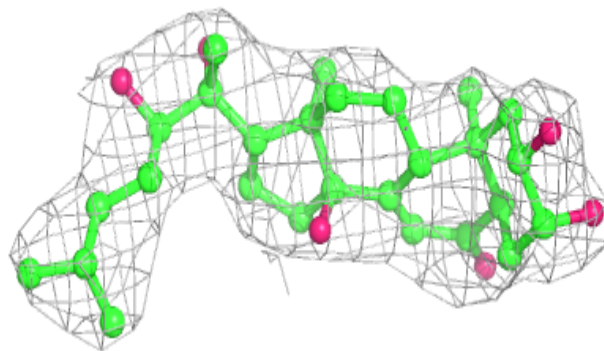
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	P1A	E	5	33/33	0.94	0.18	31,34,38,42	0
3	P1A	H	5	33/33	0.95	0.17	30,39,42,43	0
3	P1A	G	5	33/33	0.95	0.20	30,35,39,43	0
3	P1A	F	5	33/33	0.96	0.17	33,39,41,44	0

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.

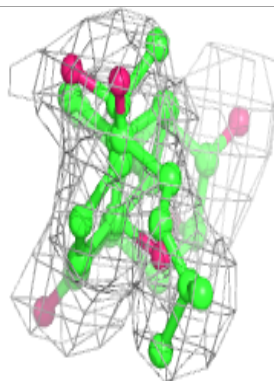
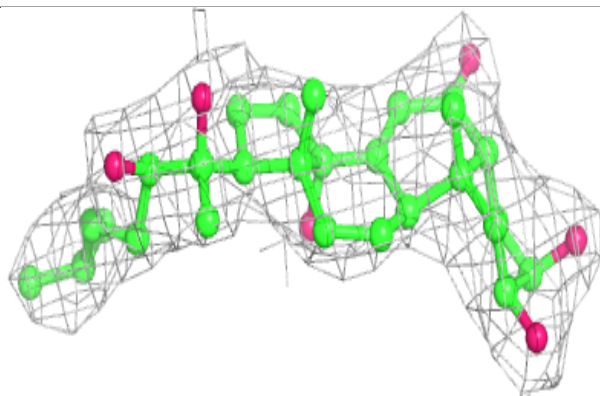
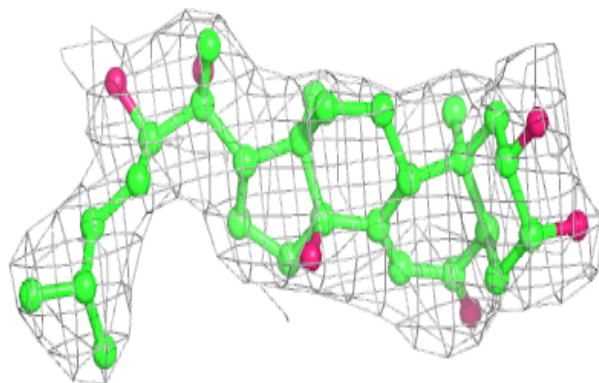
Electron density around P1A E 5:

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



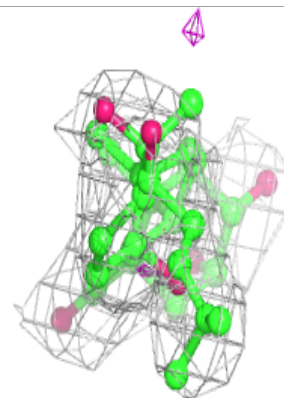
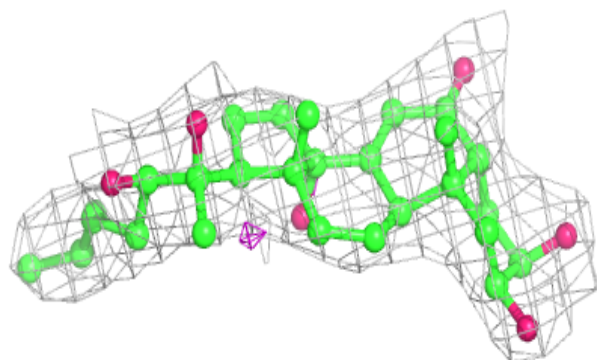
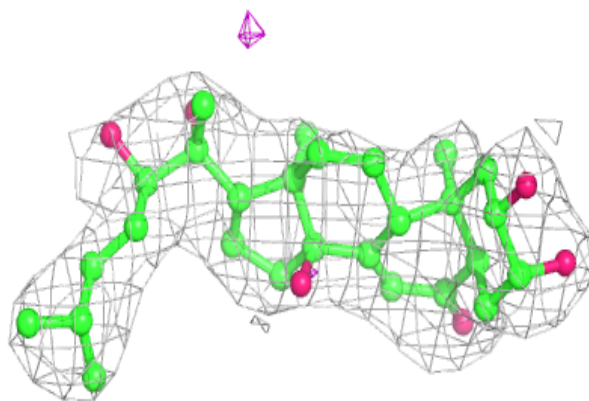
Electron density around P1A H 5:

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

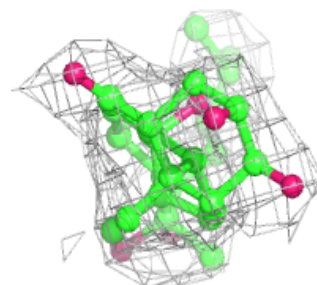
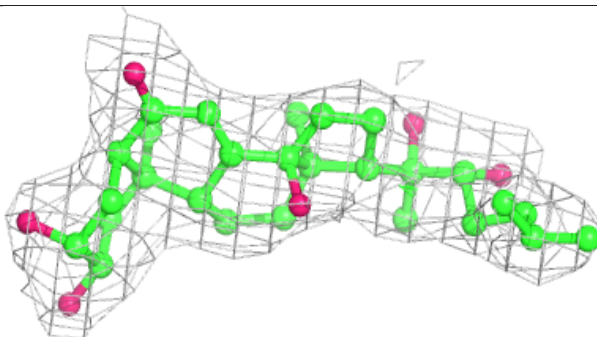
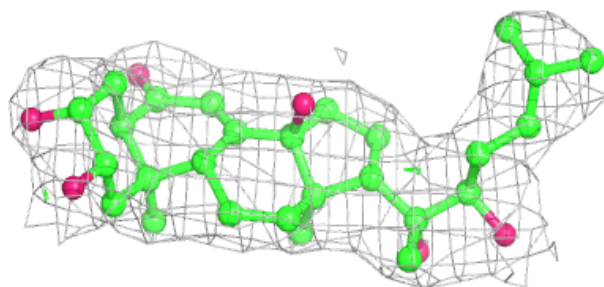


Electron density around P1A G 5:

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

**Electron density around P1A F 5:**

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



6.5 Other polymers

There are no such residues in this entry.