



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:39 AM UTC

PDB ID : 2NXX / pdb_00002nxx
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

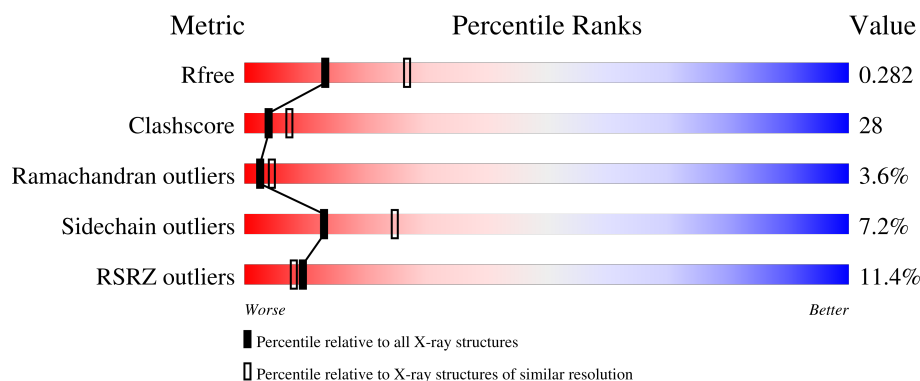
1 Overall quality at a glance

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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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

Mol	Chain	Length	Quality of chain
1	A	235	23% 49% 35% 10% 5%
1	B	235	14% 48% 38% 11% ••
1	C	235	10% 50% 35% 10% •
1	D	235	17% 47% 38% 11% •
2	E	248	6% 56% 33% 5% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	248	6% 56% 31% 6% 6%
2	G	248	6% 56% 32% 5% 6%
2	H	248	4% 54% 33% 6% 6%

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.

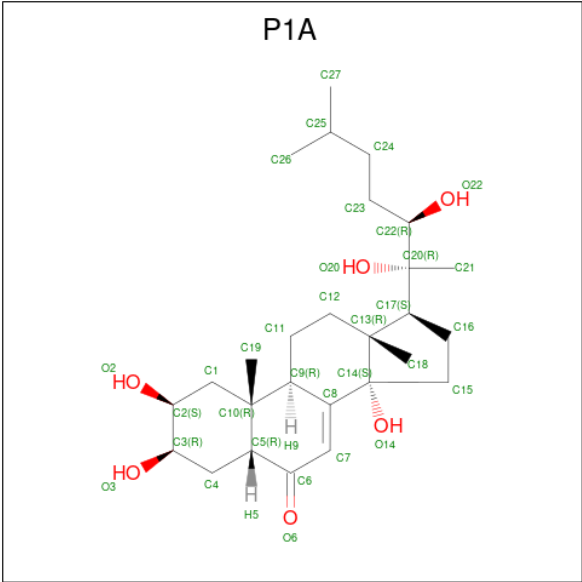
- Molecule 1 is a protein called Ultraspiracle (USP, NR2B4).

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 (CCD ID: P1A) (formula: C₂₇H₄₄O₆).



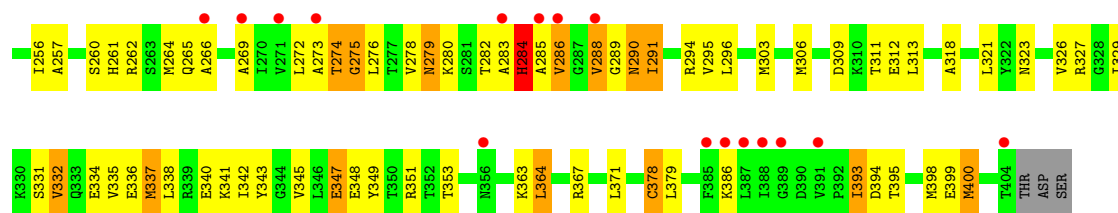
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			33	27	6		
3	F	1	Total	C	O	0	0
			33	27	6		
3	G	1	Total	C	O	0	0
			33	27	6		
3	H	1	Total	C	O	0	0
			33	27	6		

- Molecule 4 is water.

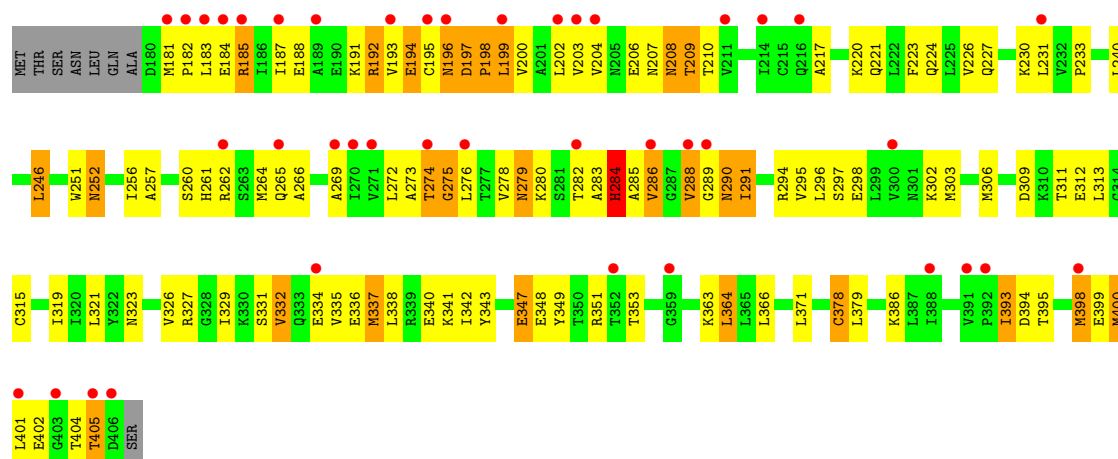
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	E	53	Total	O	0	0
			53	53		
4	B	23	Total	O	0	0
			23	23		
4	F	41	Total	O	0	0
			41	41		
4	C	16	Total	O	0	0
			16	16		
4	G	30	Total	O	0	0
			30	30		
4	D	26	Total	O	0	0
			26	26		
4	H	27	Total	O	0	0
			27	27		

- Molecule 1: Ultraspiracle (USP, NR2B4)

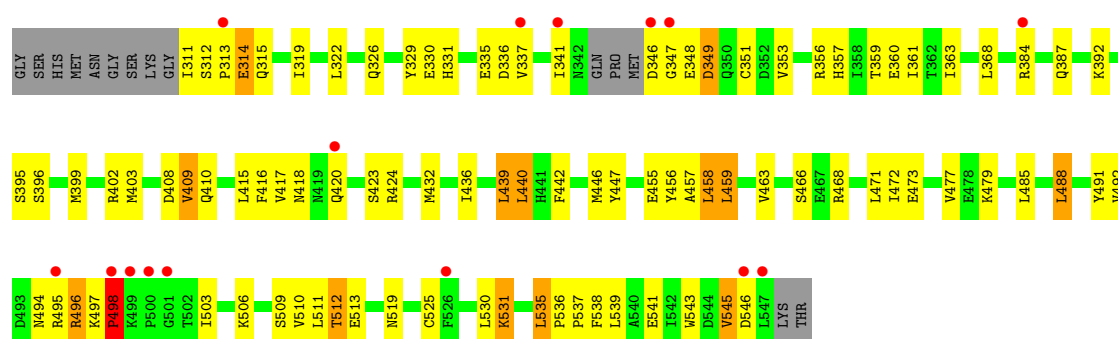




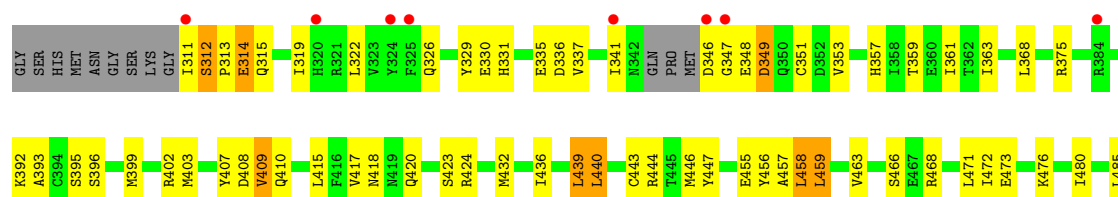
• Molecule 1: Ultraspiracle (USP, NR2B4)



• Molecule 2: Ecdysone Receptor (EcR, NRH1)

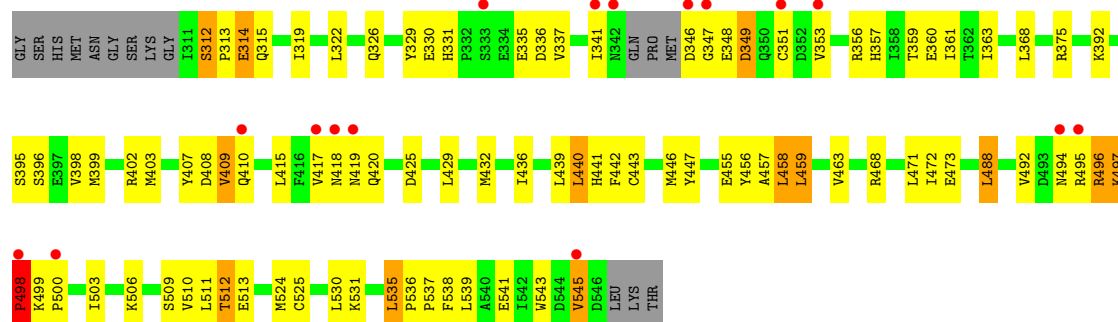


• Molecule 2: Ecdysone Receptor (EcR, NRH1)

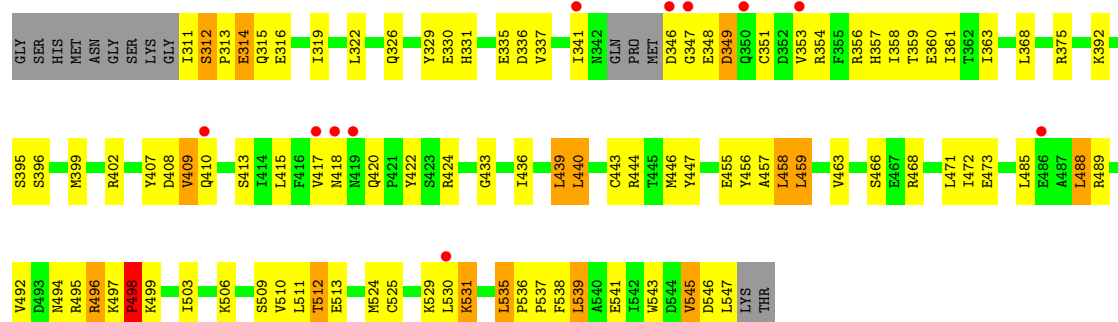




• Molecule 2: Ecdysone Receptor (EcR, NRH1)



• 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 50.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.75) 98.1 (50.00-2.75)	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 0.249 , 0.282	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)	0.34 , 69.5	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	0.50	0/1810	0.96	5/2450 (0.2%)
1	B	0.56	3/1832 (0.2%)	1.17	15/2481 (0.6%)
1	C	0.42	0/1815	0.96	8/2457 (0.3%)
1	D	0.43	0/1827	0.98	9/2474 (0.4%)
2	E	0.54	0/1957	1.36	7/2641 (0.3%)
2	F	0.50	0/1952	1.32	7/2634 (0.3%)
2	G	0.49	0/1949	1.35	6/2630 (0.2%)
2	H	0.50	0/1960	1.33	6/2645 (0.2%)
All	All	0.49	3/15102 (0.0%)	1.20	63/20412 (0.3%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	404	THR	CA-C	-10.70	1.38	1.52
1	B	404	THR	C-O	8.88	1.35	1.24
1	B	404	THR	CA-CB	-5.25	1.44	1.53

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	497	LYS	CA-C-N	36.78	165.82	119.84
2	E	497	LYS	C-N-CA	36.78	165.82	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	497	LYS	CA-C-N	36.05	164.90	119.84
2	G	497	LYS	C-N-CA	36.05	164.90	119.84
2	H	497	LYS	CA-C-N	35.26	163.92	119.84
2	H	497	LYS	C-N-CA	35.26	163.92	119.84
2	F	497	LYS	CA-C-N	34.78	163.31	119.84
2	F	497	LYS	C-N-CA	34.78	163.31	119.84
1	B	403	GLY	N-CA-C	19.59	136.04	112.33
1	B	404	THR	CA-C-N	12.62	144.43	121.70
1	B	404	THR	C-N-CA	12.62	144.43	121.70
2	H	497	LYS	C-N-CD	-12.58	73.41	125.00
2	G	497	LYS	C-N-CD	-12.56	73.52	125.00
2	E	497	LYS	C-N-CD	-12.55	73.55	125.00
2	F	497	LYS	C-N-CD	-12.45	73.96	125.00
1	B	275	GLY	N-CA-C	-10.07	102.12	115.21
1	D	275	GLY	N-CA-C	-10.03	102.17	115.21
1	A	275	GLY	N-CA-C	-9.81	102.46	115.21
2	H	531	LYS	N-CA-C	-9.68	98.18	110.19
1	C	275	GLY	N-CA-C	-9.66	102.65	115.21
2	F	531	LYS	N-CA-C	-9.52	98.39	110.19
2	G	531	LYS	N-CA-C	-9.48	98.44	110.19
1	D	405	THR	N-CA-C	9.46	123.02	110.53
1	B	291	ILE	N-CA-C	-8.98	103.64	113.43
1	C	291	ILE	N-CA-C	-8.96	103.66	113.43
1	B	404	THR	O-C-N	8.94	134.49	122.59
1	A	291	ILE	N-CA-C	-8.71	103.94	113.43
1	D	291	ILE	N-CA-C	-8.50	104.16	113.43
1	B	404	THR	CA-C-O	7.99	131.94	120.51
1	A	378	CYS	N-CA-C	7.96	119.86	111.03
1	C	378	CYS	N-CA-C	7.71	119.59	111.03
1	B	378	CYS	N-CA-C	7.68	119.55	111.03
2	E	497	LYS	N-CA-C	7.52	126.43	109.81
1	B	404	THR	N-CA-C	7.52	126.81	110.80
2	F	497	LYS	N-CA-C	7.37	126.09	109.81
2	E	531	LYS	N-CA-C	-7.29	98.45	109.60
2	H	497	LYS	N-CA-C	7.13	125.57	109.81
2	G	497	LYS	N-CA-C	6.84	124.93	109.81
1	C	386	LYS	N-CA-C	-6.77	104.76	113.16
1	A	386	LYS	N-CA-C	-6.66	104.90	113.16
1	B	386	LYS	N-CA-C	-6.62	104.95	113.16
1	D	386	LYS	N-CA-C	-6.42	105.20	113.16
2	H	498	PRO	CA-N-CD	-6.35	103.11	112.00
2	F	498	PRO	CA-N-CD	-6.32	103.15	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	378	CYS	N-CA-C	6.26	119.31	111.24
2	G	498	PRO	CA-N-CD	-6.20	103.32	112.00
1	B	297	SER	N-CA-C	6.12	118.03	111.36
1	D	297	SER	N-CA-C	6.05	117.95	111.36
2	E	498	PRO	CA-N-CD	-5.84	103.82	112.00
2	E	546	ASP	N-CA-C	-5.76	107.25	114.56
1	B	343	TYR	N-CA-C	-5.55	105.13	111.07
1	D	252	ASN	N-CA-C	5.51	116.97	111.07
1	B	404	THR	N-CA-CB	5.36	119.54	110.49
1	C	252	ASN	N-CA-C	5.35	116.79	111.07
2	F	393	ALA	N-CA-C	5.20	117.85	111.82
1	A	209	THR	N-CA-C	-5.17	106.10	112.72
1	D	343	TYR	N-CA-C	-5.16	105.55	111.07
1	B	209	THR	N-CA-C	-5.16	106.12	112.72
1	C	343	TYR	N-CA-C	-5.15	105.56	111.07
1	C	367	ARG	N-CA-C	-5.13	106.86	113.23
1	D	209	THR	N-CA-C	-5.13	106.15	112.72
1	C	209	THR	N-CA-C	-5.05	106.26	112.72
1	B	402	GLU	N-CA-C	-5.03	107.09	113.18

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	121	0
1	B	1802	0	1853	155	0
1	C	1785	0	1839	115	0
1	D	1797	0	1848	152	0
2	E	1922	0	1927	83	0
2	F	1917	0	1925	77	0
2	G	1914	0	1916	91	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1925	0	1936	91	0
3	E	33	0	44	5	0
3	F	33	0	44	4	0
3	G	33	0	44	3	0
3	H	33	0	44	2	0
4	A	51	0	0	8	0
4	B	23	0	0	4	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	4	0
4	G	30	0	0	5	0
4	H	27	0	0	3	0
All	All	15241	0	15257	846	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 28.

All (846) 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

Continued on next page...

Continued from previous page...

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:C:197:ASP:HB2	1:C:198:PRO:HD3	1.56	0.86
1:B:353:THR:CG2	2:G:419:ASN:HB3	2.06	0.86
2:F:495:ARG:O	2:F:496:ARG:HG2	1.74	0.86
1:C:288:VAL:HG12	1:C:289:GLY:N	1.89	0.86
1:D:197:ASP:HB2	1:D:198:PRO:HD3	1.57	0.86
1:B:192:ARG:HH11	1:B:192:ARG:HB2	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:HB2	1:D:192:ARG:HH11	1.42	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:D:260:SER:HB3	1:D:303:MET:HE1	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
1:A:192:ARG:HH11	1:A:192:ARG:HB2	1.42	0.82
1:D:230:LYS:HE2	1:D:405:THR:HA	1.61	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:311:ILE:HG22	2:E:312:SER:N	1.90	0.81
1:B:260:SER:HB3	1:B:303:MET:HE1	1.63	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:H	1:C:284:HIS:CD2	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
2:G:418:ASN:ND2	2:G:420:GLN:HB2	1.97	0.78
1:D:284:HIS:CD2	1:D:284:HIS:H	1.99	0.78
1:A:284:HIS:H	1:A:284:HIS:CD2	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:HD23	2:H:547:LEU:O	1.83	0.77
1:B:353:THR:HG22	2:G:419:ASN:CB	2.12	0.77
1:D:288:VAL:CG1	1:D:289:GLY:H	1.94	0.76
1:C:260:SER:HB3	1:C:303:MET:HE1	1.66	0.76
1:B:202:LEU:HD13	1:B:276:LEU:HD21	1.67	0.76
1:B:284:HIS:CD2	1:B:284:HIS:H	2.01	0.76
2:F:545:VAL:HG12	2:F:545:VAL:O	1.85	0.76
2:H:418:ASN:ND2	2:H:420:GLN:HB2	2.00	0.76
2:F:446:MET:HE1	2:F:510:VAL:CG2	2.16	0.76
1:A:221:GLN:NE2	1:A:262:ARG:HH22	1.82	0.76
2:E:545:VAL:HG12	2:E:545:VAL:O	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
2:F:446:MET:HE1	2:F:510:VAL:HG22	1.68	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
1:A:260:SER:HB3	1:A:303:MET:HE1	1.67	0.75
2:G:446:MET:HE1	2:G:510:VAL:CG2	2.16	0.75
1:B:207:ASN:HB3	1:D:265:GLN:CA	2.17	0.75
2:H:446:MET:HE1	2:H:510:VAL:CG2	2.17	0.74
4:D:415:HOH:O	2:H:512:THR:HG21	1.87	0.74
2:G:446:MET:HE1	2:G:510:VAL:HG22	1.69	0.74
2:G:545:VAL:HG12	2:G:545:VAL:O	1.86	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:446:MET:HE1	2:E:510:VAL:CG2	2.19	0.73
2:E:446:MET:HE1	2:E:510:VAL:HG22	1.70	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
1:C:185:ARG:HA	1:C:185:ARG:HE	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:H:446:MET:HE1	2:H:510:VAL:HG22	1.71	0.72
2:F:535:LEU:HD22	2:F:536:PRO:HD2	1.69	0.72
1:C:284:HIS:H	1:C:284:HIS:HD2	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
1:B:178:GLN:O	1:B:337:MET:HE1	1.91	0.70
2:H:348:GLU:HG3	2:H:349:ASP:H	1.57	0.70
1:B:205:ASN:ND2	1:D:265:GLN:HE21	1.90	0.70
1:C:203:VAL:HB	1:C:210:THR:HG22	1.74	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:H	1:A:284:HIS:HD2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:409:VAL:HG23	4:E:598:HOH:O	1.92	0.68
2:G:348:GLU:HG3	2:G:349:ASP:H	1.58	0.68
1:D:184:GLU:O	1:D:187:ILE:HG13	1.92	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
2:G:395:SER:HB2	2:G:543:TRP:HE1	1.59	0.68
1:D:323:ASN:HB3	1:D:326:VAL:HG23	1.76	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
2:E:348:GLU:HG3	2:E:349:ASP:H	1.58	0.67
1:D:203:VAL:HB	1:D:210:THR:HG22	1.76	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:E:395:SER:HB2	2:E:543:TRP:HE1	1.59	0.67
1:C:182:PRO:HB2	1:C:185:ARG:HB2	1.77	0.67
1:C:184:GLU:O	1:C:187:ILE:HG13	1.95	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: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
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:H:313:PRO:O	2:H:314:GLU:HB2	1.98	0.64
1:B:226:VAL:O	1:B:230:LYS:HG3	1.97	0.64
2:F:492:VAL:HG13	2:F:496:ARG:HG3	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:VAL:O	1:C:230:LYS:HG3	1.98	0.64
1:C:181:MET:HE1	1:C:233:PRO:HB2	1.78	0.64
2:E:313:PRO:O	2:E:314:GLU:HB2	1.98	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
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:CD2	1:D:284:HIS:N	2.67	0.63
1:A:279:ASN:H	1:A:282:THR:CG2	2.11	0.63
2:H:363:ILE:HG23	2:H:538:PHE:CD2	2.33	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
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:CD2	1:C:284:HIS:N	2.68	0.62
1:C:197:ASP:CB	1:C:198:PRO:CD	2.77	0.62
1:C:286:VAL:HG12	1:C:286:VAL:O	1.99	0.62
1:B:205:ASN:CG	1:D:265:GLN:HE21	2.08	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:D:230:LYS:HD3	1:D:404:THR:C	2.24	0.62
2:F:496:ARG:O	2:F:498:PRO:CD	2.46	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:E:432:MET:HE1	3:E:5:P1A:H272	1.80	0.62
1:D:286:VAL:HG12	1:D:286:VAL:O	2.00	0.62
1:D:400:MET:C	1:D:402:GLU:H	2.08	0.62
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:CD2	1:A:284:HIS:N	2.68	0.61
1:B:220:LYS:O	1:B:224:GLN:HG3	2.00	0.61
2:F:423:SER:HB2	4:F:583:HOH:O	1.99	0.61
1:D:183:LEU:O	1:D:187:ILE:HG23	1.99	0.61
1:D:207:ASN:OD1	1:D:209:THR:HB	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:VAL:HG12	1:A:286:VAL:O	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
1:A:187:ILE:HD12	1:A:188:GLU:N	2.15	0.61
2:F:313:PRO:O	2:F:314:GLU:HB2	1.99	0.61
2:H:496:ARG:O	2:H:498:PRO:CD	2.46	0.61
2:E:496:ARG:O	2:E:498:PRO:CD	2.45	0.61
1:D:272:LEU:HD11	1:D:286:VAL:HG11	1.83	0.61
1:A:261:HIS:O	1:A:264:MET:HG3	2.00	0.61
2:E:402:ARG:NH1	4:E:580:HOH:O	2.27	0.61
1:B:272:LEU:HD11	1:B:286:VAL:HG11	1.83	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:HG12	1:B:286:VAL:O	2.01	0.61
1:C:192:ARG:HB2	1:C:192:ARG:NH1	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:B:353:THR:HB	2:G:419:ASN:CG	2.26	0.60
1:A:207:ASN:OD1	1:A:209:THR:HB	2.01	0.60
1:D:192:ARG:HB2	1:D:192:ARG:NH1	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:HH11	1:D:327:ARG:HB3	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:207:ASN:CA	1:D:265:GLN:HA	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
2:G:509:SER:O	2:G:512:THR:HG23	2.02	0.59
1:D:302:LYS:HE3	4:D:428:HOH:O	2.01	0.59
1:D:306:MET:HE2	1:D:363:LYS:HE2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:311:ILE:HD11	2:E:491:TYR:HA	1.83	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
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
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:HB3	1:C:327:ARG:HH11	1.67	0.59
1:D:193:VAL:CG1	1:D:224:GLN:HB3	2.33	0.59
2:E:322:LEU:HD12	2:E:458:LEU:HD13	1.85	0.59
1:D:279:ASN:H	1:D:282:THR:CG2	2.09	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
2:E:311:ILE:CG2	2:E:312:SER:N	2.55	0.58
1:B:193:VAL:HG13	1:B:224:GLN:CD	2.28	0.58
1:D:193:VAL:HG13	1:D:224:GLN:CD	2.29	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:B:306:MET:HE2	1:B:363:LYS:HE2	1.86	0.57
2:F:402:ARG:NH1	4:F:580:HOH:O	2.26	0.57
1:D:398:MET:O	1:D:402:GLU:HG3	2.03	0.57
1:A:349:TYR:O	1:A:353:THR:HG23	2.04	0.57
1:A:193:VAL:HG13	1:A:224:GLN:CD	2.29	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
2:E:479:LYS:HE2	4:E:576:HOH:O	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:VAL:HB	1:B:210:THR:CG2	2.35	0.57
2:G:524:MET:HE1	4:G:554:HOH:O	2.04	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:C:187:ILE:HD12	1:C:187:ILE:C	2.30	0.57
1:D:260:SER:HB3	1:D:303:MET:CE	2.34	0.57
2:E:494:ASN:C	2:E:494:ASN:HD22	2.13	0.56
2:E:416:PHE:CZ	3:E:5:P1A:H152	2.40	0.56
1:B:187:ILE:HD12	1:B:187:ILE:C	2.30	0.56
1:D:285:ALA:O	1:D:286:VAL:HB	2.04	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
2:F:494:ASN:C	2:F:494:ASN:HD22	2.13	0.56
1:D:185:ARG:HB3	1:D:233:PRO:HG3	1.88	0.56
1:A:257:ALA:HB2	1:A:371:LEU:HD21	1.87	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:187:ILE:HD12	1:A:187:ILE:C	2.31	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:CD	2.31	0.55
1:C:193:VAL:HG13	1:C:224:GLN:HB3	1.87	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:494:ASN:C	2:H:494:ASN:HD22	2.14	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
2:F:322:LEU:HD12	2:F:458:LEU:HD13	1.87	0.55
1:C:203:VAL:HB	1:C:210:THR:CG2	2.35	0.55
1:D:187:ILE:HD12	1:D:187:ILE:C	2.31	0.55
1:B:185:ARG:HB3	1:B:233:PRO:HG3	1.89	0.55
2:G:494:ASN:C	2:G:494:ASN:HD22	2.13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:SER:CB	1:D:303:MET:HE1	2.35	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:260:SER:C	1:B:303:MET:HE1	2.33	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:C:306:MET:HE2	1:C:363:LYS:HE2	1.88	0.54
1:C:340:GLU:OE2	2:G:506:LYS:HD2	2.08	0.54
1:D:187:ILE:HG22	1:D:311:THR:HG23	1.90	0.54
1:A:193:VAL:HG12	1:A:193:VAL:O	2.07	0.54
1:C:193:VAL:HG12	1:C:193:VAL:O	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
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
2:G:402:ARG:NH1	4:G:557:HOH:O	2.41	0.53
1:D:260:SER:C	1:D:303:MET:HE1	2.34	0.53
2:H:545:VAL:O	2:H:545:VAL:CG1	2.54	0.53
1:B:207:ASN:OD1	1:B:210:THR:HG23	2.08	0.53
2:F:432:MET:HE1	3:F:5:P1A:H272	1.90	0.53
2:G:446:MET:HE1	2:G:510:VAL:HG21	1.90	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:C:207:ASN:O	1:C:209:THR:N	2.41	0.53
1:C:260:SER:C	1:C:303:MET:HE1	2.34	0.53
1:D:338:LEU:O	1:D:342:ILE:HG13	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:260:SER:HB3	1:B:303:MET:CE	2.36	0.52
1:B:260:SER:CB	1:B:303:MET:HE1	2.36	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
2:E:408:ASP:OD2	2:E:410:GLN:HB2	2.10	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:H:409:VAL:HG21	2:H:447:TYR:CZ	2.45	0.52
1:A:260:SER:C	1:A:303:MET:HE1	2.34	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: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
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:D:246:LEU:HD13	1:D:329:ILE:CD1	2.40	0.52
1:D:279:ASN:N	1:D:282:THR:HG23	2.15	0.52
1:A:221:GLN:HE22	1:A:262:ARG:NH2	1.97	0.52
2:F:396:SER:HA	2:F:399:MET:HE2	1.92	0.51
2:F:446:MET:HE1	2:F:510:VAL:HG21	1.93	0.51
1:A:260:SER:CB	1:A:303:MET:HE1	2.40	0.51
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:260:SER:HB3	1:A:303:MET:CE	2.39	0.51
1:A:187:ILE:HG22	1:A:311:THR:HG23	1.91	0.51
1:C:187:ILE:HG22	1:C:311:THR:HG23	1.92	0.51
1:B:206:GLU:C	1:B:208:ASN:H	2.19	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:VAL:CG1	1:D:196:ASN:HD21	2.18	0.50
1:C:181:MET:CE	1:C:233:PRO:HB2	2.41	0.50
1:C:206:GLU:C	1:C:208:ASN:H	2.19	0.50
2:E:436:ILE:HG13	2:E:440:LEU:HD22	1.93	0.50
1:A:206:GLU:C	1:A:208:ASN:H	2.19	0.50
1:A:306:MET:HE2	1:A:363:LYS:HE2	1.92	0.50
2:G:525:CYS:HB3	2:G:545:VAL:CG1	2.35	0.50
1:D:181:MET:CE	1:D:233:PRO:HB2	2.42	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:403:MET:HB2	3:F:5:P1A:H121	1.94	0.49
2:F:418:ASN:HD21	2:F:420:GLN:HB2	1.74	0.49
1:D:207:ASN:C	1:D:209:THR:N	2.70	0.49
1:C:207:ASN:C	1:C:209:THR:N	2.70	0.49
1:C:260:SER:HB3	1:C:303:MET:CE	2.39	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
2:F:329:TYR:O	2:F:402:ARG:NH2	2.39	0.49
1:D:206:GLU:C	1:D:208:ASN:H	2.19	0.49
1:D:291:ILE:O	1:D:295:VAL:HG23	2.12	0.49
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
2:F:463:VAL:HG22	2:F:511:LEU:HD22	1.94	0.49
1:D:252:ASN:O	1:D:256:ILE:HG13	2.12	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
2:E:357:HIS:O	2:E:361:ILE:HG13	2.13	0.48
1:B:207:ASN:C	1:B:209:THR:N	2.70	0.48
2:F:408:ASP:OD2	2:F:410:GLN:HB2	2.12	0.48
2:F:494:ASN:C	2:F:494:ASN:ND2	2.70	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:LEU:HD13	1:C:329:ILE:CD1	2.42	0.48
1:C:252:ASN:O	1:C:256:ILE:HG13	2.13	0.48
1:C:273:ALA:C	1:C:275:GLY:H	2.21	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
2:F:330:GLU:OE2	2:F:331:HIS:HB3	2.14	0.48
1:C:279:ASN:N	1:C:282:THR:HG23	2.15	0.48
2:H:446:MET:HE1	2:H:510:VAL:HG21	1.92	0.48
2:E:446:MET:HE1	2:E:510:VAL:HG21	1.95	0.48
1:B:265:GLN:HG2	1:B:266:ALA:N	2.28	0.48
2:G:455:GLU:O	2:G:459:LEU:HB2	2.14	0.48
1:D:279:ASN:OD1	1:D:280:LYS:N	2.46	0.48
1:D:290:ASN:OD1	1:D:290:ASN:N	2.47	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:E:396:SER:HA	2:E:399:MET:HE2	1.96	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
2:E:424:ARG:HG3	4:E:595:HOH:O	2.12	0.48
1:B:265:GLN:HG2	1:B:266:ALA:H	1.79	0.48
2:H:494:ASN:C	2:H:494:ASN:ND2	2.71	0.48
1:A:398:MET:O	1:A:402:GLU:HG3	2.14	0.48
1:B:353:THR:HA	2:G:419:ASN:HB3	1.95	0.48
2:F:455:GLU:O	2:F:459:LEU:HB2	2.13	0.48
2:G:495:ARG:O	2:G:496:ARG:CG	2.52	0.48
2:E:545:VAL:O	2:E:545:VAL:CG1	2.56	0.48
1:B:246:LEU:HG	1:B:321:LEU:O	2.14	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
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:D:230:LYS:HE2	1:D:405:THR:CA	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:ARG:HG2	1:D:231:LEU:HD11	1.96	0.47
2:F:335:GLU:HG3	2:F:336:ASP:N	2.29	0.47
1:C:246:LEU:HD13	1:C:329:ILE:HD13	1.95	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:494:ASN:C	2:G:494:ASN:ND2	2.71	0.47
2:G:537:PRO:O	2:G:541:GLU:HG2	2.14	0.47
2:H:396:SER:HA	2:H:399:MET:HE2	1.96	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:207:ASN:C	1:A:209:THR:N	2.70	0.47
1:A:265:GLN:HG2	1:A:266:ALA:N	2.30	0.47
1:A:278:VAL:CG1	1:A:283:ALA:HA	2.45	0.47
2:G:395:SER:CB	2:G:543:TRP:HE1	2.26	0.47
1:D:246:LEU:HG	1:D:321:LEU:O	2.14	0.47
1:D:273:ALA:C	1:D:275:GLY:H	2.23	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
2:E:455:GLU:O	2:E:459:LEU:HB2	2.15	0.47
1:B:278:VAL:HG11	1:B:283:ALA:HA	1.97	0.47
2:F:346:ASP:O	2:F:348:GLU:N	2.48	0.47
2:G:396:SER:HA	2:G:399:MET:HE2	1.96	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
2:E:346:ASP:O	2:E:348:GLU:N	2.48	0.47
1:B:279:ASN:OD1	1:B:280:LYS:N	2.47	0.47
2:F:418:ASN:C	2:F:420:GLN:H	2.22	0.47
2:F:525:CYS:HB3	2:F:545:VAL:CG1	2.35	0.47
1:C:290:ASN:OD1	1:C:290:ASN:N	2.47	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:341:ILE:HG23	2:F:341:ILE:O	2.16	0.46
1:C:278:VAL:CG1	1:C:283:ALA:HA	2.45	0.46
2:G:496:ARG:HD2	2:G:503:ILE:HG12	1.97	0.46
2:E:537:PRO:O	2:E:541:GLU:HG2	2.16	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
2:G:535:LEU:HD22	2:G:536:PRO:CD	2.44	0.46
1:D:265:GLN:HG2	1:D:266:ALA:N	2.29	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
2:E:418:ASN:C	2:E:420:GLN:H	2.24	0.46
1:B:204:VAL:HG22	1:D:196:ASN:OD1	2.15	0.46
1:B:246:LEU:HD13	1:B:329:ILE:HD13	1.97	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
2:F:417:VAL:HG23	3:F:5:P1A:O6	2.16	0.46
1:D:285:ALA:O	1:D:286:VAL:CB	2.63	0.46
1:D:309:ASP:C	1:D:309:ASP:OD2	2.58	0.46
1:B:353:THR:HB	2:G:419:ASN:ND2	2.31	0.46
2:F:537:PRO:O	2:F:541:GLU:HG2	2.16	0.46
2:G:341:ILE:O	2:G:341:ILE:HG23	2.16	0.46
1:B:273:ALA:C	1:B:275:GLY:N	2.74	0.46
2:G:418:ASN:C	2:G:420:GLN:H	2.24	0.46
1:A:273:ALA:C	1:A:275:GLY:N	2.74	0.46
1:A:331:SER:O	1:A:335:VAL:HG23	2.16	0.46
2:E:341:ILE:HG23	2:E:341:ILE:O	2.16	0.46
1:B:192:ARG:HG2	1:B:231:LEU:HD11	1.98	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
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:B:273:ALA:C	1:B:275:GLY:H	2.25	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:D:193:VAL:HG11	1:D:224:GLN:HB3	1.98	0.45
1:D:273:ALA:C	1:D:275:GLY:N	2.73	0.45
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
1:C:207:ASN:C	1:C:209:THR:H	2.24	0.45
1:C:309:ASP:OD2	1:C:309:ASP:C	2.59	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:417:VAL:HG23	3:G:5:P1A:O6	2.16	0.45
1:D:221:GLN:HE22	1:D:262:ARG:NH2	2.00	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
2:E:403:MET:HB2	3:E:5:P1A:H121	1.99	0.45
1:C:181:MET:HB3	1:C:345:VAL:HG21	1.99	0.45
1:C:265:GLN:HG2	1:C:266:ALA:N	2.31	0.45
1:C:273:ALA:C	1:C:275:GLY:N	2.71	0.45
1:D:331:SER:O	1:D:335:VAL:HG23	2.17	0.45
2:H:418:ASN:C	2:H:420:GLN:H	2.24	0.45
1:A:203:VAL:O	1:A:210:THR:HG21	2.16	0.45
1:A:283:ALA:O	1:A:284:HIS:C	2.60	0.45
1:B:398:MET:O	1:B:402:GLU:HG2	2.16	0.45
2:E:494:ASN:C	2:E:494:ASN:ND2	2.71	0.45
2:G:351:CYS:C	2:G:353:VAL:H	2.24	0.45
2:F:351:CYS:C	2:F:353:VAL:H	2.25	0.45
1:C:291:ILE:O	1:C:295:VAL:HG23	2.16	0.45
1:A:246:LEU:HD13	1:A:329:ILE:HD13	1.98	0.45
1:A:273:ALA:C	1:A:275:GLY:H	2.25	0.45
1:B:309:ASP:OD2	1:B:309:ASP:C	2.58	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:D:207:ASN:C	1:D:209:THR:H	2.25	0.45
1:D:400:MET:C	1:D:402:GLU:N	2.73	0.45
1:A:192:ARG:HG2	1:A:231:LEU:HD11	1.97	0.45
1:B:207:ASN:HD22	1:D:265:GLN:HB3	1.82	0.45
1:B:223:PHE:CD1	1:B:400:MET:HE1	2.51	0.45
1:C:278:VAL:HG12	1:C:279:ASN:N	2.31	0.45
2:G:499:LYS:O	2:G:503:ILE:HD13	2.17	0.45
1:D:327:ARG:NH1	1:D:327:ARG:CB	2.80	0.45
1:B:207:ASN:C	1:B:209:THR:H	2.25	0.45
1:B:283:ALA:O	1:B:284:HIS:C	2.60	0.45
1:C:283:ALA:O	1:C:284:HIS:C	2.60	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
2:E:496:ARG:HD2	2:E:503:ILE:HG12	1.99	0.44
1:B:330:LYS:NZ	4:B:430:HOH:O	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:322:LEU:HB3	2:F:457:ALA:HB1	1.98	0.44
2:F:545:VAL:O	2:F:545:VAL:CG1	2.57	0.44
1:C:349:TYR:CZ	1:C:353:THR:HG21	2.52	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:NH1	1:A:327:ARG:CB	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:312:GLU:HG2	1:B:364:LEU:HD21	1.99	0.44
1:B:329:ILE:CG2	1:B:332:VAL:HG22	2.47	0.44
1:C:327:ARG:NH1	1:C:327:ARG:CB	2.81	0.44
2:G:442:PHE:CE1	2:G:446:MET:HE3	2.53	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: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: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:185:ARG:HB3	1:A:233:PRO:CG	2.47	0.44
1:A:207:ASN:C	1:A:209:THR:H	2.24	0.44
2:G:322:LEU:HB3	2:G:457:ALA:HB1	2.00	0.44
1:C:246:LEU:HG	1:C:321:LEU:O	2.17	0.44
1:C:260:SER:CB	1:C:303:MET:HE1	2.40	0.44
2:G:417:VAL:HG13	4:G:577:HOH:O	2.17	0.44
1:D:327:ARG:HB3	1:D:327:ARG:NH1	2.33	0.44
1:A:349:TYR:CZ	1:A:353:THR:HG21	2.52	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: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
2:H:530:LEU:C	2:H:531:LYS:O	2.58	0.44
2:G:459:LEU:HD12	2:G:459:LEU:HA	1.83	0.43
2:G:488:LEU:HD22	2:G:492:VAL:CG2	2.48	0.43
2:E:326:GLN:HE22	2:E:456:TYR:HB3	1.83	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:HG11	1:B:224:GLN:HB3	1.99	0.43
1:B:202:LEU:HA	1:B:276:LEU:HD11	2.00	0.43
2:G:530:LEU:HD23	2:G:530:LEU:HA	1.85	0.43
1:D:202:LEU:HA	1:D:276:LEU:HD11	2.00	0.43
1:B:217:ALA:HB2	1:B:274:THR:HB	2.01	0.43
2:F:530:LEU:HD23	2:F:530:LEU:HA	1.86	0.43
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:H:433:GLY:O	4:H:564:HOH:O	2.21	0.43
2:E:351:CYS:C	2:E:353:VAL:H	2.25	0.43
1:B:274:THR:HG22	1:B:276:LEU:HB2	2.01	0.43
3:F:5:P1A:H191	3:F:5:P1A:H111	1.94	0.43
1:D:198:PRO:O	1:D:199:LEU:HB2	2.19	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
2:F:439:LEU:HD12	2:F:439:LEU:HA	1.85	0.43
1:C:327:ARG:HB3	1:C:327:ARG:NH1	2.33	0.43
2:H:375:ARG:HH11	2:H:375:ARG:HG3	1.84	0.43
1:B:193:VAL:HG13	1:B:224:GLN:NE2	2.33	0.43
1:C:198:PRO:O	1:C:199:LEU:HB2	2.18	0.43
1:C:223:PHE:CD1	1:C:400:MET:HE1	2.54	0.43
2:G:351:CYS:C	2:G:353:VAL:N	2.77	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:E:530:LEU:C	2:E:531:LYS:O	2.58	0.43
2:F:395:SER:CB	2:F:543:TRP:HE1	2.29	0.43
1:A:223:PHE:CD1	1:A:400:MET:HE1	2.53	0.43
1:A:309:ASP:OD2	1:A:309:ASP:C	2.62	0.43
4:A:443:HOH:O	2:E:519:ASN:ND2	2.51	0.43
1:C:274:THR:C	1:C:276:LEU:H	2.27	0.43
2:H:351:CYS:C	2:H:353:VAL:H	2.26	0.43
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
1:D:283:ALA:O	1:D:284:HIS:C	2.61	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
2:H:524:MET:HE1	4:H:555:HOH:O	2.18	0.42
1:A:250:GLY:O	1:A:251:TRP:C	2.62	0.42
1:A:274:THR:HG22	1:A:276:LEU:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PHE:HD1	1:B:400:MET:HE1	1.84	0.42
1:D:204:VAL:O	1:D:204:VAL:HG23	2.19	0.42
1:D:404:THR:O	1:D:404:THR:HG22	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
2:E:312:SER:HA	2:E:313:PRO:HD3	1.92	0.42
1:D:193:VAL:HG13	1:D:224:GLN:NE2	2.34	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:F:351:CYS:C	2:F:353:VAL:N	2.77	0.42
2:H:357:HIS:O	2:H:361:ILE:HG13	2.19	0.42
2:E:466:SER:O	2:E:468:ARG:HG2	2.19	0.42
1:D:274:THR:CG2	1:D:276:LEU:HB2	2.49	0.42
2:H:471:LEU:HD12	2:H:471:LEU:HA	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
2:F:375:ARG:HG3	2:F:375:ARG:HH11	1.84	0.42
1:C:198:PRO:CG	1:C:200:VAL:HG23	2.50	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
2:G:356:ARG:O	2:G:360:GLU:HG3	2.19	0.42
1:D:223:PHE:CD1	1:D:400:MET:HE1	2.55	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
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
1:D:198:PRO:CG	1:D:200:VAL:HG23	2.49	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:B:352:THR:HB	2:G:415:LEU:HD11	2.02	0.42
2:F:311:ILE:CG2	2:F:312:SER:N	2.49	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
2:H:358:ILE:HG23	3:H:5:P1A:H162	2.02	0.42
1:D:274:THR:C	1:D:276:LEU:H	2.26	0.41
2:H:311:ILE:CG2	2:H:312:SER:N	2.47	0.41
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:535:LEU:CD1	2:H:539:LEU:HB3	2.50	0.41
1:B:250:GLY:O	1:B:251:TRP:C	2.63	0.41
1:B:327:ARG:NH1	1:B:327:ARG:CB	2.83	0.41
2:F:530:LEU:C	2:F:531:LYS:O	2.61	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
2:G:432:MET:HE1	3:G:5:P1A:H263	2.03	0.41
2:G:463:VAL:HG22	2:G:511:LEU:CD2	2.51	0.41
1:D:347:GLU:HG3	1:D:348:GLU:N	2.35	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
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
2:G:425:ASP:O	2:G:429:LEU:HG	2.21	0.41
1:D:191:LYS:HA	1:D:194:GLU:HB2	2.03	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
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
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
1:C:193:VAL:HG13	1:C:224:GLN:NE2	2.36	0.41
2:G:313:PRO:O	2:G:314:GLU:CB	2.69	0.41
1:A:223:PHE:HD1	1:A:400:MET:HE1	1.86	0.41
1:A:306:MET:HE2	1:A:363:LYS:HG2	2.03	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
1:B:204:VAL:HG23	1:B:204:VAL:O	2.21	0.41
1:B:274:THR:C	1:B:276:LEU:H	2.27	0.41
1:B:353:THR:CA	2:G:419:ASN:HB3	2.51	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
2:G:312:SER:HA	2:G:313:PRO:HD3	1.96	0.41
1:D:230:LYS:HZ1	1:D:401:LEU:C	2.29	0.41
1:D:274:THR:CG2	1:D:274:THR:O	2.68	0.41
1:A:327:ARG:HB3	1:A:327:ARG:NH1	2.34	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:HD23	2:E:530:LEU:HA	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:476:LYS:O	2:F:480:ILE:HG13	2.20	0.41
2:F:524:MET:HE1	4:F:564:HOH:O	2.20	0.41
1:C:278:VAL:CG1	1:C:279:ASN:N	2.83	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:204:VAL:O	1:A:204:VAL:HG23	2.21	0.41
1:A:327:ARG:HH11	1:A:327:ARG:CB	2.33	0.41
2:H:529:LYS:O	2:H:531:LYS:O	2.39	0.41
1:B:340:GLU:OE2	2:F:506:LYS:HD2	2.21	0.41
1:D:340:GLU:OE2	2:H:506:LYS:HD2	2.21	0.41
2:H:530:LEU:HD23	2:H:530:LEU:HA	1.88	0.41
2:E:351:CYS:C	2:E:353:VAL:N	2.78	0.40
2:E:439:LEU:HD12	2:E:439:LEU:HA	1.84	0.40
2:E:442:PHE:CE1	2:E:446:MET:HE3	2.55	0.40
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:223:PHE:HD1	1:C:400:MET:HE1	1.87	0.40
1:C:318:ALA:HB1	1:C:342:ILE:HD13	2.03	0.40
2:G:472:ILE:HG22	2:G:473:GLU:HG3	2.03	0.40
1:D:334:GLU:O	1:D:338:LEU:HG	2.21	0.40
2:H:413:SER:HB3	2:H:422:TYR:O	2.21	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:A:261:HIS:CD2	1:A:264:MET:HE2	2.56	0.40
1:B:191:LYS:HA	1:B:194:GLU:HB2	2.04	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
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: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
2:E:472:ILE:HG22	2:E:473:GLU:HG3	2.03	0.40
3:E:5:P1A:H191	3:E:5:P1A:H111	1.95	0.40
1:B:193:VAL:CG1	1:B:193:VAL:O	2.70	0.40
1:B:351:ARG:HG3	1:B:352:THR:HG23	2.03	0.40
2:G:407:TYR:CG	2:G:443:CYS:HB3	2.56	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:ASN:N	1:D:282:THR:CG2	2.82	0.40
2:E:384:ARG:HD2	2:E:387:GLN:NE2	2.37	0.40
2:G:497:LYS:HG2	2:G:500:PRO:HG3	2.04	0.40
1:D:227:GLN:HA	1:D:404:THR:CG2	2.51	0.40
2:H:351:CYS:C	2:H:353:VAL:N	2.78	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	182 (92%)	16 (8%)	11	20
1	B	199/208 (96%)	183 (92%)	16 (8%)	11	20
1	C	198/208 (95%)	182 (92%)	16 (8%)	11	20
1	D	199/208 (96%)	183 (92%)	16 (8%)	11	20
2	E	213/225 (95%)	200 (94%)	13 (6%)	17	31
2	F	213/225 (95%)	199 (93%)	14 (7%)	15	29
2	G	212/225 (94%)	198 (93%)	14 (7%)	15	29
2	H	214/225 (95%)	200 (94%)	14 (6%)	15	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1646/1732 (95%)	1527 (93%)	119 (7%)	13	25

All (119) 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
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	398	MET
1	A	400	MET
2	E	349	ASP
2	E	368	LEU
2	E	392	LYS
2	E	409	VAL
2	E	439	LEU
2	E	440	LEU
2	E	458	LEU
2	E	459	LEU
2	E	488	LEU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	398	MET
1	B	400	MET
2	F	312	SER
2	F	349	ASP
2	F	368	LEU
2	F	392	LYS
2	F	409	VAL
2	F	439	LEU
2	F	440	LEU
2	F	458	LEU
2	F	459	LEU
2	F	488	LEU
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	398	MET
1	C	400	MET
2	G	312	SER
2	G	349	ASP
2	G	368	LEU
2	G	392	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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
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	398	MET
1	D	400	MET
2	H	312	SER
2	H	349	ASP
2	H	368	LEU
2	H	392	LYS
2	H	409	VAL
2	H	439	LEU
2	H	440	LEU
2	H	458	LEU
2	H	459	LEU
2	H	488	LEU
2	H	512	THR
2	H	513	GLU
2	H	535	LEU
2	H	539	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	212	ASN
1	A	267	GLN
1	A	284	HIS
2	E	315	GLN
2	E	326	GLN
2	E	342	ASN
2	E	387	GLN
2	E	494	ASN
2	E	519	ASN
1	B	205	ASN
1	B	212	ASN
1	B	234	HIS
1	B	267	GLN
1	B	284	HIS
2	F	326	GLN
2	F	342	ASN
2	F	367	GLN
2	F	387	GLN
2	F	494	ASN
2	F	520	GLN
1	C	205	ASN
1	C	212	ASN
1	C	221	GLN
1	C	267	GLN
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	267	GLN
1	D	279	ASN
1	D	284	HIS
2	H	326	GLN
2	H	342	ASN
2	H	387	GLN
2	H	494	ASN
2	H	520	GLN

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 oligosaccharides 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	G	5	-	36,36,36	2.84	16 (44%)	60,60,60	1.91	15 (25%)
3	P1A	F	5	-	36,36,36	2.69	17 (47%)	60,60,60	1.90	12 (20%)
3	P1A	H	5	-	36,36,36	2.92	17 (47%)	60,60,60	1.79	16 (26%)
3	P1A	E	5	-	36,36,36	2.81	17 (47%)	60,60,60	1.98	14 (23%)

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	G	5	-	-	2/17/87/87	0/4/4/4
3	P1A	F	5	-	-	0/17/87/87	0/4/4/4
3	P1A	H	5	-	-	2/17/87/87	0/4/4/4
3	P1A	E	5	-	-	0/17/87/87	0/4/4/4

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	5	P1A	C10-C9	7.18	1.67	1.56
3	G	5	P1A	C10-C9	7.06	1.67	1.56
3	E	5	P1A	C10-C9	6.98	1.67	1.56
3	F	5	P1A	C10-C9	6.74	1.66	1.56
3	G	5	P1A	C23-C22	5.88	1.60	1.52
3	H	5	P1A	C9-C8	5.52	1.62	1.52
3	E	5	P1A	C3-C2	5.36	1.60	1.52
3	H	5	P1A	C3-C2	5.36	1.60	1.52
3	F	5	P1A	C9-C8	5.24	1.61	1.52
3	G	5	P1A	C7-C8	5.12	1.40	1.34
3	F	5	P1A	C23-C22	5.07	1.59	1.52
3	E	5	P1A	C9-C8	4.92	1.61	1.52
3	G	5	P1A	C9-C8	4.81	1.61	1.52
3	F	5	P1A	C3-C2	4.78	1.59	1.52
3	E	5	P1A	C23-C22	4.55	1.58	1.52
3	H	5	P1A	C4-C3	4.49	1.61	1.52
3	H	5	P1A	C23-C22	4.44	1.58	1.52
3	H	5	P1A	C5-C6	4.38	1.57	1.51
3	G	5	P1A	C3-C2	4.22	1.58	1.52
3	G	5	P1A	C14-C13	4.20	1.63	1.56
3	H	5	P1A	C14-C13	4.18	1.63	1.56
3	E	5	P1A	C7-C8	4.17	1.39	1.34
3	E	5	P1A	C4-C3	4.09	1.60	1.52
3	H	5	P1A	C7-C8	4.05	1.39	1.34
3	F	5	P1A	C5-C6	3.99	1.57	1.51
3	F	5	P1A	C7-C8	3.94	1.39	1.34
3	H	5	P1A	C4-C5	3.94	1.61	1.54
3	E	5	P1A	C14-C13	3.89	1.62	1.56
3	G	5	P1A	C5-C6	3.85	1.56	1.51
3	G	5	P1A	O14-C14	3.81	1.49	1.43
3	E	5	P1A	C5-C6	3.79	1.56	1.51
3	G	5	P1A	C4-C3	3.78	1.59	1.52
3	H	5	P1A	C20-C17	3.73	1.61	1.55
3	E	5	P1A	C20-C17	3.53	1.60	1.55
3	E	5	P1A	C4-C5	3.51	1.61	1.54
3	E	5	P1A	C11-C9	3.49	1.59	1.53
3	F	5	P1A	C4-C3	3.48	1.59	1.52
3	F	5	P1A	C4-C5	3.48	1.61	1.54
3	H	5	P1A	O14-C14	3.38	1.49	1.43
3	F	5	P1A	C14-C13	3.27	1.62	1.56
3	H	5	P1A	C10-C5	3.15	1.61	1.56
3	G	5	P1A	C4-C5	3.13	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	5	P1A	C11-C9	3.11	1.59	1.53
3	H	5	P1A	C16-C17	3.10	1.60	1.54
3	F	5	P1A	C20-C17	3.01	1.60	1.55
3	F	5	P1A	C18-C13	3.00	1.59	1.54
3	F	5	P1A	C11-C9	2.98	1.58	1.53
3	G	5	P1A	C21-C20	2.96	1.57	1.52
3	G	5	P1A	C10-C5	2.90	1.60	1.56
3	E	5	P1A	C12-C13	2.89	1.59	1.54
3	E	5	P1A	C16-C17	2.88	1.59	1.54
3	F	5	P1A	C12-C13	2.81	1.59	1.54
3	E	5	P1A	O14-C14	2.81	1.48	1.43
3	E	5	P1A	C10-C5	2.81	1.60	1.56
3	E	5	P1A	C21-C20	2.81	1.57	1.52
3	G	5	P1A	C18-C13	2.77	1.59	1.54
3	E	5	P1A	C18-C13	2.67	1.59	1.54
3	G	5	P1A	C11-C9	2.66	1.58	1.53
3	H	5	P1A	C18-C13	2.63	1.59	1.54
3	G	5	P1A	C20-C17	2.62	1.59	1.55
3	H	5	P1A	C21-C20	2.53	1.57	1.52
3	F	5	P1A	C21-C20	2.50	1.57	1.52
3	F	5	P1A	C10-C5	2.45	1.60	1.56
3	H	5	P1A	C12-C13	2.43	1.58	1.54
3	G	5	P1A	C12-C13	2.31	1.58	1.54
3	F	5	P1A	O14-C14	2.22	1.47	1.43
3	F	5	P1A	C16-C17	2.08	1.58	1.54

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	P1A	C14-C13-C17	-8.52	94.64	99.90
3	F	5	P1A	C14-C13-C17	-7.97	94.98	99.90
3	G	5	P1A	C14-C13-C17	-7.76	95.11	99.90
3	H	5	P1A	C14-C13-C17	-5.91	96.25	99.90
3	E	5	P1A	C13-C14-C8	4.54	117.21	112.24
3	H	5	P1A	O14-C14-C15	-4.26	99.86	110.26
3	E	5	P1A	O14-C14-C15	-4.03	100.42	110.26
3	G	5	P1A	O14-C14-C15	-3.85	100.85	110.26
3	G	5	P1A	C13-C14-C8	3.79	116.39	112.24
3	F	5	P1A	O14-C14-C15	-3.72	101.18	110.26
3	F	5	P1A	C11-C9-C10	-3.65	107.81	113.92
3	F	5	P1A	C13-C14-C8	3.57	116.15	112.24
3	G	5	P1A	C24-C23-C22	-3.56	108.33	112.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5	P1A	C24-C23-C22	-3.49	108.41	112.86
3	H	5	P1A	C24-C23-C22	-3.38	108.56	112.86
3	G	5	P1A	C11-C9-C10	-3.34	108.33	113.92
3	G	5	P1A	C12-C11-C9	3.33	120.66	112.64
3	E	5	P1A	C11-C9-C10	-3.28	108.43	113.92
3	H	5	P1A	C13-C14-C8	3.16	115.70	112.24
3	E	5	P1A	C24-C23-C22	-3.12	108.89	112.86
3	G	5	P1A	C11-C12-C13	3.02	118.06	112.85
3	H	5	P1A	C17-C20-C22	2.96	112.15	109.59
3	H	5	P1A	C11-C9-C10	-2.95	108.99	113.92
3	F	5	P1A	C11-C12-C13	2.93	117.90	112.85
3	E	5	P1A	C21-C20-C22	2.85	111.95	110.29
3	E	5	P1A	C10-C9-C8	-2.84	108.21	112.54
3	F	5	P1A	C17-C20-C22	2.84	112.05	109.59
3	G	5	P1A	C10-C9-C8	-2.83	108.23	112.54
3	H	5	P1A	C12-C13-C14	-2.77	104.01	107.79
3	E	5	P1A	C5-C6-C7	2.76	121.05	116.54
3	H	5	P1A	C10-C9-C8	-2.72	108.39	112.54
3	F	5	P1A	C5-C6-C7	2.68	120.92	116.54
3	E	5	P1A	C15-C14-C13	2.66	105.67	103.24
3	G	5	P1A	C18-C13-C14	2.62	112.38	109.11
3	G	5	P1A	C5-C6-C7	2.62	120.83	116.54
3	G	5	P1A	C4-C5-C10	-2.60	109.26	112.75
3	E	5	P1A	C12-C11-C9	2.57	118.84	112.64
3	H	5	P1A	C5-C6-C7	2.55	120.71	116.54
3	F	5	P1A	C12-C11-C9	2.53	118.75	112.64
3	H	5	P1A	C12-C11-C9	2.52	118.72	112.64
3	F	5	P1A	C10-C9-C8	-2.48	108.76	112.54
3	H	5	P1A	C15-C14-C13	2.43	105.46	103.24
3	E	5	P1A	C12-C13-C14	-2.37	104.56	107.79
3	F	5	P1A	C4-C5-C10	-2.35	109.60	112.75
3	H	5	P1A	C11-C12-C13	2.34	116.88	112.85
3	H	5	P1A	C4-C5-C10	-2.26	109.72	112.75
3	E	5	P1A	C20-C17-C13	2.23	122.62	120.43
3	H	5	P1A	C18-C13-C14	2.22	111.88	109.11
3	F	5	P1A	C10-C1-C2	-2.19	110.57	114.17
3	E	5	P1A	C18-C13-C14	2.16	111.80	109.11
3	G	5	P1A	C12-C13-C14	-2.11	104.91	107.79
3	H	5	P1A	C10-C1-C2	-2.11	110.71	114.17
3	G	5	P1A	C23-C24-C25	2.10	121.05	113.91
3	G	5	P1A	C20-C17-C13	2.10	122.50	120.43
3	E	5	P1A	C5-C4-C3	-2.08	108.88	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5	P1A	C23-C22-C20	2.00	117.55	114.95
3	H	5	P1A	C5-C4-C3	-2.00	108.99	111.90

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

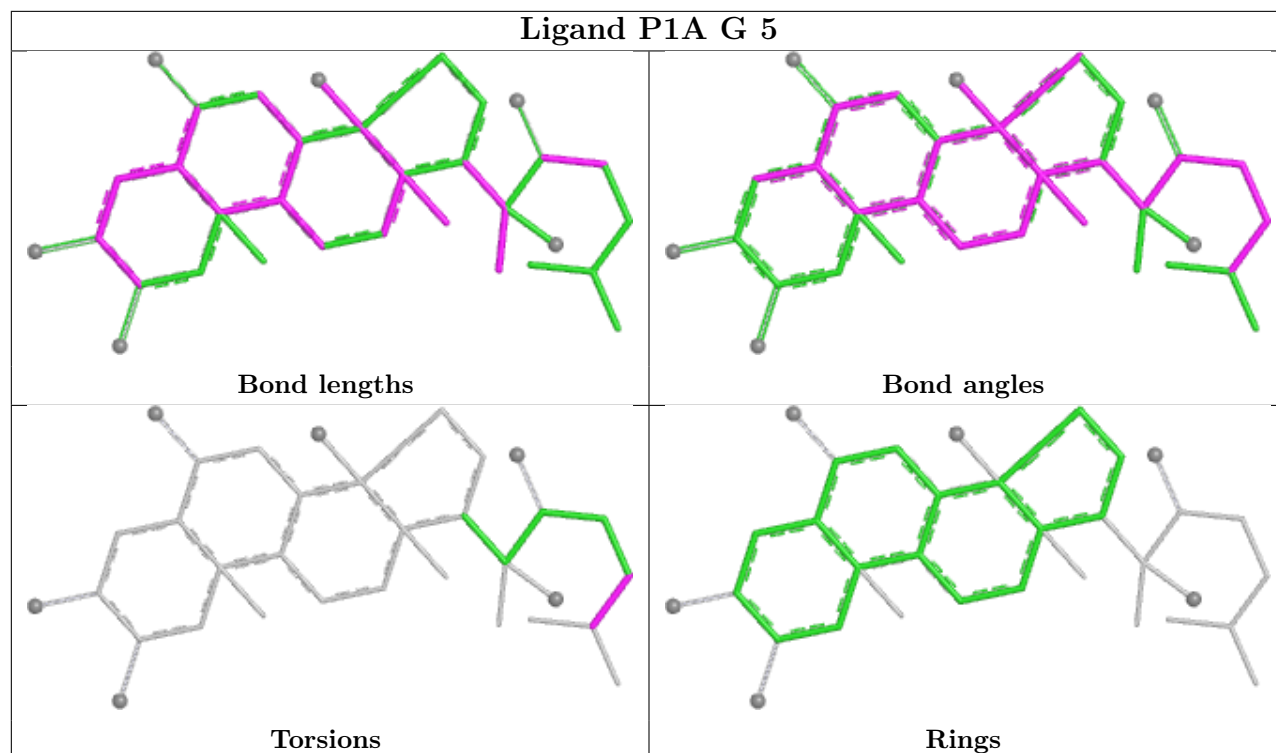
There are no ring outliers.

4 monomers are involved in 14 short contacts:

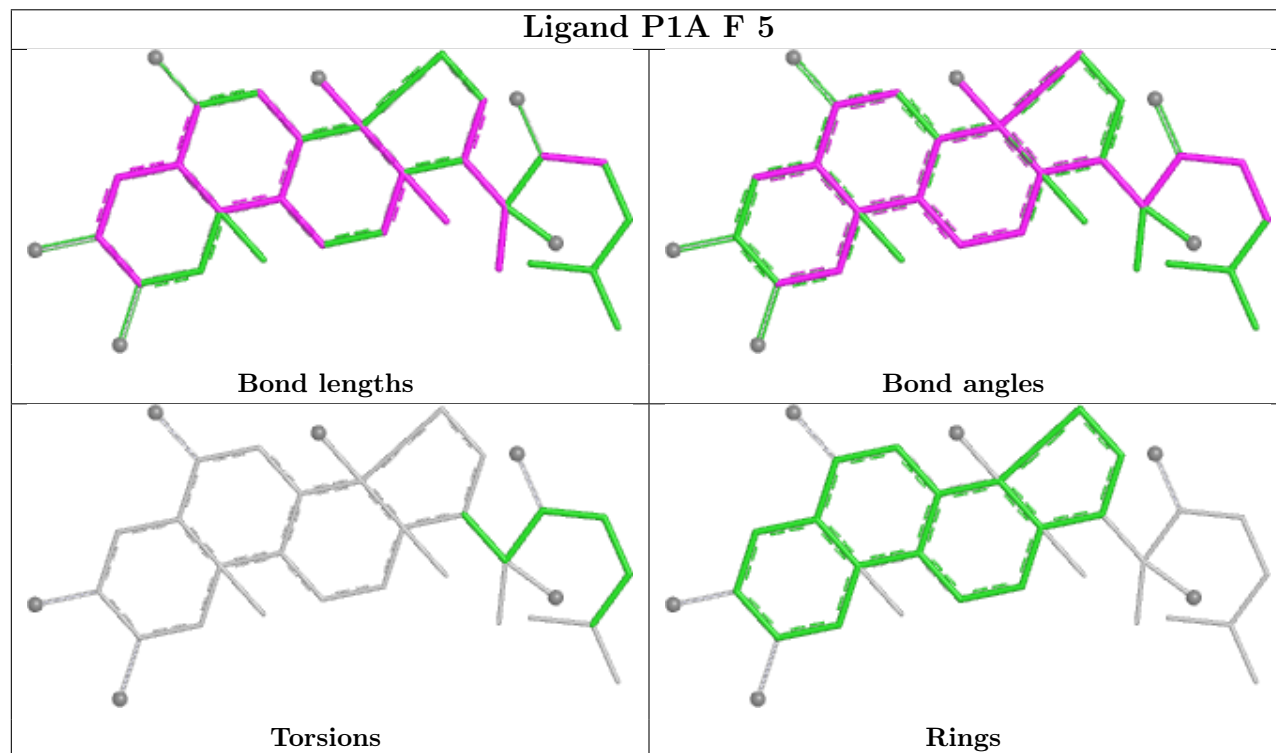
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	5	P1A	3	0
3	F	5	P1A	4	0
3	H	5	P1A	2	0
3	E	5	P1A	5	0

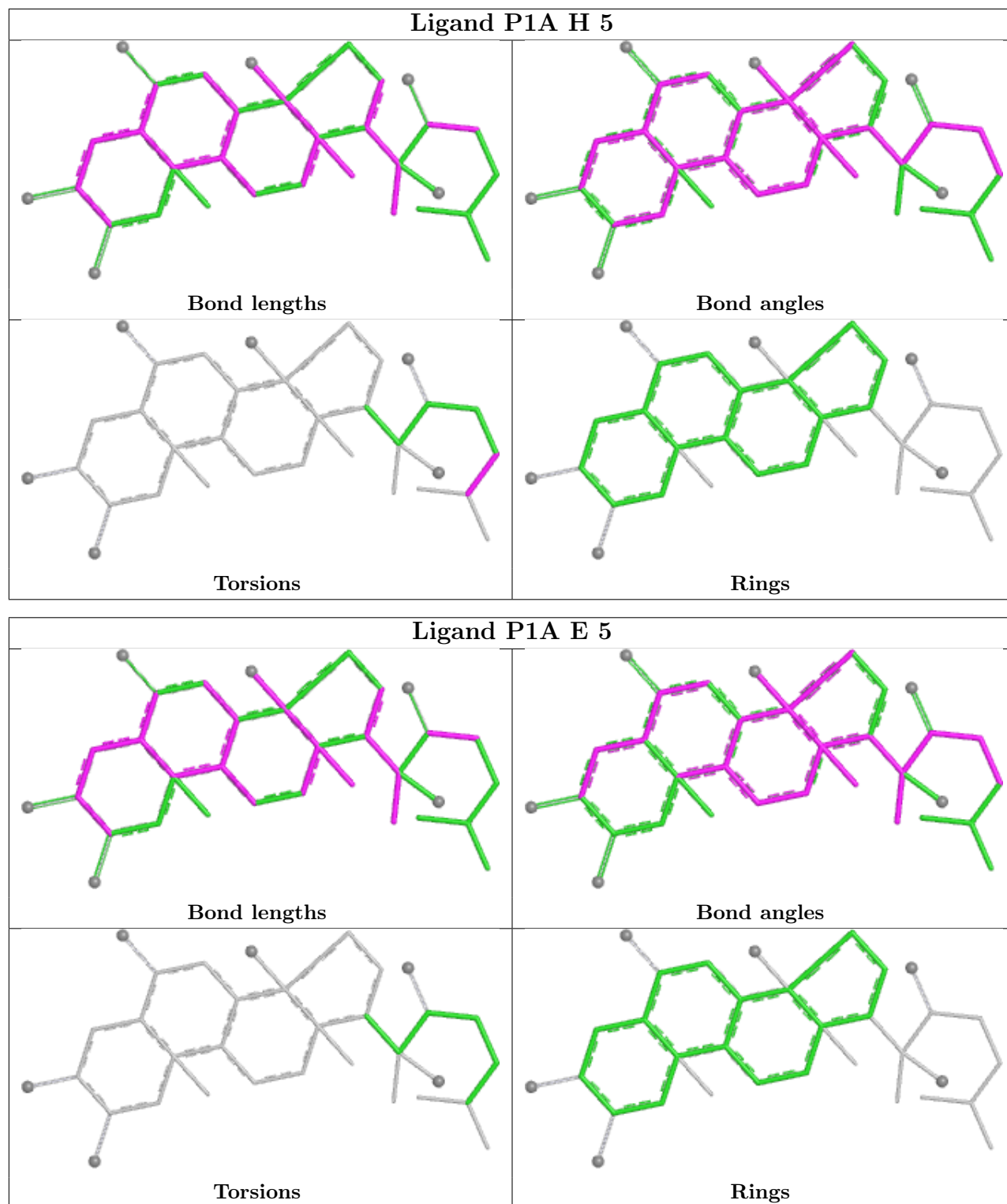
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand P1A G 5



Ligand P1A F 5





5.7 Other polymers [i](#)

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%)	1.13	54 (24%) 2 1	29, 71, 119, 158	0
1	B	228/235 (97%)	0.92	33 (14%) 6 5	30, 74, 119, 159	0
1	C	225/235 (95%)	0.87	23 (10%) 12 11	32, 74, 119, 158	0
1	D	227/235 (96%)	1.13	41 (18%) 3 3	32, 74, 124, 158	0
2	E	234/248 (94%)	0.41	15 (6%) 25 25	24, 53, 108, 158	0
2	F	233/248 (93%)	0.45	16 (6%) 23 22	25, 55, 105, 158	0
2	G	233/248 (93%)	0.43	16 (6%) 23 22	28, 54, 105, 157	0
2	H	234/248 (94%)	0.42	11 (4%) 36 36	27, 54, 106, 157	0
All	All	1838/1932 (95%)	0.72	209 (11%) 10 8	24, 62, 118, 159	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	419	ASN	10.0
1	D	406	ASP	5.1
1	B	205	ASN	4.9
1	A	201	ALA	4.6
1	A	203	VAL	4.6
2	F	324	TYR	4.5
1	A	200	VAL	4.4
1	C	404	THR	4.3
1	D	184	GLU	4.3
2	H	418	ASN	4.3
2	H	341	ILE	4.2
1	B	200	VAL	4.2
2	G	341	ILE	4.2
1	B	203	VAL	4.2
1	A	202	LEU	4.2
1	A	211	VAL	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	286	VAL	4.0
1	A	205	ASN	3.9
1	D	203	VAL	3.8
1	D	189	ALA	3.8
2	G	346	ASP	3.7
1	A	351	ARG	3.6
2	F	341	ILE	3.5
2	E	547	LEU	3.5
1	D	204	VAL	3.4
1	B	405	THR	3.4
1	A	187	ILE	3.4
2	H	486	GLU	3.4
2	H	530	LEU	3.4
1	A	390	ASP	3.4
1	C	391	VAL	3.4
1	D	182	PRO	3.3
2	G	347	GLY	3.3
2	G	418	ASN	3.3
1	A	266	ALA	3.2
1	A	391	VAL	3.2
2	H	347	GLY	3.2
1	A	207	ASN	3.2
1	B	284	HIS	3.2
2	E	341	ILE	3.1
2	E	495	ARG	3.1
1	D	202	LEU	3.1
1	A	204	VAL	3.1
1	D	265	GLN	3.0
1	C	266	ALA	3.0
1	B	211	VAL	3.0
1	D	359	GLY	3.0
1	B	201	ALA	3.0
2	F	500	PRO	3.0
1	C	388	ILE	3.0
1	B	275	GLY	3.0
1	D	193	VAL	3.0
1	C	285	ALA	2.9
1	A	278	VAL	2.9
2	F	526	PHE	2.9
2	F	311	ILE	2.9
2	F	346	ASP	2.9
2	H	346	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	282	THR	2.9
1	B	276	LEU	2.9
2	F	497	LYS	2.9
1	B	289	GLY	2.9
2	F	320	HIS	2.9
1	D	181	MET	2.8
1	A	288	VAL	2.8
1	C	385	PHE	2.8
2	G	545	VAL	2.8
1	C	356	ASN	2.8
1	C	387	LEU	2.8
1	A	274	THR	2.8
1	A	193	VAL	2.8
1	C	204	VAL	2.8
1	C	271	VAL	2.8
1	D	271	VAL	2.8
1	D	388	ILE	2.8
1	A	285	ALA	2.7
1	D	405	THR	2.7
2	H	417	VAL	2.7
1	A	265	GLN	2.7
1	D	270	ILE	2.7
1	A	199	LEU	2.7
2	G	333	SER	2.7
1	B	189	ALA	2.7
1	B	353	THR	2.7
2	G	500	PRO	2.7
1	B	193	VAL	2.7
1	C	283	ALA	2.7
1	B	388	ILE	2.7
1	B	285	ALA	2.7
1	C	181	MET	2.6
1	D	195	CYS	2.6
2	E	347	GLY	2.6
1	A	283	ALA	2.6
1	B	204	VAL	2.6
1	B	266	ALA	2.6
1	C	286	VAL	2.6
1	A	210	THR	2.6
2	F	498	PRO	2.6
1	A	209	THR	2.6
2	F	546	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	202	LEU	2.6
1	D	300	VAL	2.6
2	E	500	PRO	2.6
1	A	353	THR	2.5
1	D	352	THR	2.5
1	B	329	ILE	2.5
1	B	278	VAL	2.5
1	D	211	VAL	2.5
2	E	546	ASP	2.5
1	C	203	VAL	2.5
2	G	417	VAL	2.5
1	B	385	PHE	2.5
1	B	352	THR	2.5
2	F	499	LYS	2.5
1	D	401	LEU	2.5
1	A	354	HIS	2.5
1	D	334	GLU	2.5
1	A	352	THR	2.4
1	B	327	ARG	2.4
1	D	274	THR	2.4
1	A	356	ASN	2.4
1	A	392	PRO	2.4
1	D	392	PRO	2.4
2	E	501	GLY	2.4
2	F	495	ARG	2.4
2	F	496	ARG	2.4
1	C	386	LYS	2.4
1	A	328	GLY	2.4
2	E	313	PRO	2.4
1	C	211	VAL	2.4
2	G	353	VAL	2.4
1	D	269	ALA	2.4
2	E	526	PHE	2.4
1	B	214	ILE	2.4
1	D	199	LEU	2.4
1	B	286	VAL	2.4
1	D	391	VAL	2.4
1	D	187	ILE	2.3
1	B	389	GLY	2.3
1	D	403	GLY	2.3
2	E	384	ARG	2.3
2	E	337	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	199	LEU	2.3
1	A	214	ILE	2.3
1	A	292	TYR	2.3
2	H	419	ASN	2.3
1	D	262	ARG	2.3
1	D	286	VAL	2.3
1	A	387	LEU	2.3
1	C	269	ALA	2.3
1	A	270	ILE	2.3
1	A	388	ILE	2.3
1	A	386	LYS	2.3
2	G	410	GLN	2.3
2	H	353	VAL	2.3
1	D	398	MET	2.3
1	A	275	GLY	2.3
1	C	389	GLY	2.3
1	A	222	LEU	2.3
1	A	189	ALA	2.2
1	B	187	ILE	2.2
1	A	198	PRO	2.2
1	A	289	GLY	2.2
1	B	183	LEU	2.2
1	C	199	LEU	2.2
1	D	183	LEU	2.2
1	D	231	LEU	2.2
1	A	206	GLU	2.2
1	B	282	THR	2.2
2	F	347	GLY	2.2
1	A	240	LEU	2.2
2	G	495	ARG	2.2
1	D	276	LEU	2.2
1	A	186	ILE	2.2
1	A	273	ALA	2.2
1	A	282	THR	2.2
1	A	355	PRO	2.2
2	G	494	ASN	2.2
2	G	498	PRO	2.2
1	A	389	GLY	2.2
1	A	284	HIS	2.2
1	A	329	ILE	2.2
1	D	288	VAL	2.2
1	D	185	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	202	LEU	2.1
1	A	277	THR	2.1
1	D	289	GLY	2.1
2	E	346	ASP	2.1
2	F	384	ARG	2.1
1	A	341	LYS	2.1
2	E	420	GLN	2.1
2	G	342	ASN	2.1
2	G	351	CYS	2.1
1	C	273	ALA	2.1
2	E	498	PRO	2.1
1	D	216	GLN	2.1
2	H	410	GLN	2.1
1	A	183	LEU	2.1
1	C	193	VAL	2.1
2	F	325	PHE	2.1
1	A	357	GLU	2.0
2	E	499	LYS	2.0
2	H	350	GLN	2.0
1	B	207	ASN	2.0
1	D	196	ASN	2.0
1	B	270	ILE	2.0
1	D	214	ILE	2.0
1	B	351	ARG	2.0
1	C	288	VAL	2.0

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 ⓘ

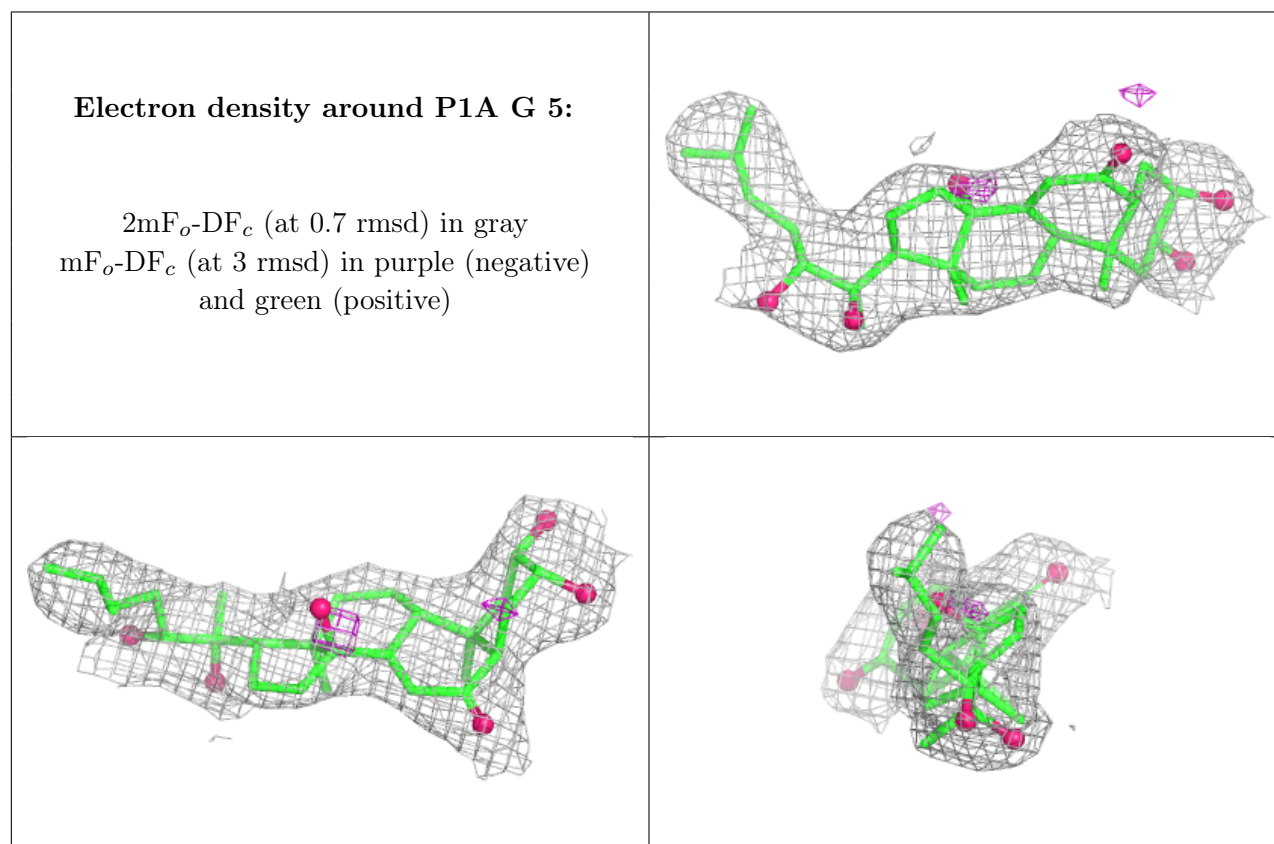
There are no oligosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

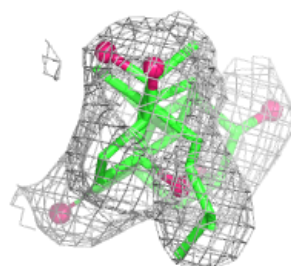
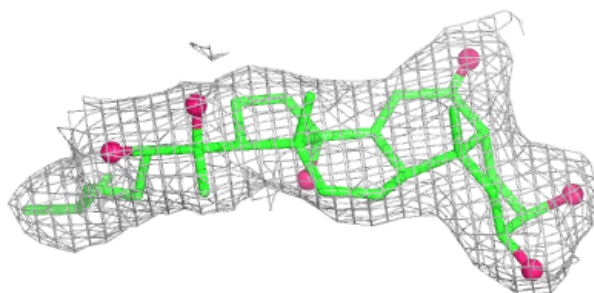
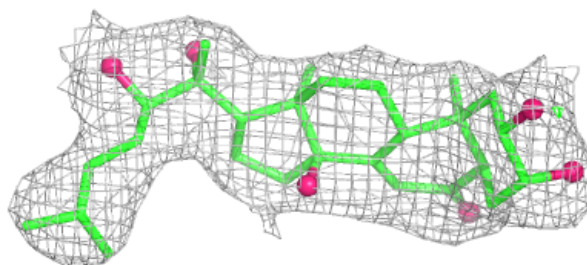
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	P1A	G	5	33/33	0.93	0.10	30,35,39,43	0
3	P1A	F	5	33/33	0.94	0.09	33,39,41,44	0
3	P1A	E	5	33/33	0.94	0.09	31,34,38,42	0
3	P1A	H	5	33/33	0.94	0.09	30,39,42,43	0

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.

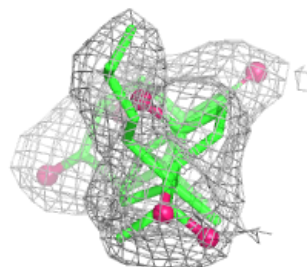
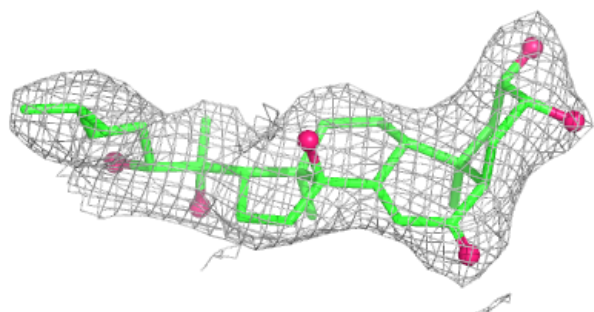
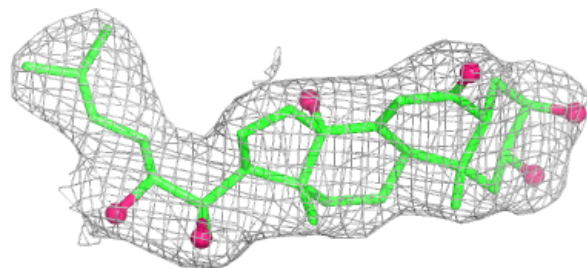


Electron density around P1A F 5:

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

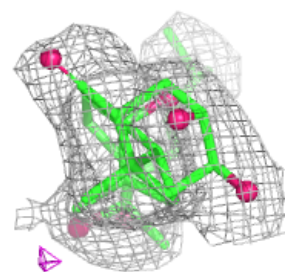
**Electron density around P1A E 5:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.