



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:46 AM UTC

PDB ID : 2FL5 / pdb_00002fl5
Title : Cofactor-containing antibodies: Crystal structure of the original yellow antibody
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2006-01-05
Resolution : 3.00 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:

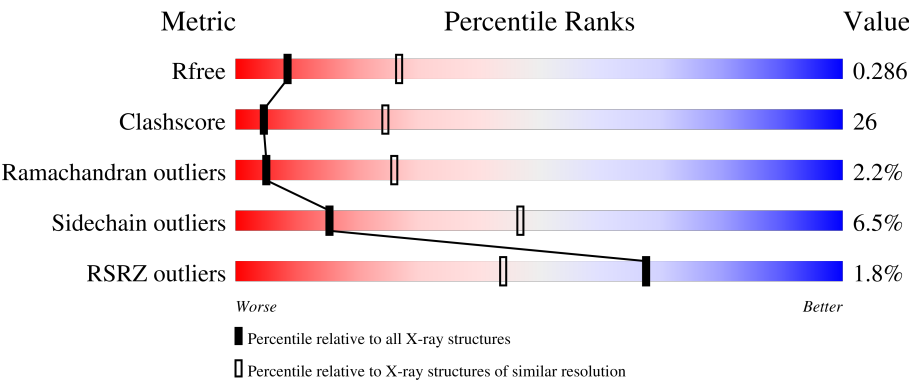
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	209	55%40%5%
1	C	209	49%46%. .
1	E	209	56%39%. .
1	L	209	4%42%52%6%
2	B	220	3%54%41%5%

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Mol	Chain	Length	Quality of chain
2	D	220	2%55%41%.•
2	F	220	%49%45%6%
2	H	220	4%50%45%5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13232 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.

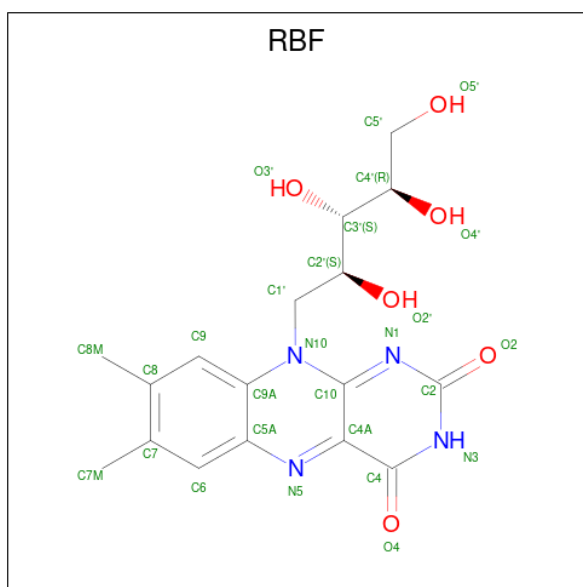
- Molecule 1 is a protein called Immunoglobulin Igg1 Lambda Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	209	Total	C	N	O	S	0	0	0
			1579	992	258	325	4			
1	A	209	Total	C	N	O	S	0	0	0
			1579	992	258	325	4			
1	C	209	Total	C	N	O	S	0	0	0
			1579	992	258	325	4			
1	E	209	Total	C	N	O	S	0	0	0
			1579	992	258	325	4			

- Molecule 2 is a protein called Immunoglobulin Igg1 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1666	1045	278	336	7			
2	B	220	Total	C	N	O	S	0	0	0
			1666	1045	278	336	7			
2	D	220	Total	C	N	O	S	0	0	0
			1666	1045	278	336	7			
2	F	220	Total	C	N	O	S	0	0	0
			1666	1045	278	336	7			

- Molecule 3 is RIBOFLAVIN (CCD ID: RBF) (formula: C₁₇H₂₀N₄O₆).

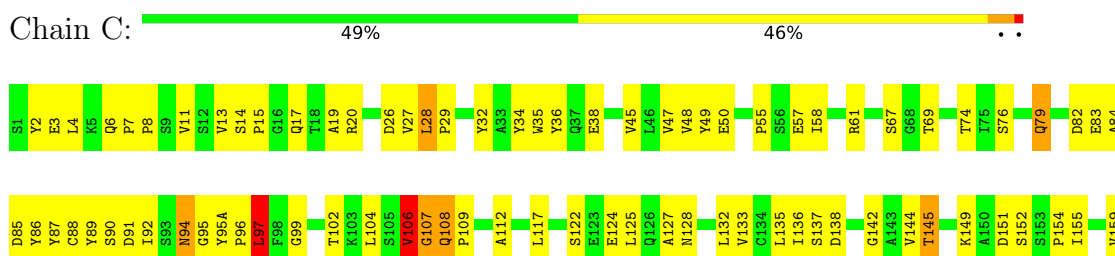
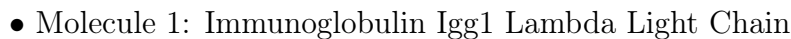


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			27	17	4	6		
3	B	1	Total	C	N	O	0	0
			27	17	4	6		
3	D	1	Total	C	N	O	0	0
			27	17	4	6		
3	F	1	Total	C	N	O	0	0
			27	17	4	6		

- Molecule 4 is water.

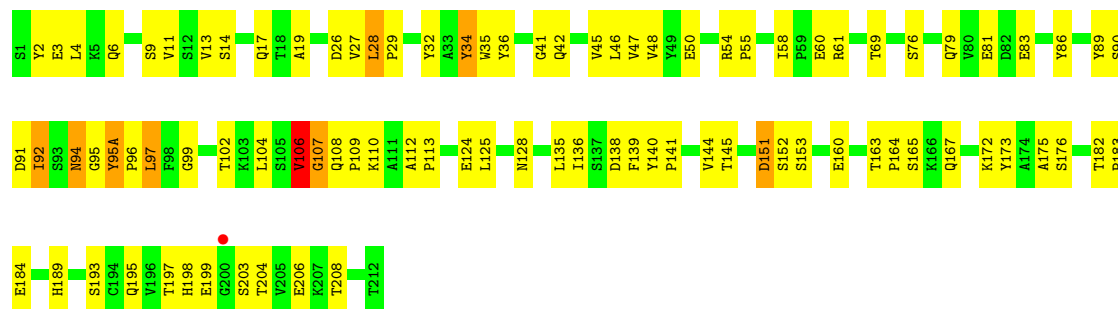
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	23	Total	O	0	0
			23	23		
4	H	17	Total	O	0	0
			17	17		
4	A	21	Total	O	0	0
			21	21		
4	B	14	Total	O	0	0
			14	14		
4	C	24	Total	O	0	0
			24	24		
4	D	16	Total	O	0	0
			16	16		
4	E	13	Total	O	0	0
			13	13		
4	F	16	Total	O	0	0
			16	16		

- Molecule 1: Immunoglobulin IgG1 Lambda Light Chain

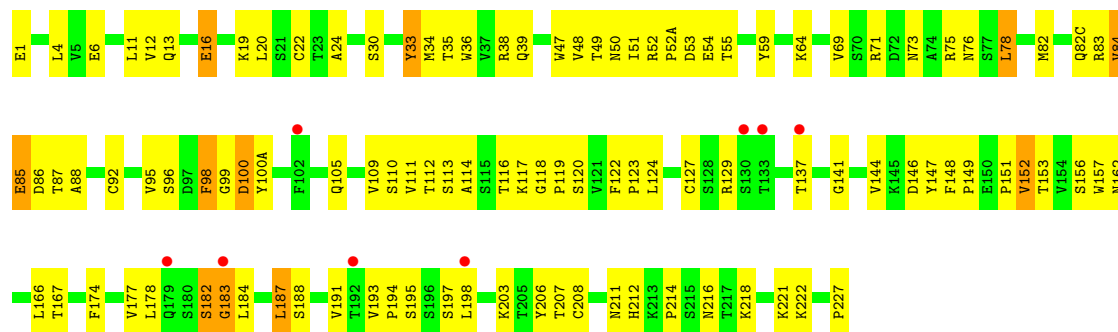




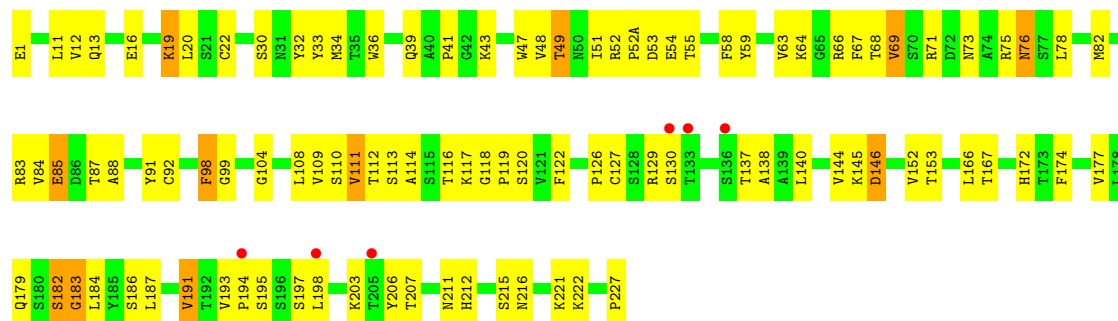
• Molecule 1: Immunoglobulin Igg1 Lambda Light Chain



• Molecule 2: Immunoglobulin Igg1 Heavy chain

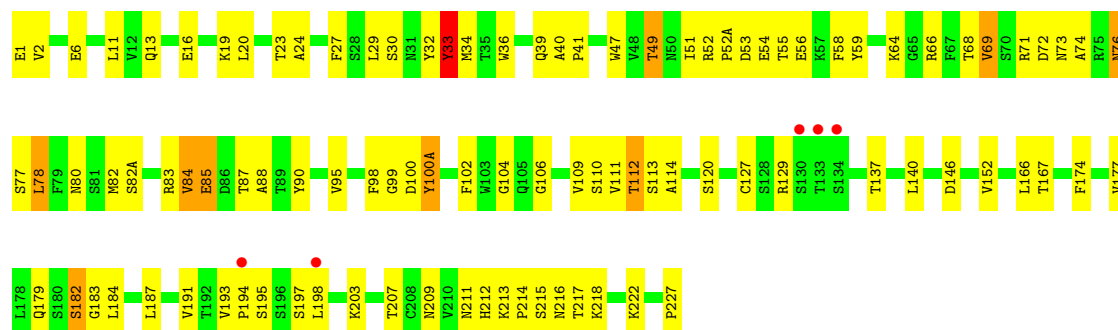


• Molecule 2: Immunoglobulin Igg1 Heavy chain

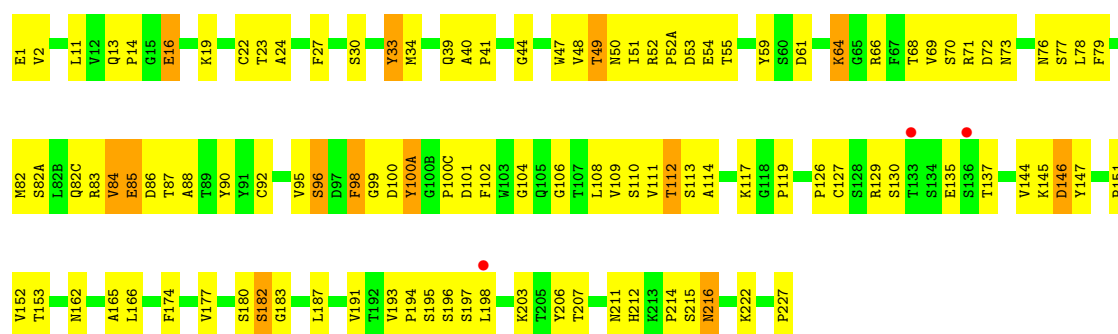


• Molecule 2: Immunoglobulin Igg1 Heavy chain





• Molecule 2: Immunoglobulin Ig1 Heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.59Å 111.11Å 188.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 93.6 (50.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.290 0.238 , 0.286	Depositor DCC
R_{free} test set	2137 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13232	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.03% 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: RBF

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	0.53	0/1620	1.06	13/2210 (0.6%)
1	C	0.61	0/1620	1.11	13/2210 (0.6%)
1	E	0.54	0/1620	1.07	11/2210 (0.5%)
1	L	0.51	0/1620	1.09	15/2210 (0.7%)
2	B	0.53	0/1706	1.01	7/2323 (0.3%)
2	D	0.61	0/1706	1.03	9/2323 (0.4%)
2	F	0.57	0/1706	1.01	7/2323 (0.3%)
2	H	0.56	0/1706	1.02	6/2323 (0.3%)
All	All	0.56	0/13304	1.05	81/18132 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	100(A)	TYR	N-CA-C	9.62	122.77	110.65
2	F	100(A)	TYR	N-CA-C	8.96	123.82	111.55
1	A	151	ASP	CB-CA-C	-8.58	100.36	111.86
1	C	107	GLY	N-CA-C	8.47	126.28	111.46
2	D	100(A)	TYR	N-CA-C	7.76	122.80	112.25
1	E	112	ALA	CA-C-N	7.72	127.48	119.76
1	E	112	ALA	C-N-CA	7.72	127.48	119.76
1	C	106	VAL	N-CA-C	7.41	124.75	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	GLU	N-CA-C	7.30	121.43	109.24
1	C	112	ALA	CA-C-N	7.11	126.87	119.76
1	C	112	ALA	C-N-CA	7.11	126.87	119.76
2	D	113	SER	N-CA-C	-7.11	102.95	113.61
1	A	3	GLU	N-CA-C	6.89	120.41	108.76
2	F	33	TYR	N-CA-C	-6.60	99.54	110.17
2	B	104	GLY	N-CA-C	-6.58	102.50	112.89
1	L	107	GLY	N-CA-C	6.56	128.73	113.18
1	E	106	VAL	N-CA-C	6.53	122.93	109.34
2	F	113	SER	N-CA-C	-6.53	103.81	113.61
1	E	95(A)	TYR	CA-C-N	6.53	126.50	119.78
1	E	95(A)	TYR	C-N-CA	6.53	126.50	119.78
1	L	57	GLU	N-CA-C	-6.47	104.81	114.64
2	H	113	SER	N-CA-C	-6.44	104.67	113.30
2	D	120	SER	N-CA-C	-6.44	99.20	109.76
1	L	3	GLU	N-CA-C	6.38	119.90	109.24
2	B	120	SER	N-CA-C	-6.37	101.06	110.48
1	L	151	ASP	CB-CA-C	-6.33	102.75	111.73
1	E	138	ASP	N-CA-C	6.30	120.10	111.54
2	D	49	THR	N-CA-C	6.26	118.47	109.14
2	F	92	CYS	N-CA-C	-6.26	99.52	109.59
1	L	137	SER	N-CA-C	6.21	119.66	109.85
1	C	95	GLY	N-CA-C	6.12	127.68	113.18
2	B	32	TYR	N-CA-C	6.03	119.37	109.85
1	L	95	GLY	N-CA-C	5.98	127.34	113.18
1	E	3	GLU	N-CA-C	5.97	119.22	109.24
1	L	106	VAL	N-CA-C	5.91	121.63	109.34
1	E	151	ASP	CB-CA-C	-5.88	103.37	111.73
2	H	92	CYS	N-CA-C	-5.88	100.12	109.59
2	H	120	SER	N-CA-C	-5.86	100.15	109.76
1	A	4	LEU	N-CA-C	-5.85	96.99	107.98
1	C	138	ASP	N-CA-C	5.84	119.48	111.54
1	E	95	GLY	N-CA-C	5.82	126.97	113.18
2	B	49	THR	N-CA-C	5.79	117.59	108.96
1	C	57	GLU	N-CA-C	-5.77	105.62	114.16
1	L	153	SER	CA-C-N	-5.77	114.81	120.98
1	L	153	SER	C-N-CA	-5.77	114.81	120.98
1	A	107	GLY	N-CA-C	5.74	126.78	113.18
1	L	138	ASP	N-CA-C	5.73	119.58	112.24
2	D	104	GLY	N-CA-C	-5.71	103.42	112.66
1	A	95	GLY	N-CA-C	5.69	126.66	113.18
2	D	33	TYR	N-CA-C	-5.68	101.02	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	113	SER	N-CA-C	-5.65	105.73	113.30
1	L	182	THR	N-CA-C	-5.62	102.37	110.40
2	D	32	TYR	N-CA-C	5.53	118.28	109.81
2	F	86	ASP	N-CA-C	-5.49	106.54	113.18
1	E	153	SER	N-CA-C	-5.45	102.61	110.40
1	C	137	SER	N-CA-C	5.43	117.94	109.52
2	H	33	TYR	N-CA-C	-5.43	101.43	110.17
1	A	182	THR	N-CA-C	-5.41	102.15	110.32
1	C	173	TYR	N-CA-C	5.41	118.37	109.72
1	A	138	ASP	N-CA-C	5.36	118.79	111.39
2	D	78	LEU	N-CA-C	-5.35	101.17	109.72
1	L	173	TYR	N-CA-C	5.34	118.44	109.95
2	B	92	CYS	N-CA-C	-5.33	101.01	109.59
1	L	47	VAL	CB-CA-C	-5.26	105.68	110.63
1	L	112	ALA	CA-C-N	5.25	125.01	119.76
1	L	112	ALA	C-N-CA	5.25	125.01	119.76
2	B	146	ASP	N-CA-C	5.22	121.92	110.80
1	C	182	THR	N-CA-C	-5.22	103.11	110.31
2	F	104	GLY	N-CA-C	-5.20	104.24	112.66
2	F	49	THR	N-CA-C	5.14	116.89	109.07
2	D	146	ASP	N-CA-C	5.12	121.71	110.80
1	A	106	VAL	N-CA-C	5.08	119.91	109.34
1	E	107	GLY	N-CA-C	5.08	125.22	113.18
1	C	159	VAL	N-CA-C	5.08	115.22	108.11
1	A	9	SER	N-CA-C	5.06	117.08	109.23
2	H	78	LEU	N-CA-C	-5.05	101.91	109.95
1	A	137	SER	N-CA-C	5.04	117.34	109.52
1	C	97	LEU	CB-CA-C	-5.02	102.06	112.44
1	A	108	GLN	N-CA-C	-5.01	98.74	109.81
1	A	153	SER	CA-C-N	-5.01	115.44	120.85
1	A	153	SER	C-N-CA	-5.01	115.44	120.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	33	TYR	Sidechain

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	1579	0	1524	80	0
1	C	1579	0	1524	95	0
1	E	1579	0	1524	74	0
1	L	1579	0	1524	103	0
2	B	1666	0	1612	85	0
2	D	1666	0	1612	83	0
2	F	1666	0	1612	81	0
2	H	1666	0	1612	103	0
3	B	27	0	20	1	0
3	D	27	0	20	1	0
3	F	27	0	20	1	0
3	H	27	0	20	2	0
4	A	21	0	0	1	0
4	B	14	0	0	3	0
4	C	24	0	0	4	0
4	D	16	0	0	2	0
4	E	13	0	0	1	0
4	F	16	0	0	1	0
4	H	17	0	0	0	0
4	L	23	0	0	2	0
All	All	13232	0	12624	665	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 (665) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:GLN:HG2	1:E:109:PRO:HD2	1.34	1.06
1:L:92:ILE:HD11	1:L:95(A):TYR:HB2	1.40	1.04
1:L:108:GLN:HG2	1:L:109:PRO:HD2	1.39	1.02
1:L:92:ILE:CD1	1:L:95(A):TYR:HB2	1.92	1.00
1:A:108:GLN:HG2	1:A:109:PRO:HD2	1.48	0.95
1:E:92:ILE:HD11	1:E:95(A):TYR:HB2	1.47	0.94
1:A:92:ILE:HD12	1:A:94:ASN:OD1	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ARG:HD3	4:A:213:HOH:O	1.71	0.90
1:C:2:TYR:CD2	1:C:97:LEU:HD11	2.07	0.89
1:C:2:TYR:HD2	1:C:97:LEU:HD11	1.38	0.89
1:A:91:ASP:HA	1:A:97:LEU:HD12	1.54	0.88
2:B:51:ILE:HD11	2:B:54:GLU:HG3	1.55	0.86
1:C:195:GLN:HB3	1:C:206:GLU:HG3	1.55	0.86
2:H:30:SER:HB3	2:H:73:ASN:HB3	1.56	0.86
1:C:108:GLN:HG2	1:C:109:PRO:HD2	1.59	0.84
2:B:117:LYS:HD3	2:B:146:ASP:O	1.78	0.84
1:C:92:ILE:CD1	1:C:95(A):TYR:HB2	2.08	0.83
2:F:48:VAL:HG12	2:F:49:THR:HG23	1.59	0.83
1:L:47:VAL:HG23	1:L:48:VAL:HG23	1.59	0.83
1:A:151:ASP:O	1:A:152:SER:HB2	1.77	0.82
1:C:92:ILE:HD11	1:C:95(A):TYR:HB2	1.62	0.81
2:D:87:THR:HG23	2:D:110:SER:HA	1.60	0.81
1:E:92:ILE:CD1	1:E:95(A):TYR:HB2	2.08	0.81
1:C:193:SER:HB3	1:C:208:THR:OG1	1.81	0.79
1:C:83:GLU:OE1	1:C:106:VAL:HG22	1.82	0.79
2:F:11:LEU:HD13	2:F:110:SER:HB2	1.65	0.79
2:F:82:MET:HB3	2:F:82(C):GLN:HE22	1.49	0.78
2:H:187:LEU:C	2:H:187:LEU:HD12	2.08	0.78
2:D:84:VAL:HG23	2:D:85:GLU:OE1	1.84	0.76
1:E:55:PRO:HB2	1:E:58:ILE:HG12	1.68	0.76
1:E:108:GLN:HA	4:E:213:HOH:O	1.86	0.75
1:L:17:GLN:HB2	4:L:226:HOH:O	1.86	0.75
2:H:39:GLN:C	2:H:88:ALA:HB1	2.12	0.75
1:L:61:ARG:HD2	1:L:76:SER:O	1.86	0.75
2:H:112:THR:HG21	2:H:183:GLY:HA3	1.67	0.75
2:D:82(A):SER:OG	2:F:196:SER:HB2	1.86	0.75
1:A:195:GLN:HB3	1:A:206:GLU:HG3	1.67	0.74
1:E:61:ARG:NH2	1:E:79:GLN:HG3	2.01	0.74
1:L:151:ASP:O	1:L:152:SER:HB2	1.87	0.74
1:L:27:VAL:C	1:L:29:PRO:HD2	2.13	0.74
1:L:61:ARG:NH2	1:L:79:GLN:HG3	2.02	0.74
1:L:117:LEU:HD23	1:L:209:VAL:HG13	1.70	0.74
2:H:162:ASN:HD22	2:H:166:LEU:HB2	1.53	0.73
1:L:91:ASP:HA	1:L:97:LEU:HD12	1.69	0.73
2:D:30:SER:HB3	2:D:73:ASN:HB3	1.70	0.73
1:E:197:THR:HG22	1:E:204:THR:HG23	1.71	0.73
2:D:187:LEU:C	2:D:187:LEU:HD12	2.14	0.72
1:A:197:THR:HG22	1:A:204:THR:HG23	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:ASP:OD1	2:B:55:THR:HG23	1.89	0.72
1:A:2:TYR:CD2	1:A:97:LEU:HD11	2.23	0.72
1:A:91:ASP:CA	1:A:97:LEU:HD12	2.18	0.72
1:L:50:GLU:HG2	2:H:99:GLY:HA3	1.70	0.72
1:A:182:THR:OG1	1:A:185:GLN:HG3	1.89	0.72
2:B:11:LEU:HD13	2:B:110:SER:HB2	1.71	0.71
1:E:195:GLN:HB3	1:E:206:GLU:HG3	1.71	0.71
1:A:92:ILE:HD11	1:A:95(A):TYR:HB2	1.72	0.71
1:A:61:ARG:HD2	1:A:76:SER:O	1.91	0.71
1:L:14:SER:O	1:L:17:GLN:HG2	1.91	0.71
1:L:91:ASP:HB3	1:L:96:PRO:HA	1.73	0.70
2:H:83:ARG:HB3	2:H:85:GLU:OE2	1.92	0.70
1:E:32:TYR:CD1	1:E:50:GLU:HA	2.26	0.70
1:L:135:LEU:HB3	2:H:174:PHE:CZ	2.27	0.70
1:C:151:ASP:O	1:C:152:SER:HB2	1.91	0.70
1:L:195:GLN:HB3	1:L:206:GLU:HG3	1.72	0.70
1:C:61:ARG:HD2	1:C:76:SER:O	1.92	0.70
1:A:2:TYR:HD2	1:A:97:LEU:HD11	1.56	0.70
1:E:50:GLU:HG2	2:F:99:GLY:HA3	1.72	0.70
1:C:95(A):TYR:HA	3:D:228:RBF:HC72	1.73	0.69
1:L:4:LEU:HB2	1:L:99:GLY:HA2	1.74	0.69
1:L:6:GLN:NE2	1:L:86:TYR:O	2.25	0.69
1:L:82:ASP:O	1:L:104:LEU:HD23	1.91	0.69
1:L:197:THR:HG22	1:L:204:THR:HG23	1.74	0.69
2:B:179:GLN:HB3	4:B:234:HOH:O	1.92	0.69
2:F:23:THR:HG22	2:F:77:SER:OG	1.92	0.69
2:F:137:THR:HG23	2:F:193:VAL:C	2.17	0.69
2:F:207:THR:OG1	2:F:222:LYS:HG2	1.92	0.69
2:H:87:THR:HG23	2:H:110:SER:HA	1.73	0.69
2:D:49:THR:HG22	2:D:58:PHE:O	1.92	0.69
1:A:92:ILE:CD1	1:A:95(A):TYR:HB2	2.23	0.68
2:F:30:SER:HB3	2:F:73:ASN:HB3	1.74	0.68
1:A:96:PRO:HG2	2:B:47:TRP:CD2	2.29	0.68
1:C:96:PRO:HG2	2:D:47:TRP:CE2	2.29	0.68
1:C:4:LEU:HB2	1:C:99:GLY:HA2	1.76	0.68
2:D:29:LEU:HD11	2:D:34:MET:HE2	1.76	0.67
2:F:197:SER:OG	2:F:203:LYS:HE2	1.95	0.67
1:L:92:ILE:HD11	1:L:95(A):TYR:CB	2.21	0.67
2:H:85:GLU:H	2:H:85:GLU:CD	2.02	0.67
1:A:83:GLU:OE1	1:A:106:VAL:HG22	1.94	0.67
2:B:85:GLU:CD	2:B:85:GLU:H	2.03	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLN:HA	4:C:213:HOH:O	1.94	0.67
2:F:13:GLN:O	2:F:16:GLU:HB2	1.94	0.67
2:H:12:VAL:O	2:H:111:VAL:HA	1.95	0.67
2:B:30:SER:HB3	2:B:73:ASN:HB3	1.75	0.67
2:B:117:LYS:HG2	2:B:118:GLY:H	1.61	0.66
1:L:96:PRO:HG2	2:H:47:TRP:CD2	2.30	0.66
1:E:96:PRO:HG2	2:F:47:TRP:CD2	2.30	0.66
1:L:136:ILE:HG12	1:L:196:VAL:HG21	1.77	0.66
1:A:92:ILE:HD11	1:A:95(A):TYR:CD1	2.31	0.66
2:D:52(A):PRO:HA	2:D:71:ARG:CZ	2.26	0.66
2:D:13:GLN:O	2:D:16:GLU:HB2	1.95	0.66
2:F:187:LEU:C	2:F:187:LEU:HD12	2.21	0.66
2:F:198:LEU:HG	2:F:227:PRO:HG3	1.78	0.66
1:A:96:PRO:HG2	2:B:47:TRP:CE2	2.30	0.65
1:E:41:GLY:O	1:E:42:GLN:HG2	1.96	0.65
1:C:117:LEU:HD23	1:C:209:VAL:HG13	1.79	0.65
1:A:4:LEU:HB2	1:A:99:GLY:HA2	1.78	0.65
1:E:2:TYR:HD2	1:E:97:LEU:CD1	2.09	0.65
2:F:83:ARG:HB3	2:F:85:GLU:OE2	1.96	0.65
2:B:198:LEU:HG	2:B:227:PRO:HG3	1.78	0.65
2:D:85:GLU:CD	2:D:85:GLU:H	2.03	0.64
2:D:198:LEU:HG	2:D:227:PRO:HG3	1.77	0.64
1:L:133:VAL:HG13	1:L:178:TYR:CE1	2.32	0.64
1:E:151:ASP:O	1:E:152:SER:HB2	1.96	0.64
2:D:212:HIS:ND1	2:D:215:SER:HB3	2.13	0.64
2:B:117:LYS:HG2	2:B:118:GLY:N	2.11	0.64
2:H:13:GLN:O	2:H:16:GLU:HB2	1.98	0.64
2:H:52(A):PRO:HA	2:H:71:ARG:CZ	2.29	0.63
1:C:96:PRO:HG2	2:D:47:TRP:CD2	2.33	0.63
2:D:53:ASP:OD1	2:D:55:THR:HG23	1.98	0.63
1:E:61:ARG:HD2	1:E:76:SER:O	1.99	0.63
2:B:198:LEU:HG	2:B:227:PRO:CG	2.29	0.62
2:D:6:GLU:OE1	2:D:106:GLY:N	2.32	0.62
2:F:162:ASN:HD22	2:F:166:LEU:HB2	1.64	0.62
1:L:28:LEU:N	1:L:29:PRO:HD2	2.15	0.62
2:B:137:THR:HG23	2:B:193:VAL:C	2.24	0.62
2:F:52(A):PRO:HA	2:F:71:ARG:CZ	2.30	0.62
2:F:82:MET:CB	2:F:82(C):GLN:HE22	2.12	0.62
2:H:47:TRP:NE1	2:H:50:ASN:OD1	2.30	0.62
1:L:92:ILE:HD13	1:L:95(A):TYR:HB2	1.79	0.62
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:TYR:CE2	2:B:177:VAL:HG11	2.35	0.61
1:C:154:PRO:O	1:C:155:ILE:HG23	2.00	0.61
1:L:154:PRO:O	1:L:155:ILE:HG23	2.01	0.61
2:H:197:SER:OG	2:H:203:LYS:HE2	2.00	0.61
2:B:110:SER:O	2:B:111:VAL:HG23	2.00	0.61
2:H:11:LEU:HD13	2:H:110:SER:HB2	1.82	0.61
2:D:207:THR:OG1	2:D:222:LYS:HG2	2.01	0.61
2:F:108:LEU:HD12	2:F:109:VAL:H	1.66	0.61
2:H:48:VAL:HG12	2:H:49:THR:HG23	1.83	0.61
2:B:13:GLN:O	2:B:16:GLU:HB2	2.01	0.61
2:B:52:ARG:CG	2:B:52(A):PRO:HD2	2.31	0.61
2:D:84:VAL:HG12	2:D:111:VAL:O	2.00	0.61
2:D:193:VAL:HB	2:D:194:PRO:HD2	1.82	0.61
2:B:51:ILE:HD11	2:B:54:GLU:CG	2.27	0.61
1:E:47:VAL:HG23	1:E:48:VAL:HG23	1.82	0.61
1:A:61:ARG:NH2	1:A:79:GLN:HG3	2.15	0.60
2:H:117:LYS:HG2	2:H:118:GLY:N	2.16	0.60
2:B:87:THR:HG23	2:B:110:SER:HA	1.83	0.60
2:B:39:GLN:C	2:B:88:ALA:HB1	2.26	0.60
2:B:212:HIS:ND1	2:B:215:SER:HB3	2.16	0.60
1:C:11:VAL:O	1:C:104:LEU:HA	2.01	0.60
2:D:137:THR:HG23	2:D:193:VAL:C	2.27	0.60
1:C:50:GLU:HG2	2:D:99:GLY:HA3	1.83	0.59
2:D:29:LEU:CD1	2:D:34:MET:HE2	2.32	0.59
2:H:12:VAL:HG23	2:H:111:VAL:HG22	1.84	0.59
1:E:151:ASP:O	1:E:152:SER:CB	2.50	0.59
1:E:193:SER:HB3	1:E:208:THR:OG1	2.02	0.59
2:B:22:CYS:HB3	2:B:78:LEU:HB3	1.84	0.59
2:D:182:SER:O	2:D:184:LEU:N	2.35	0.59
2:F:85:GLU:CD	2:F:85:GLU:H	2.10	0.59
2:H:198:LEU:HG	2:H:227:PRO:HG3	1.85	0.59
2:D:140:LEU:HD11	2:D:198:LEU:HD11	1.84	0.59
1:L:193:SER:HB3	1:L:208:THR:OG1	2.02	0.59
2:F:95:VAL:HG11	3:F:204:RBF:O4	2.02	0.59
2:D:203:LYS:HB3	4:D:230:HOH:O	2.02	0.59
1:L:25:GLY:O	1:L:69:THR:HB	2.01	0.58
2:F:108:LEU:HD12	2:F:109:VAL:N	2.18	0.58
1:L:55:PRO:HB2	1:L:58:ILE:HG12	1.85	0.58
1:E:106:VAL:HG23	1:E:107:GLY:H	1.68	0.58
1:A:50:GLU:HG2	2:B:99:GLY:HA3	1.85	0.58
2:B:129:ARG:NH1	2:B:129:ARG:HB3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:212:HIS:CD2	2:H:214:PRO:HD2	2.39	0.58
2:B:129:ARG:HB3	2:B:129:ARG:HH11	1.67	0.58
2:F:212:HIS:CD2	2:F:214:PRO:HD2	2.39	0.58
1:A:151:ASP:OD1	1:A:190:ARG:HG2	2.03	0.58
1:E:9:SER:O	1:E:11:VAL:HG23	2.03	0.58
2:F:87:THR:HG23	2:F:110:SER:HA	1.84	0.58
2:H:99:GLY:C	2:H:100:ASP:O	2.43	0.58
2:B:119:PRO:HB2	2:B:144:VAL:HG13	1.84	0.58
1:E:2:TYR:HD2	1:E:97:LEU:HD11	1.67	0.58
1:E:46:LEU:HD11	1:E:48:VAL:O	2.04	0.58
1:E:13:VAL:HG11	1:E:19:ALA:HB2	1.86	0.57
1:A:178:TYR:CD2	2:B:177:VAL:HG11	2.39	0.57
2:D:52:ARG:CG	2:D:52(A):PRO:HD2	2.34	0.57
1:A:49:TYR:HD2	1:A:50:GLU:HG3	1.69	0.57
2:D:198:LEU:HG	2:D:227:PRO:CG	2.33	0.57
1:A:197:THR:HG22	1:A:204:THR:CG2	2.33	0.57
2:H:187:LEU:HD12	2:H:187:LEU:O	2.05	0.57
1:L:61:ARG:CZ	1:L:79:GLN:HG3	2.34	0.57
1:A:95(A):TYR:HA	3:B:202:RBF:HC73	1.85	0.57
2:H:82:MET:HB3	2:H:82(C):GLN:HE22	1.70	0.57
1:C:2:TYR:CD2	1:C:97:LEU:CD1	2.84	0.57
2:B:20:LEU:HG	2:B:82:MET:HE2	1.87	0.57
2:D:52:ARG:HG2	2:D:52(A):PRO:HD2	1.86	0.57
1:L:106:VAL:HG23	1:L:107:GLY:H	1.70	0.56
1:A:92:ILE:HD11	1:A:95(A):TYR:HD1	1.69	0.56
2:B:52:ARG:HG2	2:B:52(A):PRO:HD2	1.87	0.56
2:D:211:ASN:ND2	2:D:218:LYS:HE2	2.20	0.56
2:D:11:LEU:HD13	2:D:110:SER:HB2	1.87	0.56
1:E:2:TYR:CD2	1:E:97:LEU:CD1	2.88	0.56
1:L:50:GLU:OE2	2:H:98:PHE:HB2	2.05	0.56
2:H:53:ASP:OD1	2:H:55:THR:HG23	2.06	0.56
1:A:55:PRO:HB2	1:A:58:ILE:HG12	1.86	0.56
2:F:53:ASP:OD1	2:F:55:THR:HG23	2.05	0.56
1:L:151:ASP:O	1:L:152:SER:CB	2.54	0.56
2:H:30:SER:HB3	2:H:73:ASN:CB	2.31	0.56
2:B:112:THR:HG21	2:B:183:GLY:HA3	1.88	0.56
1:E:83:GLU:OE1	1:E:106:VAL:HG22	2.06	0.56
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.05	0.56
2:H:20:LEU:HG	2:H:82:MET:HE2	1.88	0.56
1:C:61:ARG:NH2	1:C:79:GLN:HG3	2.21	0.56
2:D:207:THR:CG2	2:D:222:LYS:HG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:39:GLN:HG3	2:F:44:GLY:O	2.06	0.55
1:E:6:GLN:NE2	1:E:86:TYR:O	2.39	0.55
2:F:193:VAL:HB	2:F:194:PRO:HD2	1.89	0.55
1:L:2:TYR:HD2	1:L:97:LEU:CD1	2.18	0.55
1:L:122:SER:HA	1:L:125:LEU:HD12	1.88	0.55
1:L:62:PHE:CD2	1:L:75:ILE:HG12	2.42	0.55
1:A:149:LYS:HB2	1:A:193:SER:OG	2.06	0.55
2:B:172:HIS:HA	4:B:238:HOH:O	2.06	0.55
1:E:151:ASP:OD2	1:E:189:HIS:HB3	2.07	0.55
2:B:12:VAL:O	2:B:111:VAL:HA	2.06	0.55
1:C:92:ILE:HD11	1:C:95(A):TYR:CD1	2.41	0.55
2:D:212:HIS:HD1	2:D:215:SER:HB3	1.72	0.55
2:F:126:PRO:CB	2:F:130:SER:HB2	2.37	0.55
2:H:187:LEU:C	2:H:187:LEU:CD1	2.77	0.55
1:C:13:VAL:HG11	1:C:19:ALA:HB2	1.89	0.55
1:C:47:VAL:HA	1:C:58:ILE:HG13	1.89	0.55
1:C:106:VAL:HG23	1:C:107:GLY:H	1.72	0.54
2:B:67:PHE:CE1	2:B:82:MET:HB3	2.42	0.54
1:A:28:LEU:N	1:A:29:PRO:HD2	2.22	0.54
2:D:85:GLU:OE1	2:D:85:GLU:N	2.38	0.54
2:D:34:MET:HB2	2:D:78:LEU:HD13	1.90	0.54
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.90	0.54
1:C:92:ILE:HD13	1:C:95(A):TYR:HB2	1.88	0.54
2:D:2:VAL:HG11	2:D:102:PHE:CG	2.42	0.54
1:L:7:PRO:O	1:L:102:THR:OG1	2.25	0.54
1:A:34:TYR:O	1:A:88:CYS:HA	2.08	0.54
1:A:89:TYR:CD1	1:A:89:TYR:C	2.86	0.54
2:D:34:MET:HB3	2:D:78:LEU:HD22	1.90	0.54
2:F:100(A):TYR:CD1	2:F:100(A):TYR:N	2.75	0.54
1:A:212:THR:OXT	1:A:212:THR:HG22	2.08	0.53
2:B:140:LEU:HD11	2:B:198:LEU:HD11	1.90	0.53
2:B:198:LEU:HD12	2:B:206:TYR:CE2	2.43	0.53
1:C:160:GLU:HB3	2:D:177:VAL:HG21	1.88	0.53
2:F:52(A):PRO:HA	2:F:71:ARG:NH1	2.23	0.53
1:A:150:ALA:HB2	1:A:155:ILE:HD13	1.91	0.53
2:B:108:LEU:HD12	2:B:109:VAL:N	2.24	0.53
1:E:128:ASN:HA	1:E:183:PRO:HG2	1.89	0.53
2:F:119:PRO:HB3	2:F:147:TYR:HB3	1.90	0.53
2:B:182:SER:O	2:B:184:LEU:N	2.42	0.53
1:A:50:GLU:OE2	2:B:98:PHE:HB2	2.09	0.53
1:E:32:TYR:CE1	1:E:50:GLU:HB3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135:LEU:HD22	2:H:174:PHE:CG	2.44	0.53
1:E:14:SER:O	1:E:17:GLN:HG2	2.09	0.53
1:E:108:GLN:NE2	1:E:140:TYR:CD2	2.77	0.53
2:H:137:THR:HG23	2:H:193:VAL:C	2.34	0.53
1:L:41:GLY:O	1:L:42:GLN:HG2	2.09	0.52
2:B:52(A):PRO:HA	2:B:71:ARG:CZ	2.40	0.52
1:C:29:PRO:HD3	1:C:69:THR:HG22	1.91	0.52
2:D:39:GLN:C	2:D:88:ALA:HB1	2.33	0.52
2:B:49:THR:HG22	2:B:58:PHE:O	2.09	0.52
1:C:14:SER:O	1:C:15:PRO:C	2.53	0.52
1:C:133:VAL:HG13	1:C:178:TYR:CE2	2.45	0.52
1:C:151:ASP:OD2	1:C:189:HIS:HB3	2.10	0.52
1:A:6:GLN:NE2	1:A:86:TYR:O	2.43	0.52
1:E:32:TYR:CD1	1:E:50:GLU:CA	2.92	0.52
2:D:66:ARG:HD3	2:D:83:ARG:HH21	1.75	0.52
1:E:89:TYR:C	1:E:89:TYR:CD1	2.88	0.52
2:H:87:THR:HG23	2:H:109:VAL:O	2.10	0.52
2:H:153:THR:HB	2:H:211:ASN:HB3	1.91	0.52
1:C:34:TYR:HB2	1:C:89:TYR:HB3	1.92	0.52
1:A:151:ASP:OD2	1:A:189:HIS:HB3	2.10	0.52
2:H:124:LEU:HB2	2:H:141:GLY:C	2.35	0.51
2:H:162:ASN:ND2	2:H:166:LEU:HB2	2.22	0.51
1:C:2:TYR:CE2	1:C:97:LEU:HD11	2.45	0.51
1:C:151:ASP:O	1:C:152:SER:CB	2.55	0.51
1:E:4:LEU:HB2	1:E:99:GLY:HA2	1.92	0.51
1:L:192:TYR:O	1:L:208:THR:HG23	2.10	0.51
1:C:2:TYR:CE2	1:C:97:LEU:CD1	2.93	0.51
1:C:14:SER:O	1:C:17:GLN:HG2	2.09	0.51
2:F:135:GLU:HA	4:F:240:HOH:O	2.11	0.51
1:A:32:TYR:CD1	1:A:50:GLU:HA	2.44	0.51
2:D:72:ASP:OD1	2:D:74:ALA:HB3	2.10	0.51
1:E:28:LEU:N	1:E:29:PRO:HD2	2.25	0.51
2:H:54:GLU:OE1	2:H:71:ARG:HG2	2.11	0.51
1:A:91:ASP:HB3	1:A:96:PRO:HA	1.92	0.51
1:L:28:LEU:N	1:L:29:PRO:CD	2.73	0.51
2:H:51:ILE:HD11	2:H:54:GLU:HG3	1.93	0.51
2:B:48:VAL:HG13	2:B:63:VAL:HG21	1.91	0.51
1:L:29:PRO:HD3	1:L:69:THR:HG22	1.93	0.51
1:L:96:PRO:HG2	2:H:47:TRP:CE2	2.45	0.51
1:C:13:VAL:O	1:C:106:VAL:HA	2.10	0.51
2:F:198:LEU:HG	2:F:227:PRO:CG	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:ARG:NH1	2:H:86:ASP:HA	2.26	0.51
2:B:11:LEU:HD13	2:B:110:SER:CB	2.39	0.51
2:B:108:LEU:HD12	2:B:109:VAL:H	1.74	0.51
2:D:195:SER:HA	2:D:198:LEU:HB2	1.93	0.51
2:F:34:MET:HB3	2:F:78:LEU:HD22	1.91	0.51
1:A:29:PRO:HD3	1:A:69:THR:HG22	1.93	0.51
1:E:197:THR:HG22	1:E:204:THR:CG2	2.38	0.51
1:C:55:PRO:HB2	1:C:58:ILE:HG12	1.93	0.51
1:C:144:VAL:HG12	1:C:198:HIS:HB2	1.92	0.51
1:E:125:LEU:O	1:E:128:ASN:N	2.40	0.51
2:H:52:ARG:CG	2:H:52(A):PRO:HD2	2.41	0.50
1:E:167:GLN:HG3	1:E:172:LYS:O	2.11	0.50
2:H:12:VAL:CG2	2:H:111:VAL:HG22	2.42	0.50
2:H:49:THR:CG2	2:H:59:TYR:CD2	2.95	0.50
1:E:199:GLU:C	1:E:203:SER:H	2.20	0.50
1:L:95(A):TYR:HA	3:H:201:RBF:HC72	1.93	0.50
1:A:2:TYR:CD2	1:A:97:LEU:CD1	2.93	0.50
1:E:136:ILE:HB	1:E:175:ALA:HB3	1.93	0.50
2:B:87:THR:HG23	2:B:109:VAL:O	2.11	0.50
2:H:20:LEU:CG	2:H:82:MET:HE2	2.41	0.50
1:C:208:THR:HG22	1:C:209:VAL:N	2.26	0.50
1:L:43:ALA:HB2	2:H:105:GLN:HA	1.93	0.49
1:C:49:TYR:HD1	1:C:50:GLU:HG3	1.77	0.49
1:L:35:TRP:O	1:L:47:VAL:HG22	2.12	0.49
2:H:166:LEU:HD23	2:H:167:THR:N	2.27	0.49
2:D:197:SER:OG	2:D:203:LYS:HE2	2.12	0.49
1:L:38:GLU:HG3	1:L:42:GLN:O	2.12	0.49
1:L:38:GLU:O	1:L:84:ALA:HB1	2.12	0.49
2:H:75:ARG:O	2:H:76:ASN:C	2.55	0.49
2:H:124:LEU:HB2	2:H:141:GLY:O	2.13	0.49
1:A:41:GLY:O	1:A:42:GLN:HG2	2.13	0.49
2:B:12:VAL:HG23	2:B:111:VAL:HG22	1.95	0.49
1:C:91:ASP:HB3	1:C:96:PRO:HA	1.94	0.49
1:L:108:GLN:NE2	1:L:140:TYR:CE2	2.81	0.49
1:L:170:ASN:ND2	1:L:172:LYS:HB2	2.27	0.49
1:A:144:VAL:HG12	1:A:198:HIS:HB2	1.95	0.49
1:C:6:GLN:HE22	1:C:87:TYR:HA	1.78	0.49
1:C:91:ASP:HA	1:C:97:LEU:HD12	1.94	0.49
1:C:6:GLN:NE2	1:C:86:TYR:O	2.45	0.49
1:C:27:VAL:HG12	1:C:27:VAL:O	2.13	0.49
1:C:92:ILE:HG13	1:C:94:ASN:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLN:HG3	4:C:213:HOH:O	2.12	0.49
1:E:11:VAL:O	1:E:104:LEU:HA	2.13	0.49
2:F:2:VAL:HG11	2:F:102:PHE:CG	2.48	0.49
1:L:136:ILE:HB	1:L:175:ALA:HB3	1.94	0.49
2:H:129:ARG:HH11	2:H:129:ARG:HB3	1.78	0.49
1:A:11:VAL:O	1:A:104:LEU:HA	2.12	0.49
1:A:47:VAL:HG23	1:A:48:VAL:HG23	1.95	0.49
1:A:193:SER:HB3	1:A:208:THR:OG1	2.13	0.48
2:B:20:LEU:CG	2:B:82:MET:HE2	2.42	0.48
2:F:49:THR:HG22	2:F:59:TYR:CD2	2.48	0.48
1:L:2:TYR:CD2	1:L:97:LEU:HD13	2.48	0.48
1:L:32:TYR:CD1	1:L:50:GLU:HA	2.48	0.48
2:B:83:ARG:HB3	2:B:85:GLU:OE2	2.12	0.48
1:E:2:TYR:CD2	1:E:97:LEU:HD13	2.48	0.48
2:F:117:LYS:HD3	2:F:146:ASP:O	2.13	0.48
2:F:84:VAL:HG12	2:F:111:VAL:O	2.12	0.48
2:B:116:THR:O	2:B:116:THR:HG22	2.13	0.48
2:B:207:THR:OG1	2:B:222:LYS:HG2	2.13	0.48
1:L:135:LEU:HB3	2:H:174:PHE:CE2	2.48	0.48
2:H:119:PRO:HD3	2:H:212:HIS:ND1	2.28	0.48
1:L:83:GLU:OE1	1:L:106:VAL:HG22	2.14	0.48
1:C:20:ARG:NH1	1:C:74:THR:HG21	2.27	0.48
1:E:91:ASP:HB3	1:E:96:PRO:HA	1.95	0.48
1:L:27:VAL:HG12	1:L:27:VAL:O	2.13	0.48
1:L:46:LEU:HD11	1:L:48:VAL:O	2.14	0.48
1:C:92:ILE:HD11	1:C:95(A):TYR:CB	2.39	0.48
2:D:112:THR:HB	2:D:114:ALA:H	1.77	0.48
2:B:49:THR:HB	2:B:69:VAL:HG21	1.96	0.48
1:C:11:VAL:HG12	1:C:104:LEU:HD12	1.94	0.48
2:D:129:ARG:HH11	2:D:129:ARG:HB3	1.79	0.48
1:L:2:TYR:CD2	1:L:97:LEU:CD1	2.96	0.48
1:L:128:ASN:HA	1:L:183:PRO:HG2	1.95	0.48
2:H:112:THR:CG2	2:H:183:GLY:HA3	2.41	0.48
1:E:61:ARG:CZ	1:E:79:GLN:HG3	2.42	0.48
2:F:96:SER:HA	2:F:101:ASP:OD2	2.14	0.48
1:C:79:GLN:HE21	1:C:79:GLN:HA	1.79	0.48
2:F:87:THR:O	2:F:88:ALA:HB2	2.14	0.48
2:F:193:VAL:HG11	2:F:206:TYR:CE1	2.48	0.48
1:L:151:ASP:CG	1:L:189:HIS:HB3	2.38	0.47
1:C:36:TYR:HA	1:C:45:VAL:O	2.14	0.47
1:C:197:THR:HG22	1:C:204:THR:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:129:ARG:HH11	2:F:129:ARG:HB3	1.79	0.47
1:L:135:LEU:HD22	2:H:174:PHE:CD2	2.49	0.47
1:L:144:VAL:HG12	1:L:198:HIS:HB2	1.95	0.47
2:H:36:TRP:O	2:H:48:VAL:HB	2.14	0.47
2:B:177:VAL:HG12	2:B:186:SER:O	2.14	0.47
1:A:14:SER:O	1:A:17:GLN:HG2	2.14	0.47
1:A:2:TYR:HD2	1:A:97:LEU:CD1	2.27	0.47
1:A:92:ILE:HD11	1:A:95(A):TYR:CB	2.43	0.47
2:B:153:THR:HB	2:B:211:ASN:HB3	1.97	0.47
2:F:112:THR:HB	2:F:114:ALA:H	1.79	0.47
1:L:13:VAL:HG12	4:L:228:HOH:O	2.15	0.47
2:B:145:LYS:HG2	2:B:146:ASP:CG	2.39	0.47
2:D:20:LEU:HG	2:D:82:MET:HE2	1.97	0.47
2:H:129:ARG:HB3	2:H:129:ARG:NH1	2.30	0.47
1:A:115:VAL:O	1:A:207:LYS:HD2	2.15	0.47
2:B:197:SER:OG	2:B:203:LYS:HE2	2.14	0.47
1:C:32:TYR:CD1	1:C:50:GLU:HA	2.49	0.47
1:L:117:LEU:HD12	1:L:133:VAL:O	2.15	0.47
2:H:4:LEU:HD23	2:H:24:ALA:HB2	1.96	0.47
2:H:112:THR:HB	2:H:114:ALA:H	1.80	0.47
1:A:135:LEU:HB3	2:B:174:PHE:CZ	2.50	0.47
1:A:189:HIS:CD2	1:A:189:HIS:H	2.31	0.47
1:E:79:GLN:HB2	1:E:81:GLU:HG2	1.97	0.47
1:E:113:PRO:HB3	1:E:139:PHE:HB3	1.96	0.47
2:F:195:SER:HA	2:F:198:LEU:HB2	1.96	0.47
2:H:52:ARG:HG3	2:H:52(A):PRO:HD2	1.96	0.47
1:A:38:GLU:HG3	1:A:42:GLN:O	2.13	0.47
2:F:11:LEU:CD1	2:F:110:SER:HB2	2.43	0.47
1:C:212:THR:OXT	1:C:212:THR:CG2	2.63	0.47
1:E:13:VAL:HG11	1:E:19:ALA:CB	2.45	0.47
2:B:207:THR:CG2	2:B:222:LYS:HG2	2.45	0.46
2:F:126:PRO:HB2	2:F:130:SER:HB2	1.95	0.46
1:L:124:GLU:HA	2:H:122:PHE:CE1	2.49	0.46
2:H:82:MET:CB	2:H:82(C):GLN:HE22	2.28	0.46
2:H:119:PRO:HB2	2:H:144:VAL:HG13	1.97	0.46
2:H:198:LEU:HD12	2:H:206:TYR:CE2	2.51	0.46
2:F:49:THR:CG2	2:F:59:TYR:CD2	2.98	0.46
2:F:83:ARG:C	2:F:111:VAL:HG11	2.39	0.46
1:L:89:TYR:CD1	1:L:89:TYR:C	2.93	0.46
2:B:182:SER:C	2:B:184:LEU:H	2.24	0.46
2:D:211:ASN:HD21	2:D:218:LYS:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:137:THR:HA	2:H:194:PRO:HA	1.97	0.46
1:C:89:TYR:CD1	1:C:89:TYR:C	2.94	0.46
1:L:212:THR:OXT	1:L:212:THR:HG22	2.15	0.46
2:H:49:THR:HG21	2:H:59:TYR:CD2	2.51	0.46
3:H:201:RBF:O5'	2:D:85:GLU:OE2	2.27	0.46
1:C:28:LEU:N	1:C:29:PRO:HD2	2.31	0.46
2:F:90:TYR:O	2:F:106:GLY:HA2	2.15	0.46
1:C:92:ILE:C	1:C:94:ASN:H	2.24	0.46
1:L:49:TYR:HD2	1:L:50:GLU:HG3	1.81	0.46
1:L:132:LEU:HD12	1:L:132:LEU:N	2.30	0.46
1:A:124:GLU:HA	2:B:122:PHE:CE1	2.51	0.46
1:E:144:VAL:HG12	1:E:198:HIS:HB2	1.98	0.46
1:L:6:GLN:HG2	1:L:102:THR:OG1	2.16	0.45
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.51	0.45
2:B:41:PRO:O	2:B:43:LYS:HG2	2.16	0.45
1:C:82:ASP:O	1:C:104:LEU:HD23	2.16	0.45
1:E:29:PRO:HD3	1:E:69:THR:HG22	1.98	0.45
2:B:19:LYS:HE3	4:B:239:HOH:O	2.16	0.45
1:C:182:THR:OG1	1:C:185:GLN:HG3	2.16	0.45
2:H:111:VAL:O	2:H:111:VAL:HG12	2.16	0.45
1:A:36:TYR:HA	1:A:45:VAL:O	2.16	0.45
1:E:92:ILE:HD11	1:E:95(A):TYR:CB	2.33	0.45
2:F:153:THR:HB	2:F:211:ASN:HB3	1.97	0.45
2:H:84:VAL:HG23	2:H:85:GLU:OE1	2.16	0.45
1:C:182:THR:C	1:C:184:GLU:N	2.70	0.45
1:E:139:PHE:CE2	1:E:144:VAL:HG13	2.51	0.45
1:E:165:SER:O	1:E:173:TYR:HA	2.16	0.45
2:H:198:LEU:HG	2:H:227:PRO:CG	2.45	0.45
1:C:212:THR:OXT	1:C:212:THR:HG22	2.16	0.45
1:E:151:ASP:CG	1:E:189:HIS:HB3	2.40	0.45
2:F:24:ALA:HB1	2:F:27:PHE:CE1	2.52	0.45
1:L:120:PRO:HD2	1:L:186:TRP:CE2	2.52	0.45
2:H:211:ASN:ND2	2:H:218:LYS:HE2	2.32	0.45
1:A:148:TRP:CZ3	1:A:194:CYS:HB2	2.52	0.45
1:C:108:GLN:CA	4:C:213:HOH:O	2.57	0.45
2:D:182:SER:C	2:D:184:LEU:H	2.25	0.45
1:A:123:GLU:OE2	2:B:221:LYS:HE2	2.16	0.45
2:B:187:LEU:HD12	2:B:187:LEU:C	2.41	0.45
1:E:6:GLN:HG2	1:E:102:THR:OG1	2.17	0.45
2:F:212:HIS:ND1	2:F:215:SER:HB3	2.31	0.45
1:L:178:TYR:CD2	2:H:177:VAL:HG11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:TYR:O	1:A:208:THR:HG23	2.17	0.45
2:D:11:LEU:HD13	2:D:110:SER:CB	2.46	0.45
2:F:52:ARG:CG	2:F:52(A):PRO:HD2	2.46	0.45
2:H:39:GLN:O	2:H:88:ALA:HB1	2.17	0.45
2:H:207:THR:OG1	2:H:222:LYS:HG2	2.17	0.45
1:A:199:GLU:C	1:A:203:SER:H	2.24	0.45
2:H:195:SER:HA	2:H:198:LEU:HB2	1.99	0.45
2:H:116:THR:HG22	2:H:116:THR:O	2.17	0.44
2:H:148:PHE:HB2	2:H:184:LEU:HD23	1.98	0.44
2:F:39:GLN:C	2:F:88:ALA:HB1	2.42	0.44
1:L:47:VAL:HA	1:L:58:ILE:HG13	1.99	0.44
2:H:11:LEU:HD13	2:H:110:SER:CB	2.45	0.44
2:H:82:MET:HE1	2:H:109:VAL:HG21	1.99	0.44
2:H:98:PHE:O	2:H:100:ASP:O	2.35	0.44
2:D:87:THR:HG23	2:D:109:VAL:O	2.17	0.44
1:E:34:TYR:CD1	1:E:34:TYR:N	2.85	0.44
2:F:70:SER:OG	2:F:79:PHE:HB2	2.17	0.44
2:F:137:THR:HA	2:F:194:PRO:HA	1.97	0.44
1:A:211:PRO:O	1:A:212:THR:OG1	2.33	0.44
1:C:38:GLU:O	1:C:84:ALA:HB1	2.17	0.44
1:C:136:ILE:HG12	1:C:196:VAL:HG21	1.99	0.44
2:F:40:ALA:O	2:F:41:PRO:C	2.60	0.44
2:F:61:ASP:HA	2:F:64:LYS:HZ3	1.83	0.44
1:E:35:TRP:HB2	1:E:48:VAL:HB	1.99	0.44
2:F:72:ASP:O	2:F:73:ASN:C	2.59	0.44
2:H:156:SER:C	2:H:157:TRP:CD1	2.96	0.44
2:D:34:MET:CB	2:D:78:LEU:HD13	2.47	0.44
2:D:129:ARG:HB3	2:D:129:ARG:NH1	2.33	0.44
1:E:92:ILE:C	1:E:94:ASN:H	2.26	0.44
2:F:129:ARG:HB3	2:F:129:ARG:NH1	2.33	0.44
2:H:207:THR:CG2	2:H:222:LYS:HG2	2.47	0.44
1:A:83:GLU:HG3	1:A:104:LEU:O	2.18	0.44
1:L:140:TYR:HA	1:L:141:PRO:C	2.42	0.44
1:A:128:ASN:HA	1:A:183:PRO:HG2	1.99	0.44
1:C:13:VAL:HG11	1:C:19:ALA:CB	2.47	0.44
1:C:107:GLY:O	1:C:108:GLN:HB2	2.18	0.44
1:C:125:LEU:C	1:C:127:ALA:N	2.75	0.44
1:E:27:VAL:HG12	1:E:27:VAL:O	2.18	0.44
1:L:170:ASN:HD21	1:L:172:LYS:HB2	1.83	0.44
1:A:96:PRO:CG	2:B:47:TRP:CE2	3.01	0.44
1:C:122:SER:HA	1:C:125:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:VAL:C	1:E:29:PRO:HD2	2.43	0.44
1:L:140:TYR:CG	1:L:141:PRO:HA	2.54	0.43
2:B:66:ARG:HD3	2:B:83:ARG:HH21	1.82	0.43
1:C:117:LEU:CD2	1:C:209:VAL:HG13	2.48	0.43
2:D:66:ARG:HD3	2:D:83:ARG:NH2	2.31	0.43
2:D:99:GLY:C	2:D:100:ASP:O	2.59	0.43
2:F:187:LEU:C	2:F:187:LEU:CD1	2.91	0.43
1:A:2:TYR:CD2	1:A:97:LEU:HD21	2.53	0.43
1:A:82:ASP:O	1:A:104:LEU:HD23	2.18	0.43
2:B:34:MET:HB2	2:B:78:LEU:HD13	2.00	0.43
1:C:136:ILE:HB	1:C:175:ALA:HB3	2.00	0.43
1:L:2:TYR:HD2	1:L:97:LEU:HD11	1.81	0.43
2:H:147:TYR:CE2	2:H:152:VAL:HG23	2.53	0.43
1:L:212:THR:OXT	1:L:212:THR:CG2	2.66	0.43
2:H:182:SER:O	2:H:184:LEU:N	2.52	0.43
1:C:92:ILE:HD11	1:C:95(A):TYR:HD1	1.82	0.43
1:E:140:TYR:HA	1:E:141:PRO:C	2.43	0.43
2:F:54:GLU:OE1	2:F:71:ARG:HG2	2.18	0.43
1:L:11:VAL:O	1:L:104:LEU:HA	2.17	0.43
1:A:27:VAL:HG12	1:A:27:VAL:O	2.18	0.43
2:D:49:THR:CG2	2:D:59:TYR:CD2	3.02	0.43
2:D:54:GLU:OE1	2:D:71:ARG:HG2	2.18	0.43
2:D:207:THR:HG23	2:D:222:LYS:HG2	2.00	0.43
1:L:29:PRO:HB3	1:L:68:GLY:O	2.19	0.43
2:H:207:THR:HG23	2:H:222:LYS:HG2	2.00	0.43
2:B:55:THR:OG1	2:F:83:ARG:NH2	2.49	0.43
1:E:47:VAL:C	1:E:48:VAL:HG23	2.43	0.43
1:E:54:ARG:NH1	1:E:60:GLU:HG3	2.33	0.43
1:L:151:ASP:OD2	1:L:189:HIS:CD2	2.72	0.43
1:C:7:PRO:HA	1:C:8:PRO:HD2	1.87	0.43
1:C:124:GLU:O	1:C:124:GLU:HG2	2.18	0.43
1:L:50:GLU:HG2	2:H:99:GLY:CA	2.44	0.43
1:L:117:LEU:CD2	1:L:209:VAL:HG13	2.43	0.43
1:C:34:TYR:O	1:C:88:CYS:HA	2.19	0.43
1:C:128:ASN:HA	1:C:183:PRO:HG2	2.01	0.43
2:D:179:GLN:HB2	2:D:184:LEU:O	2.19	0.43
1:L:54:ARG:NH1	1:L:60:GLU:HA	2.34	0.43
2:H:148:PHE:HB2	2:H:184:LEU:CD2	2.48	0.43
1:E:135:LEU:HB3	2:F:174:PHE:CZ	2.54	0.43
1:L:9:SER:O	1:L:11:VAL:HG23	2.19	0.42
2:H:35:THR:HG22	2:H:95:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:LYS:HG2	2:F:146:ASP:CG	2.43	0.42
1:C:6:GLN:OE1	1:C:88:CYS:SG	2.77	0.42
1:C:178:TYR:CD1	2:D:177:VAL:HG11	2.54	0.42
2:D:23:THR:HG22	2:D:77:SER:OG	2.19	0.42
2:D:24:ALA:HB1	2:D:27:PHE:CE1	2.54	0.42
2:H:87:THR:OG1	2:H:111:VAL:HB	2.19	0.42
2:B:111:VAL:O	2:B:111:VAL:HG12	2.19	0.42
1:C:149:LYS:HG3	4:C:219:HOH:O	2.18	0.42
2:D:52:ARG:HD3	2:D:55:THR:OG1	2.20	0.42
2:D:52:ARG:NH1	2:D:56:GLU:OE1	2.52	0.42
2:F:51:ILE:HD11	2:F:54:GLU:HG3	2.01	0.42
2:B:126:PRO:CB	2:B:130:SER:HB2	2.49	0.42
1:C:35:TRP:HB2	1:C:48:VAL:HB	2.02	0.42
1:C:199:GLU:C	1:C:203:SER:H	2.27	0.42
1:E:160:GLU:HB3	2:F:177:VAL:HG21	2.02	0.42
2:H:51:ILE:O	2:H:51:ILE:HG23	2.20	0.42
2:H:98:PHE:CD1	2:H:98:PHE:N	2.88	0.42
1:C:61:ARG:CZ	1:C:79:GLN:HG3	2.50	0.42
1:C:132:LEU:HD22	1:C:179:LEU:HD23	2.01	0.42
2:D:83:ARG:C	2:D:111:VAL:HG11	2.45	0.42
2:D:16:GLU:HG2	4:D:232:HOH:O	2.20	0.42
2:D:66:ARG:HB3	2:D:82(A):SER:O	2.20	0.42
2:F:52:ARG:HD3	2:F:55:THR:OG1	2.20	0.42
1:L:36:TYR:HA	1:L:45:VAL:O	2.19	0.42
1:L:150:ALA:HB2	1:L:155:ILE:HD13	2.02	0.42
2:H:4:LEU:CD2	2:H:24:ALA:HB2	2.49	0.42
2:H:82(C):GLN:HG2	2:H:111:VAL:HG21	2.02	0.42
2:B:75:ARG:O	2:B:76:ASN:C	2.61	0.42
2:D:53:ASP:CG	2:D:55:THR:HG23	2.45	0.42
1:L:165:SER:O	1:L:173:TYR:HA	2.19	0.42
2:B:193:VAL:HB	2:B:194:PRO:HD2	2.01	0.42
2:D:51:ILE:O	2:D:51:ILE:HG23	2.19	0.42
2:D:111:VAL:O	2:D:112:THR:HG23	2.20	0.42
1:E:83:GLU:HG3	1:E:104:LEU:O	2.20	0.42
1:L:4:LEU:HB2	1:L:99:GLY:CA	2.45	0.42
1:C:125:LEU:C	1:C:127:ALA:H	2.27	0.42
2:D:213:LYS:N	2:D:214:PRO:CD	2.83	0.42
2:F:22:CYS:HB3	2:F:78:LEU:HB3	2.02	0.42
2:F:119:PRO:HB2	2:F:144:VAL:HG13	2.00	0.42
1:A:120:PRO:HD2	1:A:186:TRP:CE2	2.55	0.41
1:A:178:TYR:CE2	2:B:177:VAL:CG1	3.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:LEU:HD23	2:B:167:THR:N	2.35	0.41
1:C:151:ASP:OD1	1:C:190:ARG:HG2	2.20	0.41
1:C:208:THR:CG2	1:C:209:VAL:N	2.83	0.41
2:D:36:TRP:CE2	2:D:80:ASN:HB2	2.55	0.41
1:E:2:TYR:CD2	1:E:97:LEU:HD11	2.50	0.41
1:L:92:ILE:HG23	1:L:97:LEU:HD11	2.01	0.41
2:H:6:GLU:OE1	2:H:6:GLU:N	2.53	0.41
2:H:117:LYS:HG2	2:H:118:GLY:H	1.82	0.41
2:B:98:PHE:N	2:B:98:PHE:CD1	2.79	0.41
2:F:66:ARG:HB3	2:F:82(A):SER:O	2.20	0.41
1:E:108:GLN:HG2	1:E:109:PRO:CD	2.25	0.41
2:H:124:LEU:N	2:H:141:GLY:O	2.47	0.41
1:A:126:GLN:HA	1:A:126:GLN:NE2	2.36	0.41
1:A:185:GLN:O	1:A:188:SER:HB3	2.20	0.41
2:B:49:THR:CG2	2:B:59:TYR:CD2	3.04	0.41
2:B:130:SER:O	2:B:138:ALA:HB2	2.20	0.41
2:D:49:THR:HB	2:D:69:VAL:HG21	2.02	0.41
2:D:95:VAL:HG13	2:D:100(A):TYR:O	2.21	0.41
2:F:47:TRP:NE1	2:F:50:ASN:OD1	2.45	0.41
2:D:90:TYR:O	2:D:106:GLY:HA2	2.21	0.41
2:F:52:ARG:HG2	2:F:52(A):PRO:HD2	2.01	0.41
1:L:138:ASP:O	1:L:172:LYS:HD3	2.21	0.41
1:L:199:GLU:C	1:L:203:SER:H	2.29	0.41
2:H:212:HIS:HD2	2:H:214:PRO:HD2	1.84	0.41
2:B:126:PRO:HB2	2:B:130:SER:HB2	2.02	0.41
1:C:85:ASP:HA	1:C:102:THR:O	2.20	0.41
1:C:135:LEU:HB3	2:D:174:PHE:CZ	2.56	0.41
2:D:49:THR:HG21	2:D:59:TYR:CD2	2.56	0.41
2:F:216:ASN:HD22	2:F:216:ASN:HA	1.73	0.41
1:L:47:VAL:HG12	1:L:58:ILE:HD12	2.02	0.41
1:L:92:ILE:HD11	1:L:95(A):TYR:CD1	2.55	0.41
2:H:34:MET:HB2	2:H:78:LEU:HD13	2.01	0.41
2:B:207:THR:HG23	2:B:222:LYS:HG2	2.02	0.41
1:E:36:TYR:OH	2:F:100(C):PRO:HD2	2.21	0.41
1:E:182:THR:C	1:E:184:GLU:N	2.76	0.41
2:F:34:MET:HB2	2:F:78:LEU:HD13	2.03	0.41
2:F:51:ILE:O	2:F:51:ILE:HG23	2.21	0.41
2:H:34:MET:CB	2:H:78:LEU:HD13	2.50	0.41
1:A:2:TYR:HD2	1:A:97:LEU:HD21	1.86	0.41
1:A:4:LEU:HD12	1:A:98:PHE:C	2.45	0.41
1:A:151:ASP:CG	1:A:189:HIS:HB3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:SER:OG	2:D:217:THR:OG1	2.29	0.41
1:L:133:VAL:HG11	2:H:188:SER:OG	2.20	0.41
1:A:28:LEU:N	1:A:29:PRO:CD	2.84	0.41
1:A:95(A):TYR:HA	1:A:96:PRO:HD2	1.95	0.41
2:B:112:THR:HB	2:B:114:ALA:H	1.86	0.41
2:B:193:VAL:HG11	2:B:206:TYR:CE1	2.56	0.41
2:B:195:SER:HA	2:B:198:LEU:HB2	2.03	0.41
2:D:182:SER:O	2:D:184:LEU:HG	2.20	0.41
1:E:124:GLU:O	1:E:124:GLU:HG2	2.20	0.41
2:F:13:GLN:O	2:F:14:PRO:C	2.64	0.41
1:A:2:TYR:CE2	1:A:97:LEU:CD1	3.03	0.41
1:A:170:ASN:ND2	1:A:172:LYS:HB2	2.36	0.41
1:C:160:GLU:HB3	2:D:177:VAL:CG2	2.50	0.41
2:D:166:LEU:HD23	2:D:167:THR:N	2.35	0.41
2:F:98:PHE:O	2:F:100:ASP:O	2.38	0.41
2:H:87:THR:O	2:H:88:ALA:HB2	2.21	0.40
2:B:112:THR:HG21	2:B:183:GLY:CA	2.51	0.40
2:B:191:VAL:HG22	2:B:193:VAL:HG13	2.03	0.40
1:C:49:TYR:O	1:C:50:GLU:C	2.64	0.40
1:E:95(A):TYR:HA	1:E:96:PRO:HD2	1.83	0.40
1:L:123:GLU:OE2	2:H:221:LYS:HE2	2.22	0.40
2:H:123:PRO:HD3	2:H:221:LYS:HE3	2.03	0.40
2:D:187:LEU:C	2:D:187:LEU:CD1	2.86	0.40
1:L:13:VAL:HG21	1:L:19:ALA:HB2	2.02	0.40
1:L:66:SER:O	1:L:67:SER:HB2	2.22	0.40
2:H:156:SER:O	2:H:208:CYS:HA	2.21	0.40
1:C:2:TYR:CE2	1:C:97:LEU:HD13	2.56	0.40
1:C:6:GLN:OE1	1:C:99:GLY:HA3	2.20	0.40
1:C:145:THR:HB	1:C:197:THR:OG1	2.22	0.40
2:D:40:ALA:O	2:D:41:PRO:C	2.64	0.40
2:F:197:SER:HG	2:F:203:LYS:HE2	1.86	0.40
2:H:96:SER:HB2	2:H:98:PHE:CE1	2.55	0.40
1:A:34:TYR:CD1	1:A:34:TYR:N	2.89	0.40
2:B:198:LEU:HD12	2:B:206:TYR:HE2	1.86	0.40
2:D:29:LEU:HD22	2:D:76:ASN:C	2.47	0.40
1:L:39:ARG:O	1:L:40:SER:C	2.65	0.40
1:A:108:GLN:NE2	1:A:140:TYR:CE1	2.90	0.40
2:B:36:TRP:HA	2:B:91:TYR:O	2.20	0.40
1:C:182:THR:O	1:C:183:PRO:C	2.65	0.40
1:E:36:TYR:HA	1:E:45:VAL:O	2.21	0.40
1:E:94:ASN:OD1	1:E:94:ASN:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:HIS:O	1:E:203:SER:HB2	2.22	0.40
2:F:180:SER:OG	2:F:182:SER:N	2.55	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	207/209 (99%)	184 (89%)	19 (9%)	4 (2%)	6	30
1	C	207/209 (99%)	178 (86%)	24 (12%)	5 (2%)	4	24
1	E	207/209 (99%)	181 (87%)	22 (11%)	4 (2%)	6	30
1	L	207/209 (99%)	182 (88%)	19 (9%)	6 (3%)	3	20
2	B	218/220 (99%)	192 (88%)	22 (10%)	4 (2%)	6	31
2	D	218/220 (99%)	190 (87%)	25 (12%)	3 (1%)	9	36
2	F	218/220 (99%)	190 (87%)	22 (10%)	6 (3%)	4	21
2	H	218/220 (99%)	189 (87%)	23 (11%)	6 (3%)	4	21
All	All	1700/1716 (99%)	1486 (87%)	176 (10%)	38 (2%)	5	26

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	127	CYS
2	D	127	CYS
2	D	183	GLY
2	F	127	CYS
1	L	95	GLY
2	H	100	ASP
2	H	183	GLY
2	B	111	VAL

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Mol	Chain	Res	Type
2	B	127	CYS
2	B	182	SER
2	B	183	GLY
1	E	92	ILE
1	E	110	LYS
2	F	96	SER
2	F	182	SER
1	L	90	SER
2	H	16	GLU
1	A	90	SER
1	C	108	GLN
2	F	165	ALA
1	L	67	SER
1	L	211	PRO
2	H	146	ASP
2	H	182	SER
1	C	67	SER
2	D	182	SER
2	F	146	ASP
1	A	188	SER
1	A	211	PRO
1	C	90	SER
1	E	90	SER
2	F	183	GLY
1	C	142	GLY
1	L	106	VAL
1	E	106	VAL
1	L	142	GLY
1	A	106	VAL
1	C	106	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	177/177 (100%)	169 (96%)	8 (4%)	24 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	177/177 (100%)	169 (96%)	8 (4%)	24	59
1	E	177/177 (100%)	168 (95%)	9 (5%)	21	55
1	L	177/177 (100%)	165 (93%)	12 (7%)	14	45
2	B	191/191 (100%)	178 (93%)	13 (7%)	14	45
2	D	191/191 (100%)	176 (92%)	15 (8%)	11	39
2	F	191/191 (100%)	175 (92%)	16 (8%)	10	37
2	H	191/191 (100%)	176 (92%)	15 (8%)	11	39
All	All	1472/1472 (100%)	1376 (94%)	96 (6%)	15	47

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	11	VAL
1	L	26	ASP
1	L	28	LEU
1	L	92	ILE
1	L	97	LEU
1	L	105	SER
1	L	145	THR
1	L	156	LYS
1	L	163	THR
1	L	164	PRO
1	L	176	SER
1	L	193	SER
2	H	1	GLU
2	H	19	LYS
2	H	33	TYR
2	H	64	LYS
2	H	69	VAL
2	H	84	VAL
2	H	85	GLU
2	H	98	PHE
2	H	149	PRO
2	H	151	PRO
2	H	152	VAL
2	H	178	LEU
2	H	187	LEU
2	H	191	VAL
2	H	216	ASN
1	A	26	ASP

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Mol	Chain	Res	Type
1	A	28	LEU
1	A	89	TYR
1	A	94	ASN
1	A	137	SER
1	A	145	THR
1	A	163	THR
1	A	176	SER
2	B	1	GLU
2	B	19	LYS
2	B	33	TYR
2	B	64	LYS
2	B	68	THR
2	B	69	VAL
2	B	76	ASN
2	B	84	VAL
2	B	85	GLU
2	B	98	PHE
2	B	152	VAL
2	B	191	VAL
2	B	216	ASN
1	C	26	ASP
1	C	28	LEU
1	C	79	GLN
1	C	94	ASN
1	C	97	LEU
1	C	145	THR
1	C	164	PRO
1	C	176	SER
2	D	1	GLU
2	D	19	LYS
2	D	33	TYR
2	D	64	LYS
2	D	68	THR
2	D	69	VAL
2	D	76	ASN
2	D	84	VAL
2	D	85	GLU
2	D	98	PHE
2	D	112	THR
2	D	152	VAL
2	D	191	VAL
2	D	209	ASN

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Mol	Chain	Res	Type
2	D	216	ASN
1	E	26	ASP
1	E	28	LEU
1	E	34	TYR
1	E	94	ASN
1	E	97	LEU
1	E	145	THR
1	E	163	THR
1	E	164	PRO
1	E	176	SER
2	F	1	GLU
2	F	16	GLU
2	F	19	LYS
2	F	33	TYR
2	F	64	LYS
2	F	68	THR
2	F	69	VAL
2	F	76	ASN
2	F	84	VAL
2	F	85	GLU
2	F	98	PHE
2	F	112	THR
2	F	151	PRO
2	F	152	VAL
2	F	191	VAL
2	F	216	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	171	ASN
1	L	198	HIS
2	H	13	GLN
2	H	82(C)	GLN
2	H	162	ASN
2	H	179	GLN
2	H	216	ASN
1	A	79	GLN
1	A	126	GLN
2	B	13	GLN
2	B	31	ASN
2	B	82(C)	GLN

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Mol	Chain	Res	Type
2	B	179	GLN
2	B	216	ASN
1	C	42	GLN
1	C	79	GLN
1	C	108	GLN
1	C	195	GLN
2	D	31	ASN
2	D	39	GLN
2	D	82(C)	GLN
2	D	105	GLN
2	D	162	ASN
2	D	179	GLN
2	D	216	ASN
1	E	6	GLN
1	E	79	GLN
1	E	108	GLN
1	E	198	HIS
2	F	13	GLN
2	F	31	ASN
2	F	82(C)	GLN
2	F	162	ASN
2	F	179	GLN
2	F	216	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 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	RBF	F	204	-	29,29,29	2.03	11 (37%)	42,43,43	2.18	14 (33%)
3	RBF	H	201	-	29,29,29	2.10	11 (37%)	42,43,43	2.15	15 (35%)
3	RBF	D	228	-	29,29,29	2.09	11 (37%)	42,43,43	2.17	14 (33%)
3	RBF	B	202	-	29,29,29	1.99	11 (37%)	42,43,43	2.13	14 (33%)

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	RBF	F	204	-	-	2/14/14/14	0/3/3/3
3	RBF	H	201	-	-	2/14/14/14	0/3/3/3
3	RBF	D	228	-	-	2/14/14/14	0/3/3/3
3	RBF	B	202	-	-	2/14/14/14	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	201	RBF	C9A-N10	4.76	1.49	1.41
3	D	228	RBF	C9A-N10	4.40	1.48	1.41
3	F	204	RBF	C9A-N10	4.17	1.48	1.41
3	H	201	RBF	C2'-C3'	-4.00	1.46	1.53
3	B	202	RBF	C9A-N10	3.97	1.48	1.41
3	F	204	RBF	C6-C5A	3.94	1.46	1.40
3	D	228	RBF	C5'-C4'	3.87	1.61	1.52
3	H	201	RBF	C10-N1	3.56	1.40	1.33
3	F	204	RBF	C5'-C4'	3.53	1.60	1.52
3	D	228	RBF	C6-C5A	3.52	1.45	1.40
3	B	202	RBF	C5'-C4'	3.37	1.60	1.52
3	H	201	RBF	C6-C5A	3.31	1.45	1.40
3	B	202	RBF	C2'-C3'	-3.29	1.47	1.53
3	D	228	RBF	C9-C9A	3.22	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	RBF	C6-C5A	3.22	1.44	1.40
3	F	204	RBF	C9-C9A	3.18	1.44	1.39
3	F	204	RBF	C8M-C8	3.11	1.56	1.51
3	B	202	RBF	C8M-C8	3.08	1.56	1.51
3	H	201	RBF	C9-C9A	3.04	1.44	1.39
3	D	228	RBF	C1'-C2'	3.02	1.56	1.52
3	D	228	RBF	C8M-C8	2.97	1.56	1.51
3	B	202	RBF	C10-N1	2.92	1.39	1.33
3	H	201	RBF	C8M-C8	2.89	1.56	1.51
3	D	228	RBF	C10-N1	2.86	1.39	1.33
3	F	204	RBF	C8-C7	2.79	1.47	1.40
3	B	202	RBF	C9-C9A	2.77	1.44	1.39
3	D	228	RBF	C2'-C3'	-2.62	1.48	1.53
3	D	228	RBF	C8-C7	2.57	1.47	1.40
3	F	204	RBF	C10-N1	2.57	1.38	1.33
3	H	201	RBF	C5'-C4'	2.57	1.58	1.52
3	H	201	RBF	C8-C7	2.56	1.47	1.40
3	B	202	RBF	C8-C7	2.55	1.47	1.40
3	F	204	RBF	C2'-C3'	-2.44	1.49	1.53
3	D	228	RBF	C4A-C4	2.43	1.53	1.44
3	H	201	RBF	O4-C4	-2.37	1.19	1.23
3	F	204	RBF	O4-C4	-2.27	1.19	1.23
3	D	228	RBF	C9A-C5A	2.27	1.44	1.41
3	B	202	RBF	C1'-C2'	2.24	1.55	1.52
3	F	204	RBF	C1'-C2'	2.19	1.55	1.52
3	B	202	RBF	C4A-C4	2.15	1.52	1.44
3	B	202	RBF	O2-C2	-2.11	1.20	1.24
3	H	201	RBF	C9A-C5A	2.10	1.44	1.41
3	H	201	RBF	C4'-C3'	-2.10	1.49	1.53
3	F	204	RBF	C9A-C5A	2.10	1.44	1.41

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	201	RBF	C5'-C4'-C3'	-4.96	102.06	112.17
3	B	202	RBF	C5'-C4'-C3'	-4.75	102.48	112.17
3	F	204	RBF	C5'-C4'-C3'	-4.65	102.70	112.17
3	F	204	RBF	O2-C2-N3	4.64	127.49	118.58
3	D	228	RBF	O2-C2-N3	4.60	127.41	118.58
3	F	204	RBF	O2'-C2'-C3'	-4.47	98.79	109.25
3	H	201	RBF	O2-C2-N3	4.46	127.14	118.58
3	B	202	RBF	O2-C2-N3	4.46	127.14	118.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	228	RBF	C5'-C4'-C3'	-4.46	103.09	112.17
3	D	228	RBF	O2'-C2'-C3'	-4.44	98.86	109.25
3	H	201	RBF	O2'-C2'-C3'	-4.40	98.95	109.25
3	H	201	RBF	C9-C8-C7	4.29	125.99	119.69
3	F	204	RBF	C9-C8-C7	4.24	125.91	119.69
3	D	228	RBF	C9-C8-C7	4.23	125.90	119.69
3	B	202	RBF	C9-C8-C7	4.21	125.87	119.69
3	F	204	RBF	O4'-C4'-C3'	4.12	118.89	109.25
3	B	202	RBF	O2'-C2'-C3'	-4.08	99.70	109.25
3	D	228	RBF	O4'-C4'-C3'	4.01	118.64	109.25
3	B	202	RBF	O4'-C4'-C3'	3.97	118.53	109.25
3	H	201	RBF	O4'-C4'-C3'	3.91	118.39	109.25
3	D	228	RBF	C10-N1-C2	3.40	124.21	116.85
3	F	204	RBF	C10-N1-C2	3.36	124.12	116.85
3	B	202	RBF	C10-N1-C2	3.19	123.75	116.85
3	D	228	RBF	C4A-C10-N10	3.18	121.04	116.48
3	F	204	RBF	C4A-C10-N10	3.08	120.90	116.48
3	H	201	RBF	C10-N1-C2	3.06	123.48	116.85
3	B	202	RBF	C6-C5A-C9A	3.03	123.22	119.05
3	B	202	RBF	C9A-C9-C8	-3.01	113.16	119.22
3	B	202	RBF	C5A-C6-C7	-2.95	115.36	120.83
3	D	228	RBF	C9A-C9-C8	-2.95	113.29	119.22
3	H	201	RBF	C9A-C9-C8	-2.95	113.29	119.22
3	B	202	RBF	O2-C2-N1	-2.88	117.02	121.80
3	F	204	RBF	C5A-C6-C7	-2.87	115.50	120.83
3	D	228	RBF	C5A-C6-C7	-2.86	115.52	120.83
3	H	201	RBF	C6-C5A-C9A	2.86	122.98	119.05
3	H	201	RBF	C5A-C6-C7	-2.86	115.53	120.83
3	F	204	RBF	C9A-C9-C8	-2.83	113.53	119.22
3	B	202	RBF	C4A-C10-N10	2.82	120.52	116.48
3	D	228	RBF	C1'-C2'-C3'	2.81	117.27	109.66
3	F	204	RBF	C6-C5A-C9A	2.76	122.84	119.05
3	F	204	RBF	C1'-C2'-C3'	2.75	117.11	109.66
3	D	228	RBF	O2-C2-N1	-2.74	117.25	121.80
3	F	204	RBF	O2-C2-N1	-2.68	117.35	121.80
3	D	228	RBF	C6-C5A-C9A	2.67	122.71	119.05
3	H	201	RBF	C4A-C10-N10	2.64	120.27	116.48
3	H	201	RBF	O2-C2-N1	-2.62	117.45	121.80
3	H	201	RBF	C1'-C2'-C3'	2.45	116.30	109.66
3	B	202	RBF	C1'-C2'-C3'	2.39	116.14	109.66
3	B	202	RBF	C8M-C8-C9	-2.27	115.57	119.57
3	F	204	RBF	C8M-C8-C9	-2.24	115.63	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	RBF	C6-C5A-N5	-2.19	114.80	118.44
3	D	228	RBF	C8M-C8-C9	-2.16	115.76	119.57
3	H	201	RBF	O5'-C5'-C4'	-2.10	106.74	111.16
3	H	201	RBF	C8M-C8-C9	-2.07	115.93	119.57
3	F	204	RBF	N3-C2-N1	-2.04	115.16	119.50
3	H	201	RBF	C6-C5A-N5	-2.03	115.08	118.44
3	D	228	RBF	C4-N3-C2	2.02	129.23	125.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	228	RBF	C3'-C4'-C5'-O5'
3	F	204	RBF	C3'-C4'-C5'-O5'
3	D	228	RBF	O4'-C4'-C5'-O5'
3	H	201	RBF	C3'-C4'-C5'-O5'
3	B	202	RBF	C3'-C4'-C5'-O5'
3	H	201	RBF	O4'-C4'-C5'-O5'
3	F	204	RBF	O4'-C4'-C5'-O5'
3	B	202	RBF	O4'-C4'-C5'-O5'

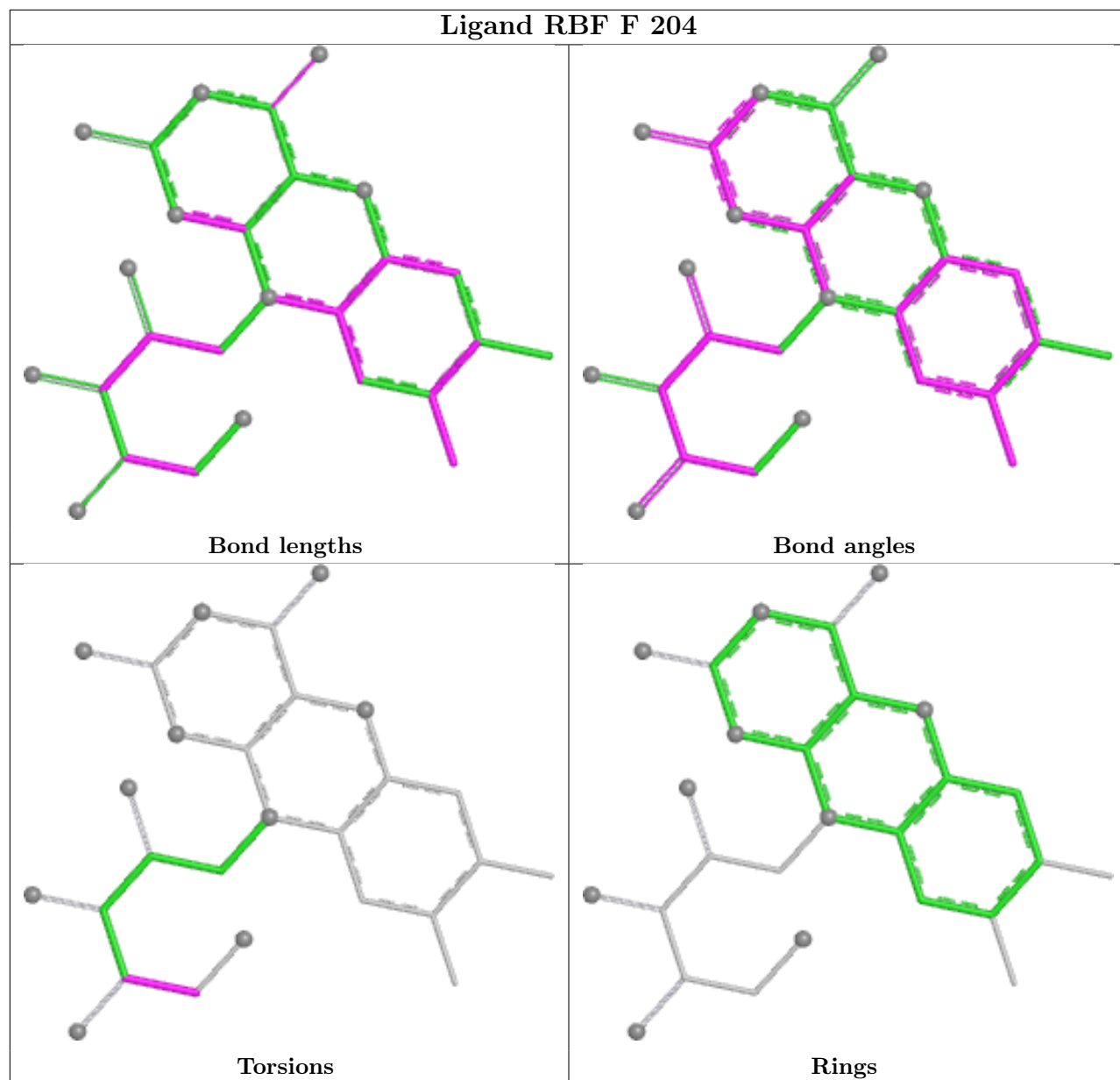
There are no ring outliers.

4 monomers are involved in 5 short contacts:

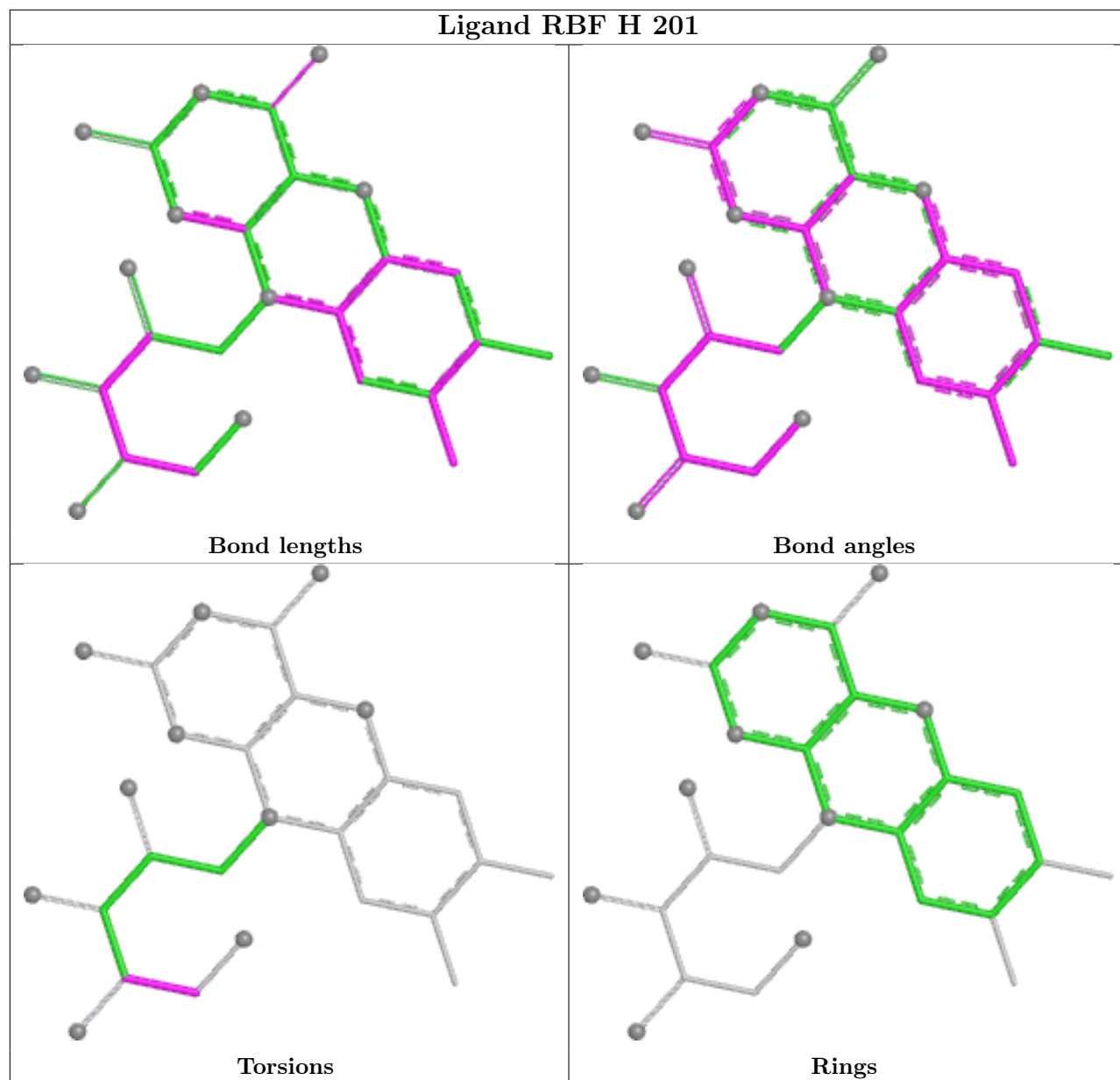
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	204	RBF	1	0
3	H	201	RBF	2	0
3	D	228	RBF	1	0
3	B	202	RBF	1	0

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.

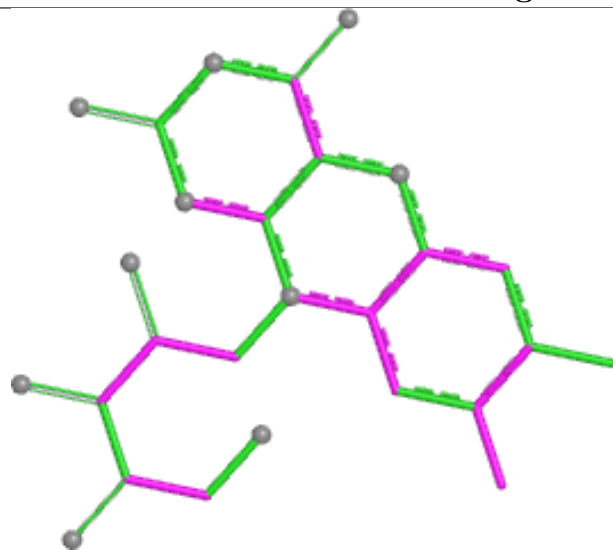
Ligand RBF F 204



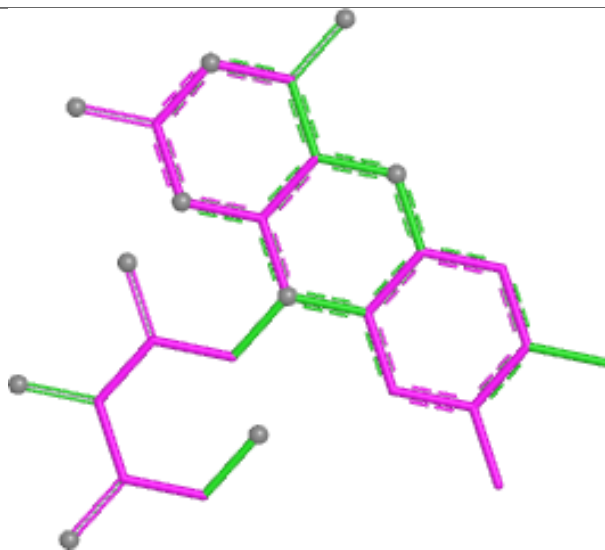
Ligand RBF H 201



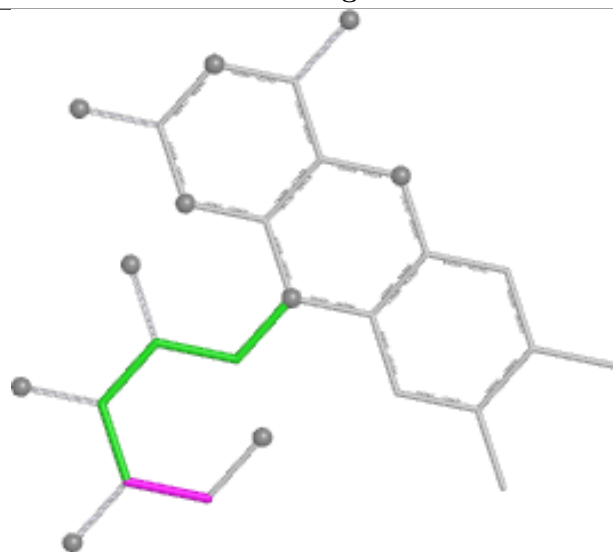
Ligand RBF D 228



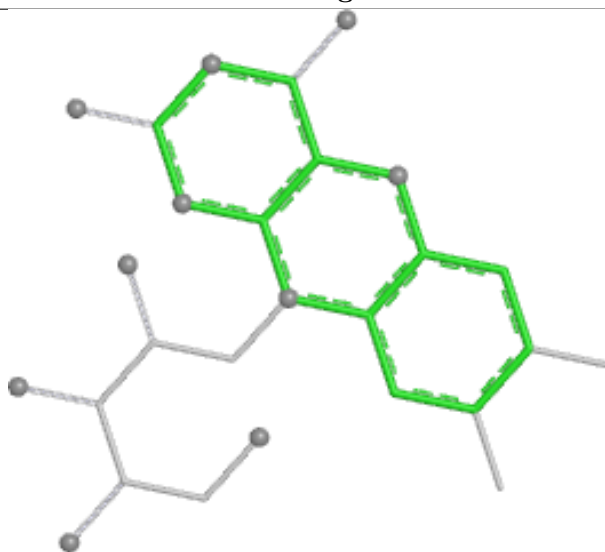
Bond lengths



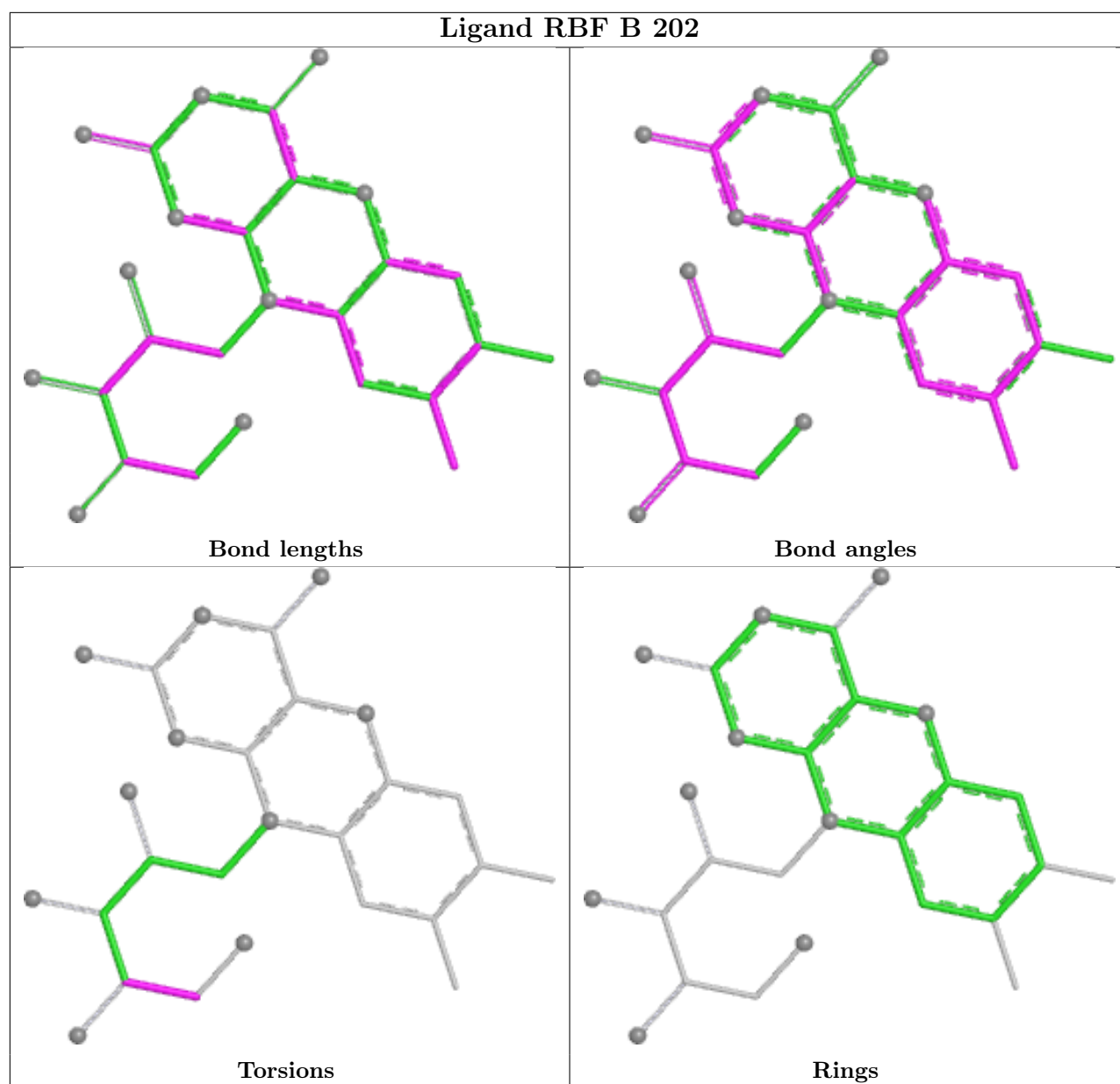
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	209/209 (100%)	-0.06	0 100 100	37, 60, 80, 89	0
1	C	209/209 (100%)	-0.14	0 100 100	29, 50, 71, 85	0
1	E	209/209 (100%)	0.14	1 (0%) 87 72	31, 61, 84, 92	0
1	L	209/209 (100%)	0.47	8 (3%) 44 24	41, 70, 95, 106	0
2	B	220/220 (100%)	0.19	6 (2%) 56 33	40, 64, 118, 138	0
2	D	220/220 (100%)	-0.06	5 (2%) 61 38	30, 48, 116, 140	0
2	F	220/220 (100%)	0.06	3 (1%) 73 51	33, 56, 119, 138	0
2	H	220/220 (100%)	0.19	8 (3%) 46 26	31, 60, 120, 139	0
All	All	1716/1716 (100%)	0.10	31 (1%) 67 44	29, 59, 97, 140	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	133	THR	4.2
2	B	133	THR	3.6
2	F	133	THR	3.5
1	L	196	VAL	3.1
2	H	192	THR	2.9
2	D	130	SER	2.8
2	B	136	SER	2.8
2	D	198	LEU	2.7
2	B	130	SER	2.7
2	B	198	LEU	2.5
2	D	134	SER	2.5
1	L	146	VAL	2.5
2	F	136	SER	2.4
2	H	133	THR	2.4
1	L	106	VAL	2.4
2	H	179	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	137	THR	2.3
1	L	13	VAL	2.3
2	H	198	LEU	2.3
2	F	198	LEU	2.3
2	H	102	PHE	2.2
2	H	130	SER	2.2
1	L	112	ALA	2.2
2	D	194	PRO	2.2
1	L	205	VAL	2.1
1	L	197	THR	2.1
2	B	205	THR	2.1
1	L	109	PRO	2.1
1	E	200	GLY	2.1
2	B	194	PRO	2.1
2	H	183	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

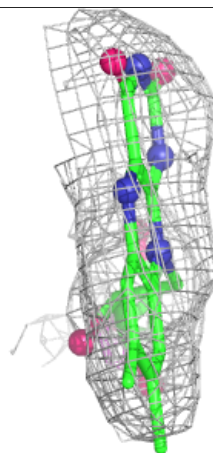
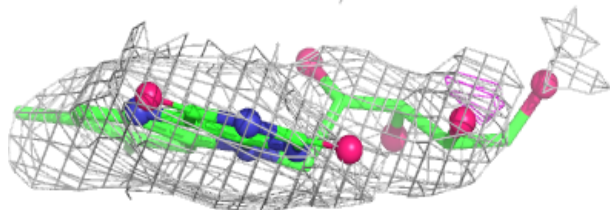
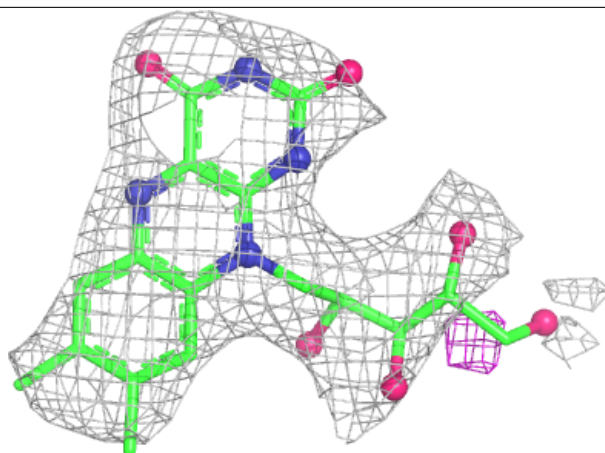
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	RBF	D	228	27/27	0.88	0.14	66,74,89,89	0
3	RBF	B	202	27/27	0.90	0.10	55,61,63,65	0
3	RBF	H	201	27/27	0.90	0.12	50,54,58,59	0
3	RBF	F	204	27/27	0.91	0.12	70,76,82,83	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.

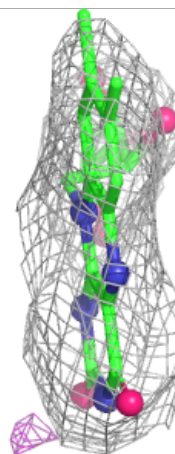
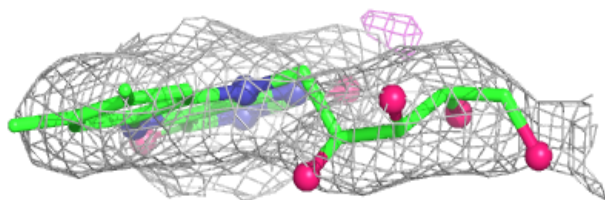
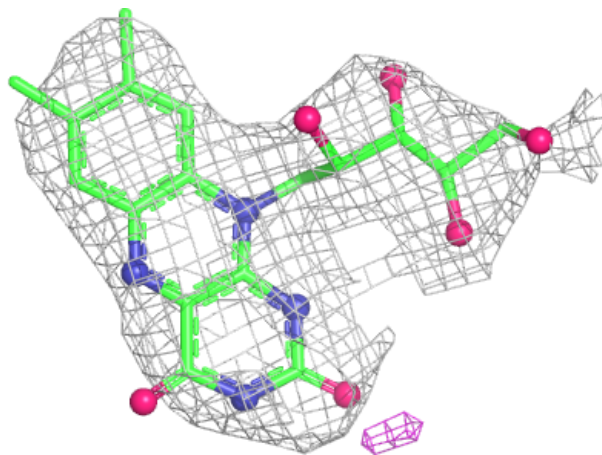
Electron density around RBF D 228:

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



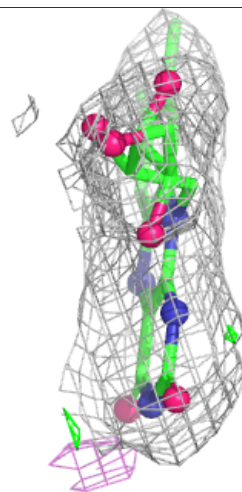
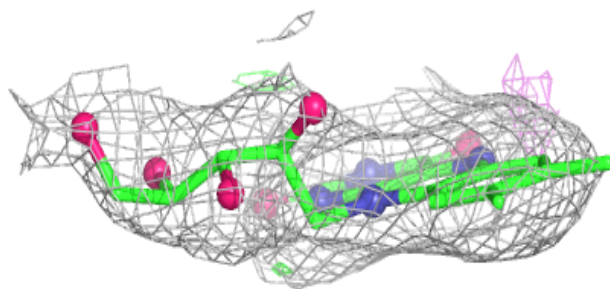
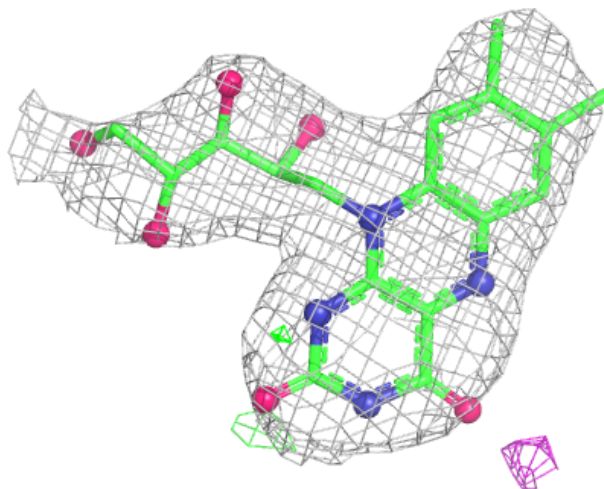
Electron density around RBF B 202:

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



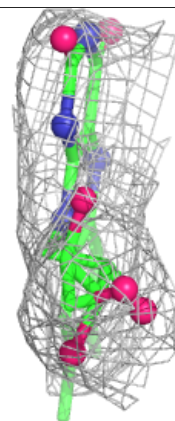
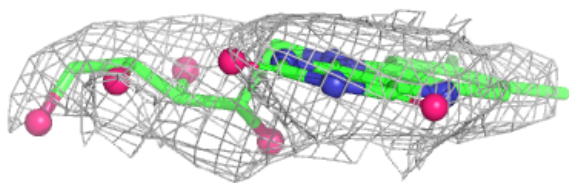
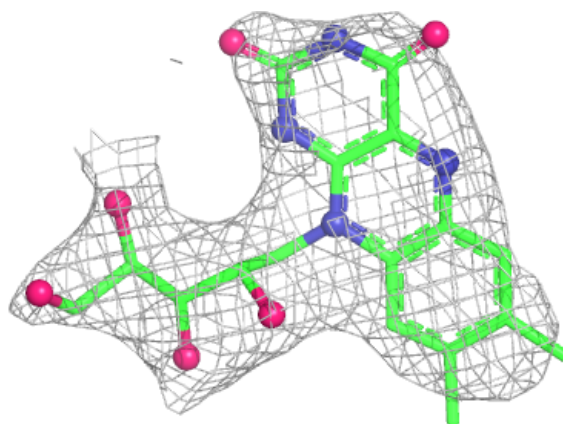
Electron density around RBF H 201:

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



Electron density around RBF F 204:

$2mF_o - DF_c$ (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.