



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:27 AM UTC

PDB ID : 1A4K / pdb_00001a4k
Title : DIELS ALDER CATALYTIC ANTIBODY WITH TRANSITION STATE ANALOGUE
Authors : Spiller, B.W.; Romesburg, F.E.; Schultz, P.G.; Stevens, R.C.
Deposited on : 1998-01-30
Resolution : 2.40 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

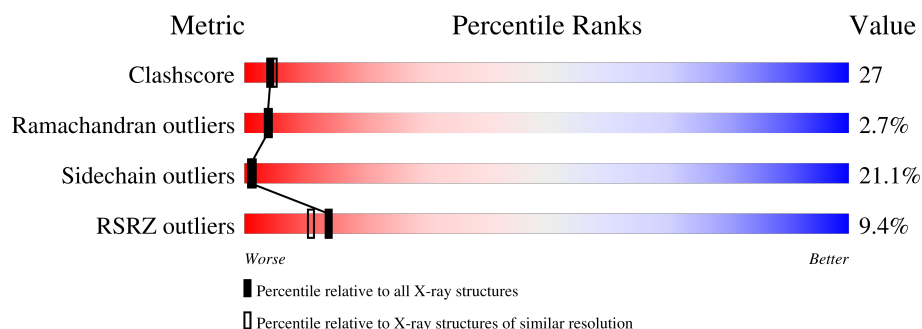
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	217	4% 56% 37% 6%
1	L	217	6% 48% 41% 8% .
2	B	219	13% 38% 44% 17%
2	H	219	16% 47% 39% 12% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6921 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 ANTIBODY FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	217	Total	C	N	O	S	0	0	0
			1670	1049	284	332	5			
1	A	216	Total	C	N	O	S	0	0	0
			1665	1047	283	330	5			

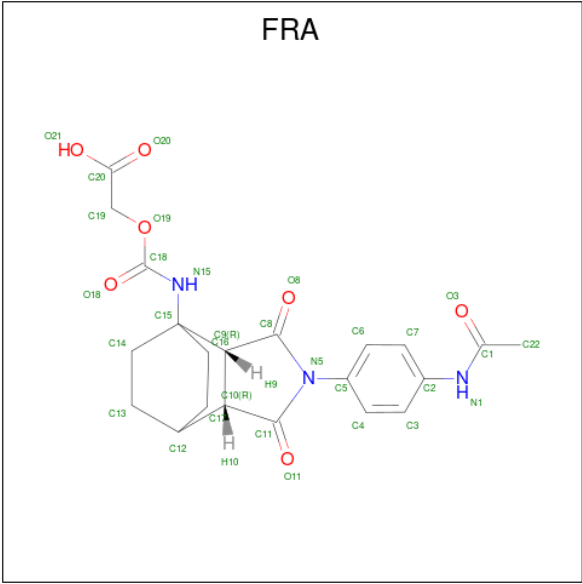
- Molecule 2 is a protein called ANTIBODY FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1645	1046	271	322	6			
2	B	219	Total	C	N	O	S	0	0	0
			1662	1056	273	327	6			

- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	2	Total	Cd	0	0
			2	2		
3	A	2	Total	Cd	0	0
			2	2		

- Molecule 4 is [4-(4-ACETYLAMINO-PHENYL)-3,5-DIOXO-4-AZA-TRICYCLO[5.2.2.0 2,6]UNDEC-1-YLCARBAMOXYLOXY]-ACETIC ACID (CCD ID: FRA) (formula: C₂₁H₂₃N₃O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			31	21	3	7		
4	B	1	Total	C	N	O	0	0
			31	21	3	7		

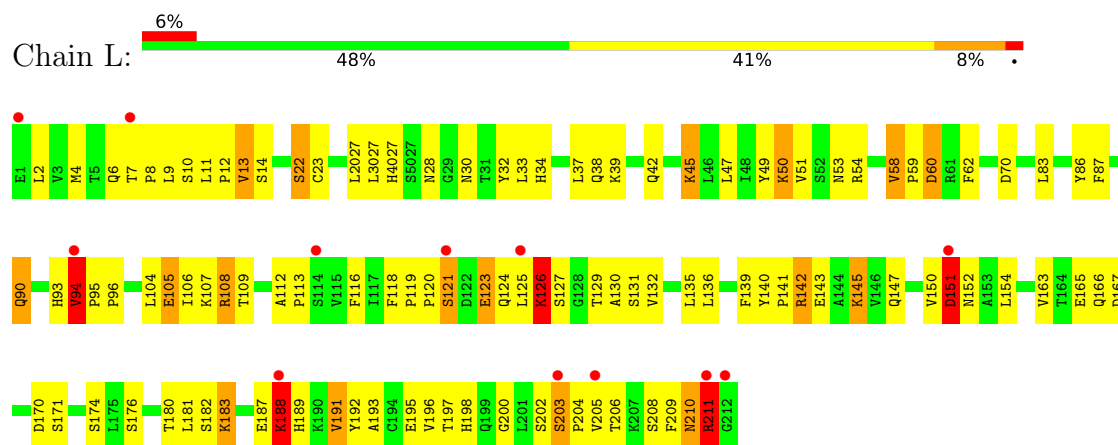
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	50	Total	O	0	0
			50	50		
5	H	51	Total	O	0	0
			51	51		
5	A	69	Total	O	0	0
			69	69		
5	B	43	Total	O	0	0
			43	43		

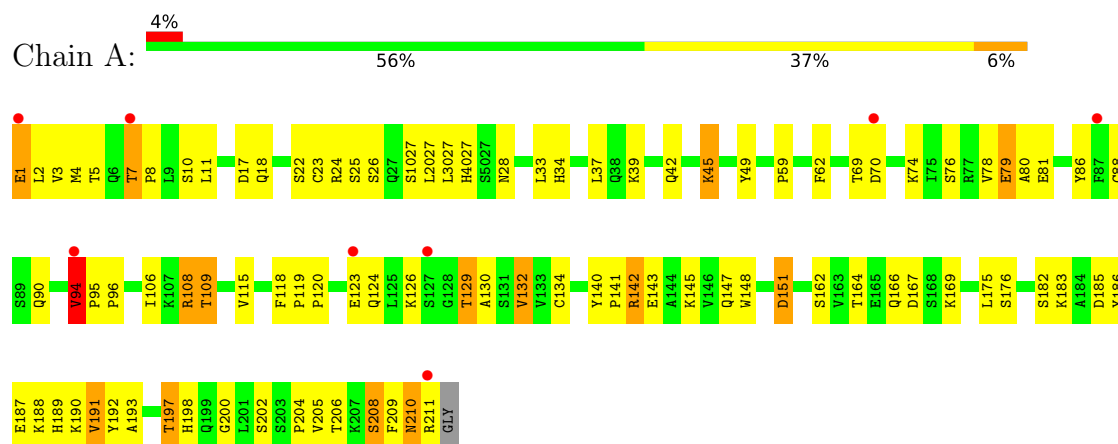
3 Residue-property plots [i](#)

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

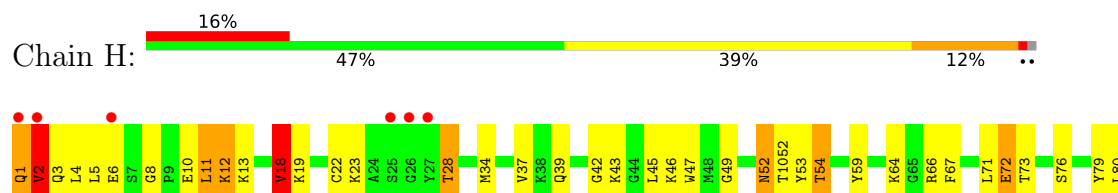
• Molecule 1: ANTIBODY FAB

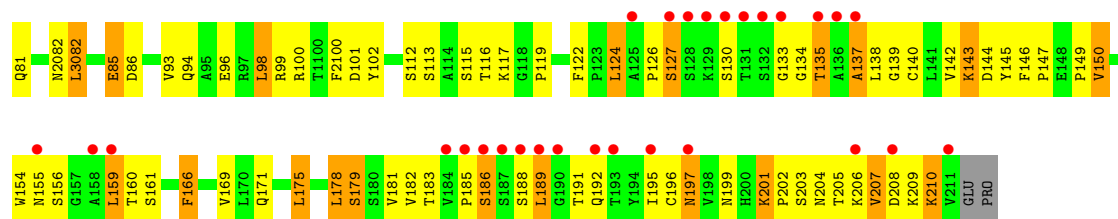


• Molecule 1: ANTIBODY FAB

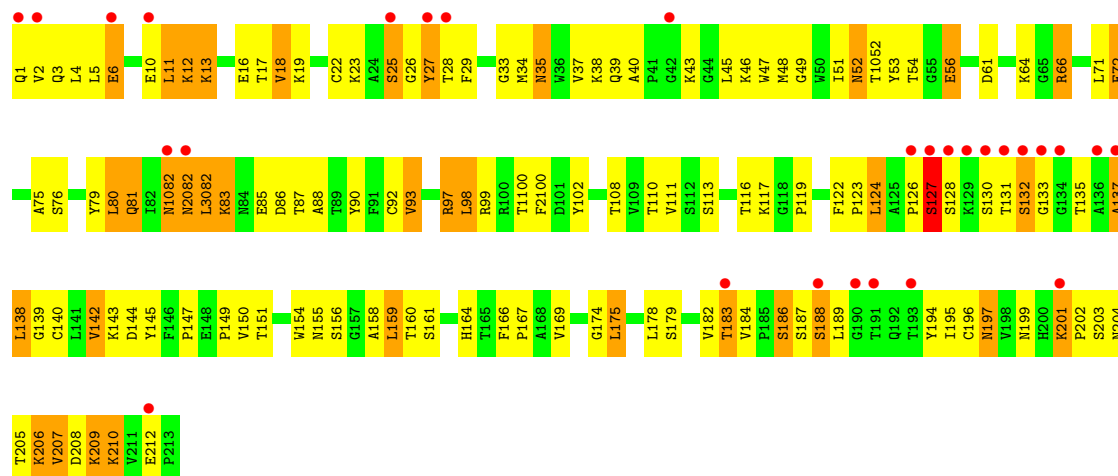


• Molecule 2: ANTIBODY FAB





• Molecule 2: ANTIBODY FAB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.32Å 96.82Å 172.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.40) 98.0 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.72 (at 2.41Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.211 , 0.291 0.231 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6921	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.42% 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: CD, FRA

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	0.45	0/1702	0.96	7/2310 (0.3%)
1	L	0.43	0/1707	0.92	7/2315 (0.3%)
2	B	0.43	0/1705	0.95	6/2322 (0.3%)
2	H	0.45	0/1687	0.96	8/2298 (0.3%)
All	All	0.44	0/6801	0.94	28/9245 (0.3%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	151	ASP	N-CA-C	-8.02	104.00	113.38
1	A	79	GLU	N-CA-C	7.66	122.14	111.56
2	B	97	ARG	N-CA-C	7.46	119.06	111.07
2	H	143	LYS	N-CA-C	6.82	119.30	109.14
1	A	151	ASP	N-CA-C	-6.80	104.57	112.86
2	B	143	LYS	N-CA-C	6.70	119.90	109.52
2	H	101	ASP	N-CA-C	6.42	117.94	111.07
2	B	93	VAL	N-CA-C	6.40	117.07	108.11
1	L	94	VAL	CA-C-N	-6.39	113.80	120.38
1	L	94	VAL	C-N-CA	-6.39	113.80	120.38
2	B	33	GLY	N-CA-C	-6.27	100.03	111.25
2	H	8	GLY	CA-C-N	6.02	125.98	119.78
2	H	8	GLY	C-N-CA	6.02	125.98	119.78
1	A	115	VAL	N-CA-C	5.93	117.12	108.58
2	H	98	LEU	N-CA-C	5.89	117.70	111.28
1	L	53	ASN	N-CA-C	5.83	117.79	108.41
2	H	18	VAL	CB-CA-C	-5.80	102.55	110.90
1	A	94	VAL	CA-C-N	-5.65	114.56	120.38
1	A	94	VAL	C-N-CA	-5.65	114.56	120.38
1	L	58	VAL	N-CA-C	5.53	113.34	107.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	GLU	N-CA-C	-5.49	106.56	113.20
1	A	191	VAL	N-CA-C	5.33	115.99	108.36
2	H	160	THR	N-CA-C	-5.32	108.05	114.75
1	L	51	VAL	N-CA-C	5.28	120.31	109.34
2	H	166	PHE	N-CA-C	5.18	117.30	110.36
2	B	174	GLY	N-CA-C	-5.17	108.14	115.43
1	L	93	HIS	N-CA-C	5.14	118.11	110.14
2	B	83	LYS	N-CA-C	-5.05	102.99	110.46

There are no chirality outliers.

There are no planarity outliers.

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	1665	0	1638	75	0
1	L	1670	0	1641	94	0
2	B	1662	0	1628	114	0
2	H	1645	0	1615	96	0
3	A	2	0	0	0	0
3	L	2	0	0	0	0
4	B	31	0	21	2	0
4	H	31	0	22	1	0
5	A	69	0	0	4	0
5	B	43	0	0	2	0
5	H	51	0	0	4	0
5	L	50	0	0	2	0
All	All	6921	0	6565	360	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 27.

All (360) 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:L:94:VAL:HB	1:L:95:PRO:HD3	1.30	1.10
1:L:94:VAL:HB	1:L:95:PRO:CD	1.91	1.00
2:H:18:VAL:HG22	2:H:3082:LEU:HD21	1.43	0.99
1:L:193:ALA:HB2	1:L:208:SER:HB3	1.50	0.93
1:A:7:THR:HB	1:A:8:PRO:HD3	1.49	0.92
1:L:197:THR:HG22	1:L:204:PRO:HB3	1.50	0.92
1:A:94:VAL:HB	1:A:95:PRO:HD3	1.52	0.90
2:B:52:ASN:HD22	2:B:53:TYR:H	1.19	0.90
2:B:18:VAL:HG22	2:B:3082:LEU:HD21	1.54	0.90
1:L:118:PHE:CZ	2:H:137:ALA:HB1	2.09	0.88
1:L:7:THR:HB	1:L:8:PRO:HD3	1.60	0.83
2:H:156:SER:H	2:H:197:ASN:HD21	1.27	0.82
2:B:52:ASN:ND2	2:B:53:TYR:H	1.78	0.81
1:L:193:ALA:CB	1:L:208:SER:HB3	2.11	0.80
2:B:52:ASN:ND2	2:B:54:THR:H	1.79	0.80
1:A:210:ASN:HD21	1:A:211:ARG:HE	1.29	0.80
2:B:127:SER:HB3	2:B:130:SER:HB3	1.63	0.80
1:L:123:GLU:HA	1:L:126:LYS:HD2	1.65	0.79
1:L:145:LYS:HD3	1:L:147:GLN:HG3	1.65	0.78
2:H:85:GLU:H	2:H:85:GLU:CD	1.91	0.78
2:H:143:LYS:HE3	2:H:171:GLN:HE22	1.46	0.78
1:A:124:GLN:HG3	2:B:122:PHE:CE2	2.19	0.77
1:L:142:ARG:NH1	1:L:163:VAL:HG11	2.00	0.76
1:L:2027:LEU:HD22	1:L:90:GLN:HG3	1.68	0.76
2:B:156:SER:H	2:B:197:ASN:HD21	1.33	0.76
1:A:120:PRO:HG3	1:A:130:ALA:HB1	1.67	0.76
2:B:52:ASN:HD21	2:B:53:TYR:HB3	1.49	0.75
2:H:52:ASN:ND2	2:H:54:THR:H	1.84	0.75
1:L:106:ILE:H	1:L:166:GLN:HE22	1.31	0.75
2:H:28:THR:HG23	2:H:94:GLN:HE22	1.52	0.74
2:H:156:SER:N	2:H:197:ASN:HD21	1.85	0.74
2:H:1:GLN:HG2	2:H:3:GLN:HB3	1.68	0.73
2:H:100:ARG:HG2	4:H:3083:FRA:H161	1.69	0.73
1:L:83:LEU:HD21	1:L:106:ILE:HG12	1.70	0.72
1:A:4027:HIS:HD2	1:A:28:ASN:H	1.36	0.72
1:A:94:VAL:HB	1:A:95:PRO:CD	2.19	0.72
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.71	0.72
1:A:185:ASP:HA	1:A:188:LYS:HG2	1.71	0.72
2:B:3:GLN:HA	2:B:25:SER:HB3	1.72	0.72
2:B:210:LYS:HD3	2:B:212:GLU:HG2	1.72	0.72
1:A:2027:LEU:HD22	1:A:90:GLN:HG3	1.73	0.70
2:H:116:THR:HG21	2:H:202:PRO:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:VAL:HG11	2:B:2100:PHE:HB3	1.74	0.69
2:H:18:VAL:CG2	2:H:3082:LEU:HD21	2.21	0.69
1:L:34:HIS:CD2	1:L:50:LYS:H	2.09	0.69
2:H:52:ASN:HD22	2:H:53:TYR:H	1.40	0.68
1:A:198:HIS:CD2	1:A:200:GLY:H	2.12	0.68
2:B:123:PRO:HD3	2:B:209:LYS:HE2	1.76	0.67
1:A:210:ASN:CG	1:A:211:ARG:H	1.99	0.67
1:A:188:LYS:HG3	1:A:189:HIS:CD2	2.30	0.67
2:B:4:LEU:HD22	2:B:22:CYS:SG	2.35	0.67
1:A:151:ASP:CG	1:A:189:HIS:HD1	2.02	0.66
2:B:66:ARG:NH2	2:B:86:ASP:OD2	2.26	0.66
2:H:127:SER:HB3	2:H:130:SER:HB3	1.77	0.66
2:H:42:GLY:O	2:H:43:LYS:HD3	1.96	0.66
1:A:4:MET:HE3	1:A:23:CYS:SG	2.34	0.66
1:L:96:PRO:HD2	2:H:47:TRP:CE3	2.31	0.66
2:B:203:SER:HG	2:B:205:THR:HG1	1.41	0.66
1:L:151:ASP:CG	1:L:189:HIS:HD1	2.03	0.66
2:B:119:PRO:HD2	2:B:205:THR:HG21	1.78	0.66
1:A:185:ASP:HB3	1:A:188:LYS:HE3	1.77	0.65
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.78	0.65
1:L:39:LYS:H	1:L:45:LYS:NZ	1.94	0.65
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.29	0.65
2:H:178:LEU:HD12	2:H:179:SER:N	2.11	0.65
1:L:39:LYS:HB2	1:L:42:GLN:HE21	1.62	0.65
1:A:118:PHE:CZ	2:B:137:ALA:HB1	2.31	0.65
1:L:34:HIS:HD2	1:L:50:LYS:H	1.43	0.65
2:H:1:GLN:C	2:H:2:VAL:HG23	2.22	0.65
1:L:4:MET:HE3	1:L:23:CYS:SG	2.37	0.64
2:H:11:LEU:C	2:H:12:LYS:HG2	2.23	0.64
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.80	0.64
1:A:49:TYR:CE1	2:B:99:ARG:HD2	2.33	0.63
2:B:39:GLN:HB2	2:B:45:LEU:HD23	1.79	0.63
1:L:39:LYS:HB2	1:L:42:GLN:NE2	2.14	0.63
1:A:37:LEU:HD13	1:A:86:TYR:CZ	2.34	0.63
2:H:85:GLU:CD	2:H:85:GLU:N	2.57	0.62
1:L:108:ARG:HG2	1:L:171:SER:HB2	1.80	0.62
1:L:211:ARG:NH1	1:L:211:ARG:HG2	2.13	0.62
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.35	0.62
1:L:106:ILE:H	1:L:166:GLN:NE2	1.96	0.62
1:A:2:LEU:HD21	1:A:25:SER:HB2	1.82	0.62
1:L:94:VAL:CB	1:L:95:PRO:HD3	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:SER:HB2	2:H:130:SER:O	2.00	0.62
2:B:61:ASP:HA	2:B:64:LYS:HD2	1.81	0.62
2:H:28:THR:CG2	2:H:94:GLN:HE22	2.13	0.61
2:H:52:ASN:ND2	2:H:53:TYR:H	1.98	0.61
2:B:48:MET:HE1	2:B:80:LEU:HD11	1.82	0.61
1:L:112:ALA:HB2	1:L:200:GLY:O	2.00	0.61
2:B:117:LYS:HD3	2:B:144:ASP:O	2.00	0.61
2:H:116:THR:HG22	2:H:203:SER:HB3	1.83	0.61
1:A:210:ASN:CG	1:A:211:ARG:N	2.59	0.61
2:H:28:THR:HG23	2:H:94:GLN:NE2	2.16	0.60
2:H:126:PRO:HA	2:H:137:ALA:HB3	1.82	0.60
2:H:1052:THR:HA	2:H:71:LEU:HD11	1.82	0.60
2:B:4:LEU:HB2	2:B:102:TYR:HE2	1.66	0.60
2:B:27:TYR:C	2:B:29:PHE:H	2.09	0.60
2:B:72:GLU:HB2	2:B:79:TYR:HE2	1.66	0.60
1:L:143:GLU:CD	1:L:143:GLU:H	2.10	0.59
2:B:1052:THR:HA	2:B:71:LEU:HD11	1.82	0.59
1:L:197:THR:HG22	1:L:204:PRO:CB	2.29	0.59
1:L:94:VAL:CB	1:L:95:PRO:CD	2.77	0.59
1:A:7:THR:CB	1:A:8:PRO:HD3	2.28	0.58
1:A:141:PRO:O	1:A:198:HIS:HE1	1.85	0.58
1:L:151:ASP:OD2	1:L:189:HIS:ND1	2.35	0.58
1:A:198:HIS:HD2	1:A:200:GLY:H	1.49	0.58
2:B:1082:ASN:O	2:B:2082:ASN:HB2	2.04	0.58
2:B:156:SER:N	2:B:197:ASN:HD21	1.99	0.58
1:L:12:PRO:HB3	1:L:105:GLU:HG2	1.85	0.58
2:B:1:GLN:NE2	2:B:25:SER:HB2	2.19	0.58
1:L:37:LEU:HD13	1:L:86:TYR:CZ	2.38	0.58
2:H:52:ASN:HD21	2:H:53:TYR:HB3	1.67	0.58
1:A:118:PHE:CE2	2:B:137:ALA:HB1	2.39	0.58
2:B:159:LEU:CD1	2:B:182:VAL:HG11	2.34	0.58
2:B:116:THR:HG22	2:B:117:LYS:H	1.68	0.58
2:B:155:ASN:HB3	2:B:158:ALA:HB3	1.86	0.58
2:H:144:ASP:HA	2:H:175:LEU:HB3	1.86	0.57
2:H:156:SER:CA	2:H:197:ASN:HD21	2.17	0.57
1:A:162:SER:OG	2:B:167:PRO:HD2	2.04	0.57
2:B:23:LYS:HD2	2:B:75:ALA:O	2.04	0.57
2:H:207:VAL:HG23	2:H:208:ASP:N	2.19	0.57
2:B:164:HIS:HD2	5:B:3113:HOH:O	1.86	0.57
1:A:33:LEU:C	1:A:33:LEU:HD13	2.30	0.57
1:L:211:ARG:HG2	1:L:211:ARG:HH11	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2027:LEU:CD2	1:A:90:GLN:HG3	2.35	0.57
1:L:167:ASP:HB3	1:L:170:ASP:OD1	2.04	0.57
2:H:11:LEU:O	2:H:12:LYS:HG2	2.03	0.57
1:A:192:TYR:O	1:A:208:SER:HB2	2.04	0.57
2:B:27:TYR:O	2:B:29:PHE:N	2.38	0.56
1:L:211:ARG:HH11	1:L:211:ARG:CG	2.19	0.56
2:B:116:THR:HG21	2:B:202:PRO:O	2.05	0.56
1:L:150:VAL:C	1:L:152:ASN:H	2.12	0.56
1:L:188:LYS:HG3	1:L:189:HIS:CD2	2.40	0.56
2:H:66:ARG:HH22	2:H:86:ASP:CG	2.12	0.56
2:B:159:LEU:HD13	2:B:182:VAL:HG11	1.86	0.56
2:H:119:PRO:HB2	2:H:142:VAL:HG23	1.88	0.56
2:H:156:SER:HA	2:H:197:ASN:ND2	2.21	0.56
2:H:197:ASN:N	2:H:197:ASN:OD1	2.37	0.56
1:A:4027:HIS:CD2	1:A:28:ASN:H	2.20	0.56
2:B:126:PRO:HA	2:B:137:ALA:HB3	1.88	0.56
1:L:198:HIS:CD2	1:L:200:GLY:H	2.23	0.56
1:A:3:VAL:HG13	5:A:5035:HOH:O	2.06	0.56
1:L:96:PRO:HD2	2:H:47:TRP:CD2	2.41	0.56
2:H:201:LYS:NZ	2:H:201:LYS:H	2.04	0.56
1:A:124:GLN:HG3	2:B:122:PHE:CD2	2.41	0.56
1:L:2027:LEU:CD2	1:L:90:GLN:HG3	2.36	0.55
1:L:39:LYS:H	1:L:45:LYS:HZ1	1.53	0.55
1:A:18:GLN:NE2	1:A:74:LYS:HD3	2.21	0.55
2:H:199:ASN:ND2	2:H:201:LYS:HE3	2.22	0.55
1:A:94:VAL:CB	1:A:95:PRO:HD3	2.33	0.55
2:B:10:GLU:OE1	2:B:12:LYS:HE3	2.07	0.55
1:L:2:LEU:C	1:L:2:LEU:HD23	2.32	0.55
1:L:106:ILE:N	1:L:166:GLN:HE22	2.04	0.55
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.47	0.55
1:A:94:VAL:CB	1:A:95:PRO:CD	2.85	0.54
1:A:143:GLU:H	1:A:143:GLU:CD	2.14	0.54
1:A:210:ASN:ND2	1:A:211:ARG:HE	2.01	0.54
1:L:150:VAL:C	1:L:152:ASN:N	2.61	0.54
1:L:7:THR:HB	1:L:8:PRO:CD	2.35	0.54
1:L:32:TYR:CE1	2:H:100:ARG:HD2	2.43	0.54
2:H:2:VAL:HG11	2:H:102:TYR:HB2	1.90	0.54
2:H:2:VAL:HG12	2:H:94:GLN:OE1	2.08	0.54
1:A:2027:LEU:HD22	1:A:90:GLN:CG	2.38	0.54
2:B:119:PRO:HB2	2:B:142:VAL:HG23	1.90	0.54
1:L:54:ARG:NE	1:L:60:ASP:HA	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:195:ILE:HG12	2:H:210:LYS:HA	1.89	0.53
1:A:106:ILE:H	1:A:166:GLN:HE22	1.54	0.53
2:H:119:PRO:HD2	2:H:205:THR:HG21	1.89	0.53
2:H:149:PRO:HA	5:H:3128:HOH:O	2.08	0.53
2:H:124:LEU:HB2	2:H:139:GLY:C	2.33	0.53
2:B:116:THR:HG22	2:B:117:LYS:N	2.23	0.53
1:L:124:GLN:HE22	1:L:131:SER:CB	2.22	0.53
2:B:52:ASN:HD22	2:B:53:TYR:N	2.00	0.53
2:H:93:VAL:HG11	2:H:2100:PHE:HB3	1.90	0.53
1:A:96:PRO:HD2	2:B:47:TRP:CE3	2.43	0.53
1:A:108:ARG:HD3	1:A:109:THR:O	2.08	0.53
2:H:116:THR:HG21	2:H:202:PRO:C	2.34	0.53
1:A:1027:SER:HA	1:A:69:THR:HG22	1.91	0.53
2:B:212:GLU:OE1	2:B:212:GLU:HA	2.08	0.52
1:A:188:LYS:NZ	1:A:189:HIS:NE2	2.41	0.52
1:L:37:LEU:HD13	1:L:86:TYR:CE1	2.45	0.52
2:H:59:TYR:HB2	2:H:64:LYS:HD3	1.92	0.52
1:A:1:GLU:HG2	1:A:2:LEU:N	2.23	0.52
2:B:207:VAL:HG23	2:B:208:ASP:N	2.24	0.52
1:L:125:LEU:C	1:L:127:SER:H	2.18	0.52
2:H:135:THR:HA	2:H:185:PRO:HA	1.92	0.52
2:B:154:TRP:CH2	2:B:196:CYS:HB3	2.45	0.52
1:L:192:TYR:HB2	1:L:209:PHE:CE1	2.45	0.52
1:A:17:ASP:O	1:A:78:VAL:HG23	2.10	0.52
1:A:70:ASP:HB2	5:A:5054:HOH:O	2.08	0.52
2:B:83:LYS:HD3	2:B:85:GLU:OE1	2.08	0.52
1:A:119:PRO:HB3	1:A:209:PHE:CZ	2.44	0.52
1:L:182:SER:O	1:L:183:LYS:C	2.52	0.51
2:H:2082:ASN:ND2	5:H:3091:HOH:O	2.43	0.51
1:L:129:THR:HG23	1:L:181:LEU:O	2.11	0.51
1:A:7:THR:HB	1:A:8:PRO:CD	2.31	0.51
2:H:156:SER:H	2:H:197:ASN:ND2	2.04	0.51
2:B:72:GLU:HB2	2:B:79:TYR:CE2	2.46	0.51
2:B:138:LEU:HD11	2:B:194:TYR:CD2	2.46	0.51
2:H:155:ASN:ND2	2:H:195:ILE:H	2.09	0.51
1:L:140:TYR:CG	1:L:141:PRO:HA	2.46	0.51
2:H:159:LEU:HD13	2:H:182:VAL:HG11	1.93	0.50
2:B:11:LEU:HG	2:B:147:PRO:HG3	1.94	0.50
2:B:97:ARG:HB2	4:B:3083:FRA:C2	2.41	0.50
2:B:40:ALA:HB3	2:B:43:LYS:CB	2.41	0.50
1:A:79:GLU:O	1:A:80:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:37:LEU:O	1:L:45:LYS:HD2	2.11	0.50
2:H:81:GLN:HG2	5:H:3104:HOH:O	2.12	0.49
2:H:116:THR:HA	2:H:146:PHE:O	2.12	0.49
1:L:6:GLN:HA	1:L:22:SER:O	2.12	0.49
1:A:1:GLU:CG	1:A:2:LEU:N	2.72	0.49
1:A:124:GLN:NE2	1:A:129:THR:HG22	2.27	0.49
1:L:150:VAL:HA	1:L:191:VAL:O	2.13	0.49
1:L:6:GLN:OE1	1:L:87:PHE:HA	2.13	0.49
2:H:154:TRP:CH2	2:H:196:CYS:HB3	2.48	0.49
1:A:39:LYS:HB2	1:A:42:GLN:HE21	1.77	0.49
2:B:186:SER:O	2:B:189:LEU:HB2	2.12	0.49
2:H:3082:LEU:HD12	2:H:86:ASP:OD2	2.12	0.48
2:H:144:ASP:HB3	2:H:175:LEU:HD23	1.95	0.48
2:B:2:VAL:HG13	2:B:102:TYR:OH	2.13	0.48
2:B:199:ASN:HB2	2:B:206:LYS:HE2	1.95	0.48
1:L:34:HIS:HD2	1:L:49:TYR:HA	1.77	0.48
1:A:210:ASN:O	1:A:211:ARG:C	2.57	0.48
2:B:80:LEU:HD22	2:B:81:GLN:N	2.29	0.48
2:B:93:VAL:CG1	2:B:2100:PHE:HB3	2.43	0.48
2:H:10:GLU:OE1	2:H:12:LYS:HE3	2.12	0.48
2:H:156:SER:HA	2:H:197:ASN:HD21	1.79	0.48
2:B:66:ARG:HH22	2:B:86:ASP:CG	2.22	0.48
2:B:155:ASN:CB	2:B:158:ALA:HB3	2.44	0.48
1:A:39:LYS:HG3	1:A:45:LYS:HE3	1.96	0.47
1:A:119:PRO:HB3	1:A:209:PHE:CE1	2.49	0.47
2:B:27:TYR:C	2:B:29:PHE:N	2.72	0.47
1:L:12:PRO:CB	1:L:105:GLU:HG2	2.44	0.47
1:L:28:ASN:OD1	1:L:30:ASN:HB2	2.14	0.47
1:L:38:GLN:HA	1:L:45:LYS:HZ3	1.79	0.47
1:L:151:ASP:O	1:L:152:ASN:HB3	2.14	0.47
2:B:131:THR:HG23	2:B:189:LEU:HD12	1.96	0.47
2:B:138:LEU:C	2:B:138:LEU:HD23	2.39	0.47
1:L:4027:HIS:HE1	5:L:5062:HOH:O	1.98	0.47
2:B:11:LEU:C	2:B:12:LYS:HG2	2.40	0.47
2:H:11:LEU:HG	2:H:147:PRO:HG3	1.95	0.47
1:L:120:PRO:HD3	1:L:132:VAL:HG22	1.96	0.47
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.97	0.47
2:B:207:VAL:CG2	2:B:208:ASP:N	2.77	0.47
2:H:186:SER:HA	2:H:189:LEU:HG	1.96	0.47
1:A:5:THR:HG21	1:A:24:ARG:NH2	2.29	0.47
2:B:2:VAL:HG12	2:B:4:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:LYS:N	2:B:202:PRO:CD	2.77	0.47
2:H:116:THR:CG2	2:H:203:SER:HB3	2.43	0.46
2:H:201:LYS:N	2:H:202:PRO:CD	2.78	0.46
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.96	0.46
1:L:12:PRO:HA	1:L:105:GLU:HG2	1.98	0.46
1:L:13:VAL:HG11	1:L:104:LEU:HD11	1.98	0.46
1:L:94:VAL:HG22	5:L:5039:HOH:O	2.16	0.46
2:H:127:SER:CB	2:H:130:SER:HB3	2.45	0.46
1:L:108:ARG:HD3	1:L:109:THR:O	2.16	0.46
2:B:51:ILE:CD1	2:B:71:LEU:HG	2.46	0.46
1:A:108:ARG:HD2	1:A:140:TYR:CB	2.46	0.46
1:A:59:PRO:HG2	1:A:62:PHE:CD2	2.51	0.45
2:B:149:PRO:HA	5:B:3106:HOH:O	2.16	0.45
2:H:1:GLN:O	2:H:2:VAL:HG23	2.16	0.45
2:B:54:THR:CG2	2:B:56:GLU:HG2	2.47	0.45
2:B:127:SER:CB	2:B:130:SER:HB3	2.41	0.45
2:B:147:PRO:HD2	2:B:202:PRO:CB	2.47	0.45
2:B:178:LEU:C	2:B:178:LEU:HD12	2.41	0.45
1:A:167:ASP:OD2	1:A:169:LYS:HB2	2.16	0.45
1:L:34:HIS:HD2	1:L:50:LYS:N	2.13	0.45
1:L:121:SER:OG	2:H:122:PHE:HB3	2.17	0.45
1:L:197:THR:CG2	1:L:204:PRO:HB3	2.36	0.45
2:B:126:PRO:O	2:B:127:SER:O	2.35	0.45
1:L:150:VAL:HG22	1:L:192:TYR:CD2	2.52	0.45
1:A:188:LYS:HD2	1:A:189:HIS:NE2	2.32	0.45
2:B:205:THR:HG22	2:B:207:VAL:HG12	1.99	0.45
1:L:54:ARG:NH1	1:L:62:PHE:O	2.50	0.44
2:H:150:VAL:HG12	2:H:178:LEU:HD21	1.98	0.44
2:B:12:LYS:O	2:B:111:VAL:HA	2.16	0.44
2:H:1:GLN:C	2:H:2:VAL:CG2	2.90	0.44
1:A:39:LYS:HD3	5:A:5042:HOH:O	2.17	0.44
1:L:32:TYR:CD1	2:H:100:ARG:HD2	2.52	0.44
1:L:129:THR:HG22	1:L:130:ALA:N	2.31	0.44
2:H:134:GLY:O	2:H:185:PRO:HA	2.17	0.44
1:A:120:PRO:HG2	1:A:186:TYR:CZ	2.52	0.44
1:L:96:PRO:HG2	2:H:47:TRP:CG	2.52	0.44
1:L:116:PHE:CD1	1:L:116:PHE:N	2.85	0.44
2:H:138:LEU:C	2:H:138:LEU:HD23	2.43	0.43
2:H:72:GLU:HB2	2:H:79:TYR:HE2	1.82	0.43
1:A:108:ARG:HD2	1:A:140:TYR:CG	2.54	0.43
2:B:124:LEU:HB2	2:B:139:GLY:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:58:VAL:HA	1:L:59:PRO:HD2	1.91	0.43
2:B:97:ARG:H	4:B:3083:FRA:H221	1.83	0.43
1:L:147:GLN:HB3	1:L:154:LEU:CD1	2.47	0.43
2:B:38:LYS:HD2	2:B:90:TYR:CE1	2.54	0.43
1:L:135:LEU:HD22	2:H:181:VAL:HG11	1.99	0.43
1:A:175:LEU:C	1:A:175:LEU:HD23	2.43	0.43
1:A:182:SER:OG	1:A:185:ASP:OD1	2.36	0.43
1:A:197:THR:HG22	1:A:204:PRO:HB3	2.01	0.43
1:A:134:CYS:HB2	1:A:148:TRP:CH2	2.54	0.43
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.99	0.42
2:H:146:PHE:HA	2:H:147:PRO:HA	1.76	0.42
1:A:96:PRO:HD2	2:B:47:TRP:CD2	2.54	0.42
1:A:164:THR:HG23	2:B:166:PHE:CD2	2.54	0.42
2:B:156:SER:HA	2:B:197:ASN:ND2	2.34	0.42
2:B:52:ASN:ND2	2:B:53:TYR:N	2.58	0.42
2:B:127:SER:HB2	2:B:130:SER:O	2.19	0.42
2:H:199:ASN:HD21	2:H:201:LYS:HG3	1.84	0.42
2:B:13:LYS:HG3	2:B:16:GLU:OE1	2.19	0.42
1:L:6:GLN:HE21	1:L:6:GLN:HB3	1.66	0.42
2:H:10:GLU:OE2	5:H:3111:HOH:O	2.21	0.42
2:H:72:GLU:HB2	2:H:79:TYR:CE2	2.55	0.42
2:B:13:LYS:O	2:B:16:GLU:HG3	2.20	0.42
2:B:16:GLU:O	2:B:3082:LEU:HD22	2.19	0.42
1:A:7:THR:CB	1:A:8:PRO:CD	2.94	0.42
2:B:3:GLN:HA	2:B:25:SER:CB	2.47	0.42
2:B:187:SER:C	2:B:189:LEU:H	2.28	0.42
1:L:2027:LEU:CD1	1:L:33:LEU:HD23	2.50	0.42
1:L:125:LEU:C	1:L:127:SER:N	2.75	0.42
1:L:151:ASP:O	1:L:152:ASN:CB	2.67	0.42
2:B:27:TYR:CD1	2:B:27:TYR:N	2.85	0.42
2:B:151:THR:OG1	2:B:199:ASN:HB3	2.19	0.42
1:A:4027:HIS:HD2	1:A:28:ASN:N	2.13	0.42
2:B:87:THR:O	2:B:88:ALA:HB2	2.20	0.42
2:B:116:THR:HG21	2:B:202:PRO:C	2.44	0.42
2:H:119:PRO:HB2	2:H:142:VAL:CG2	2.48	0.42
2:H:188:SER:HB2	2:H:192:GLN:OE1	2.19	0.42
2:B:117:LYS:HD2	2:B:175:LEU:HD21	2.02	0.42
1:L:145:LYS:HE3	1:L:147:GLN:OE1	2.20	0.42
2:B:35:ASN:HD22	2:B:35:ASN:N	2.18	0.42
1:L:37:LEU:HB2	1:L:47:LEU:HD11	2.01	0.41
2:H:155:ASN:HD22	2:H:155:ASN:HA	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:SER:O	2:B:189:LEU:N	2.53	0.41
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.94	0.41
1:A:142:ARG:HH11	1:A:142:ARG:CG	2.33	0.41
5:A:5071:HOH:O	2:B:183:THR:HG21	2.20	0.41
2:H:178:LEU:HD12	2:H:178:LEU:C	2.44	0.41
2:B:98:LEU:HD12	2:B:98:LEU:HA	1.92	0.41
1:L:34:HIS:CD2	1:L:49:TYR:HA	2.55	0.41
2:H:154:TRP:CZ3	2:H:196:CYS:HB3	2.54	0.41
1:A:4:MET:HE3	1:A:88:CYS:SG	2.61	0.41
2:B:71:LEU:HD23	2:B:71:LEU:HA	1.90	0.41
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.54	0.41
2:H:96:GLU:OE1	2:H:99:ARG:HG3	2.20	0.41
2:B:47:TRP:CH2	2:B:49:GLY:HA2	2.56	0.41
2:B:52:ASN:HD22	2:B:52:ASN:C	2.28	0.41
2:B:61:ASP:HA	2:B:64:LYS:CD	2.49	0.41
2:B:11:LEU:O	2:B:12:LYS:HG2	2.21	0.41
2:H:189:LEU:N	2:H:189:LEU:HD23	2.36	0.41
2:H:67:PHE:HA	2:H:81:GLN:O	2.21	0.41
1:L:136:LEU:HD21	1:L:196:VAL:HG13	2.03	0.41
2:B:132:SER:HA	2:B:186:SER:HB3	2.03	0.41
1:L:203:SER:O	1:L:204:PRO:C	2.64	0.41
2:H:1:GLN:C	2:H:3:GLN:H	2.28	0.41
1:A:34:HIS:CD2	2:B:1100:THR:HG22	2.55	0.41
1:L:49:TYR:O	1:L:50:LYS:C	2.64	0.40
1:L:174:SER:O	2:H:166:PHE:HE1	2.05	0.40
2:B:18:VAL:CG2	2:B:3082:LEU:HD11	2.51	0.40
2:B:135:THR:HA	2:B:184:VAL:O	2.22	0.40
1:A:193:ALA:HB2	1:A:208:SER:HB2	2.03	0.40
2:B:4:LEU:HD12	2:B:102:TYR:HD2	1.87	0.40
2:B:6:GLU:OE2	2:B:92:CYS:HB3	2.21	0.40
2:B:17:THR:HG22	2:B:18:VAL:N	2.36	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	214/217 (99%)	199 (93%)	12 (6%)	3 (1%)	9	13
1	L	215/217 (99%)	192 (89%)	18 (8%)	5 (2%)	5	6
2	B	217/219 (99%)	186 (86%)	21 (10%)	10 (5%)	2	1
2	H	215/219 (98%)	189 (88%)	21 (10%)	5 (2%)	5	6
All	All	861/872 (99%)	766 (89%)	72 (8%)	23 (3%)	4	4

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	94	VAL
1	L	210	ASN
1	L	211	ARG
2	H	137	ALA
1	A	94	VAL
1	A	210	ASN
2	B	27	TYR
2	B	137	ALA
2	H	2	VAL
2	B	127	SER
1	L	126	LYS
1	L	188	LYS
2	H	127	SER
2	H	133	GLY
2	B	28	THR
2	B	133	GLY
2	B	188	SER
2	H	186	SER
2	B	25	SER
2	B	138	LEU
1	A	7	THR
2	B	26	GLY
2	B	132	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/193 (100%)	165 (86%)	28 (14%)	3	4
1	L	193/193 (100%)	157 (81%)	36 (19%)	1	2
2	B	185/185 (100%)	137 (74%)	48 (26%)	0	0
2	H	183/185 (99%)	136 (74%)	47 (26%)	0	0
All	All	754/756 (100%)	595 (79%)	159 (21%)	1	1

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	9	LEU
1	L	10	SER
1	L	11	LEU
1	L	13	VAL
1	L	14	SER
1	L	22	SER
1	L	3027	LEU
1	L	45	LYS
1	L	50	LYS
1	L	60	ASP
1	L	70	ASP
1	L	90	GLN
1	L	94	VAL
1	L	105	GLU
1	L	107	LYS
1	L	108	ARG
1	L	121	SER
1	L	123	GLU
1	L	126	LYS
1	L	142	ARG
1	L	145	LYS
1	L	151	ASP
1	L	165	GLU
1	L	176	SER
1	L	180	THR
1	L	183	LYS
1	L	187	GLU
1	L	188	LYS
1	L	191	VAL
1	L	195	GLU

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Mol	Chain	Res	Type
1	L	202	SER
1	L	203	SER
1	L	205	VAL
1	L	206	THR
1	L	210	ASN
1	L	211	ARG
2	H	1	GLN
2	H	2	VAL
2	H	5	LEU
2	H	6	GLU
2	H	11	LEU
2	H	12	LYS
2	H	13	LYS
2	H	18	VAL
2	H	19	LYS
2	H	23	LYS
2	H	28	THR
2	H	34	MET
2	H	37	VAL
2	H	46	LYS
2	H	52	ASN
2	H	54	THR
2	H	72	GLU
2	H	73	THR
2	H	76	SER
2	H	80	LEU
2	H	3082	LEU
2	H	85	GLU
2	H	98	LEU
2	H	112	SER
2	H	113	SER
2	H	115	SER
2	H	117	LYS
2	H	124	LEU
2	H	135	THR
2	H	140	CYS
2	H	150	VAL
2	H	159	LEU
2	H	161	SER
2	H	169	VAL
2	H	175	LEU
2	H	178	LEU

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Mol	Chain	Res	Type
2	H	179	SER
2	H	183	THR
2	H	189	LEU
2	H	191	THR
2	H	197	ASN
2	H	201	LYS
2	H	204	ASN
2	H	206	LYS
2	H	207	VAL
2	H	209	LYS
2	H	210	LYS
1	A	1	GLU
1	A	10	SER
1	A	11	LEU
1	A	22	SER
1	A	26	SER
1	A	3027	LEU
1	A	45	LYS
1	A	76	SER
1	A	94	VAL
1	A	108	ARG
1	A	109	THR
1	A	123	GLU
1	A	126	LYS
1	A	129	THR
1	A	132	VAL
1	A	142	ARG
1	A	145	LYS
1	A	147	GLN
1	A	176	SER
1	A	183	LYS
1	A	187	GLU
1	A	190	LYS
1	A	191	VAL
1	A	197	THR
1	A	202	SER
1	A	205	VAL
1	A	206	THR
1	A	208	SER
2	B	5	LEU
2	B	6	GLU
2	B	11	LEU

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Mol	Chain	Res	Type
2	B	12	LYS
2	B	13	LYS
2	B	18	VAL
2	B	19	LYS
2	B	34	MET
2	B	35	ASN
2	B	37	VAL
2	B	46	LYS
2	B	52	ASN
2	B	56	GLU
2	B	66	ARG
2	B	72	GLU
2	B	76	SER
2	B	80	LEU
2	B	81	GLN
2	B	1082	ASN
2	B	2082	ASN
2	B	3082	LEU
2	B	98	LEU
2	B	108	THR
2	B	110	THR
2	B	113	SER
2	B	124	LEU
2	B	127	SER
2	B	128	SER
2	B	140	CYS
2	B	142	VAL
2	B	150	VAL
2	B	159	LEU
2	B	160	THR
2	B	161	SER
2	B	169	VAL
2	B	175	LEU
2	B	179	SER
2	B	183	THR
2	B	186	SER
2	B	188	SER
2	B	195	ILE
2	B	197	ASN
2	B	201	LYS
2	B	204	ASN
2	B	206	LYS

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Mol	Chain	Res	Type
2	B	207	VAL
2	B	209	LYS
2	B	210	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	4027	HIS
1	L	34	HIS
1	L	42	GLN
1	L	90	GLN
1	L	124	GLN
1	L	137	ASN
1	L	152	ASN
1	L	166	GLN
1	L	198	HIS
1	L	210	ASN
2	H	31	ASN
2	H	39	GLN
2	H	52	ASN
2	H	81	GLN
2	H	2082	ASN
2	H	94	GLN
2	H	155	ASN
2	H	164	HIS
2	H	171	GLN
2	H	197	ASN
2	H	199	ASN
1	A	18	GLN
1	A	4027	HIS
1	A	38	GLN
1	A	42	GLN
1	A	53	ASN
1	A	152	ASN
1	A	166	GLN
1	A	198	HIS
1	A	199	GLN
1	A	210	ASN
2	B	3	GLN
2	B	31	ASN
2	B	52	ASN
2	B	81	GLN

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Mol	Chain	Res	Type
2	B	155	ASN
2	B	197	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 ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FRA	B	3083	-	34,34,34	2.73	11 (32%)	48,51,51	2.83	16 (33%)
4	FRA	H	3083	-	34,34,34	2.69	11 (32%)	48,51,51	2.69	18 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FRA	B	3083	-	-	9/18/60/60	0/5/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FRA	H	3083	-	-	2/18/60/60	0/5/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3083	FRA	C14-C13	-6.60	1.40	1.53
4	H	3083	FRA	C14-C13	-6.54	1.40	1.53
4	H	3083	FRA	C14-C15	6.18	1.63	1.54
4	H	3083	FRA	C10-C12	6.15	1.64	1.54
4	B	3083	FRA	C10-C12	6.12	1.64	1.54
4	B	3083	FRA	C14-C15	5.86	1.63	1.54
4	B	3083	FRA	C16-C15	4.96	1.61	1.54
4	H	3083	FRA	C16-C15	4.72	1.61	1.54
4	B	3083	FRA	C5-N5	4.55	1.51	1.44
4	H	3083	FRA	C16-C17	4.32	1.62	1.53
4	H	3083	FRA	C17-C12	3.88	1.62	1.53
4	B	3083	FRA	C16-C17	3.81	1.61	1.53
4	B	3083	FRA	C17-C12	3.80	1.62	1.53
4	H	3083	FRA	C5-N5	3.41	1.49	1.44
4	B	3083	FRA	C4-C5	2.84	1.44	1.39
4	H	3083	FRA	C8-N5	-2.66	1.36	1.40
4	H	3083	FRA	C4-C5	2.61	1.44	1.39
4	B	3083	FRA	C8-N5	-2.42	1.36	1.40
4	B	3083	FRA	C3-C2	2.41	1.43	1.39
4	H	3083	FRA	C9-C10	2.27	1.57	1.54
4	B	3083	FRA	C6-C5	2.23	1.43	1.39
4	H	3083	FRA	C3-C2	2.14	1.42	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3083	FRA	C9-C8-N5	7.34	113.80	108.12
4	H	3083	FRA	C9-C8-N5	7.21	113.70	108.12
4	B	3083	FRA	C22-C1-N1	6.82	125.21	114.95
4	H	3083	FRA	O8-C8-C9	-6.60	119.93	127.50
4	B	3083	FRA	O8-C8-C9	-6.53	120.01	127.50
4	H	3083	FRA	C22-C1-N1	5.96	123.91	114.95
4	B	3083	FRA	O11-C11-C10	-5.93	119.94	127.51
4	B	3083	FRA	O3-C1-N1	-5.58	115.41	123.06
4	B	3083	FRA	C2-N1-C1	5.47	138.20	127.98
4	H	3083	FRA	O11-C11-C10	-5.03	121.09	127.51
4	H	3083	FRA	O3-C1-N1	-4.96	116.25	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	3083	FRA	C2-N1-C1	4.71	136.77	127.98
4	B	3083	FRA	C10-C9-C8	-4.28	101.34	104.55
4	B	3083	FRA	C8-N5-C11	-4.27	108.31	112.81
4	B	3083	FRA	C10-C11-N5	4.05	113.22	108.24
4	H	3083	FRA	C14-C15-N15	3.95	121.32	110.06
4	H	3083	FRA	O19-C19-C20	-3.93	102.47	110.93
4	B	3083	FRA	C19-O19-C18	3.78	120.06	115.67
4	H	3083	FRA	C8-N5-C11	-3.56	109.06	112.81
4	H	3083	FRA	C10-C9-C8	-3.48	101.94	104.55
4	H	3083	FRA	C4-C5-N5	3.36	123.68	119.65
4	H	3083	FRA	C10-C11-N5	3.33	112.34	108.24
4	H	3083	FRA	C13-C14-C15	3.14	116.77	109.98
4	B	3083	FRA	C13-C14-C15	3.07	116.61	109.98
4	B	3083	FRA	C14-C15-N15	3.02	118.67	110.06
4	B	3083	FRA	C4-C5-N5	3.00	123.24	119.65
4	H	3083	FRA	C19-O19-C18	2.86	118.99	115.67
4	H	3083	FRA	C9-C15-N15	-2.55	106.53	110.36
4	H	3083	FRA	C9-C10-C11	-2.51	102.95	104.85
4	H	3083	FRA	C5-N5-C11	2.48	126.58	123.59
4	B	3083	FRA	O11-C11-N5	2.32	126.84	124.30
4	B	3083	FRA	C9-C15-N15	-2.26	106.96	110.36
4	H	3083	FRA	O11-C11-N5	2.07	126.57	124.30
4	B	3083	FRA	C9-C10-C11	-2.02	103.32	104.85

There are no chirality outliers.

All (11) torsion outliers are listed below:

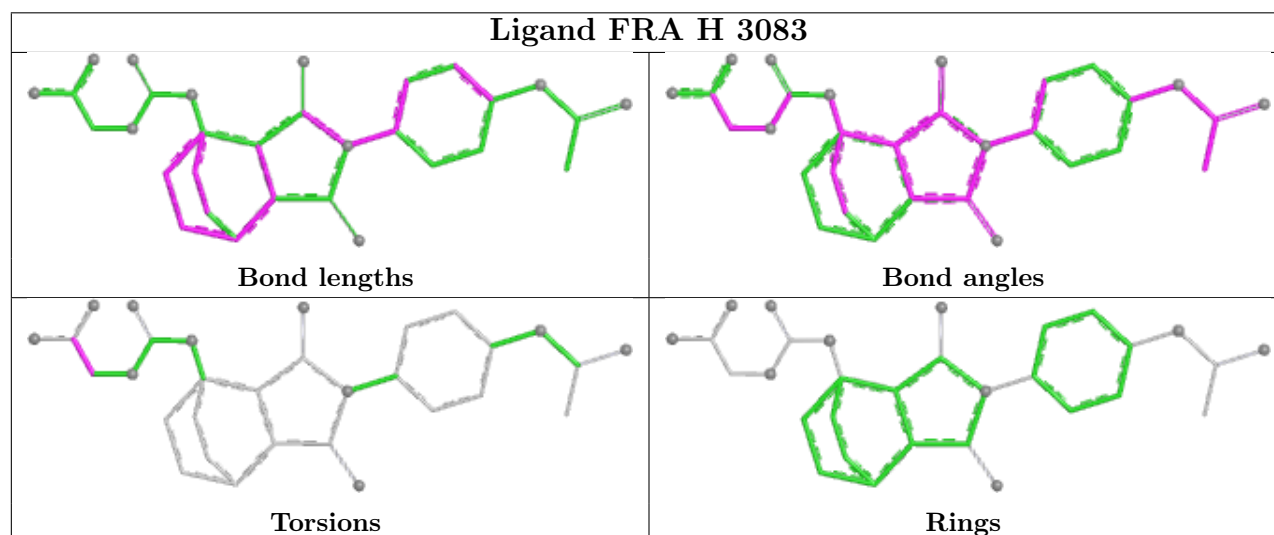
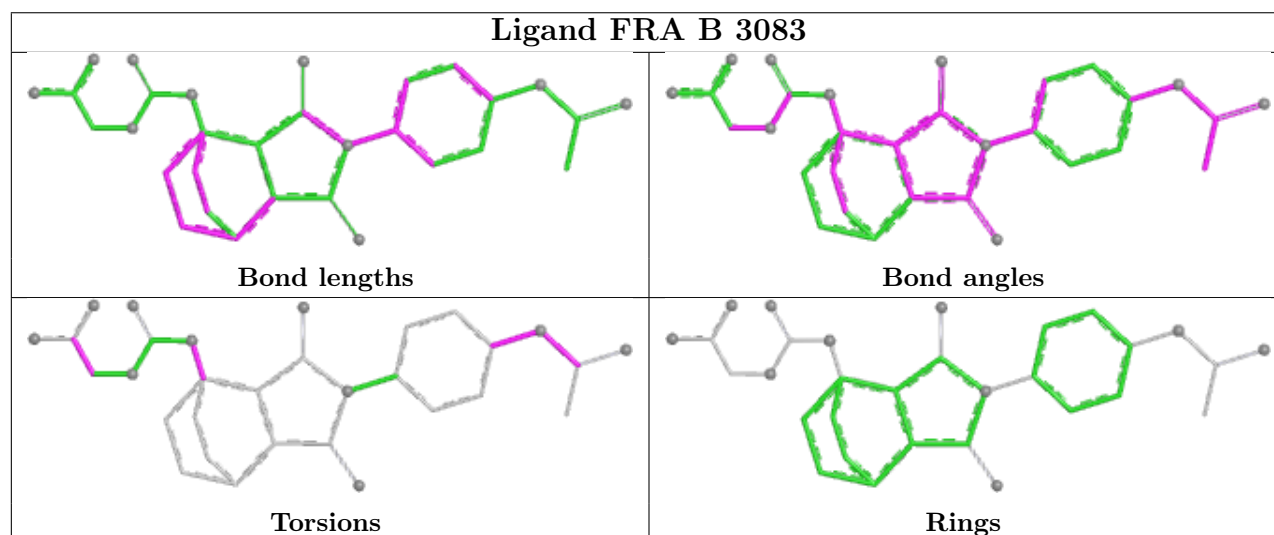
Mol	Chain	Res	Type	Atoms
4	H	3083	FRA	O19-C19-C20-O21
4	B	3083	FRA	O3-C1-N1-C2
4	B	3083	FRA	C22-C1-N1-C2
4	H	3083	FRA	O19-C19-C20-O20
4	B	3083	FRA	C14-C15-N15-C18
4	B	3083	FRA	C9-C15-N15-C18
4	B	3083	FRA	C3-C2-N1-C1
4	B	3083	FRA	O19-C19-C20-O20
4	B	3083	FRA	C7-C2-N1-C1
4	B	3083	FRA	O19-C19-C20-O21
4	B	3083	FRA	C16-C15-N15-C18

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3083	FRA	2	0
4	H	3083	FRA	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.



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	216/217 (99%)	0.16	8 (3%) 45 41	16, 33, 60, 79	0
1	L	217/217 (100%)	0.42	12 (5%) 30 27	17, 40, 68, 76	0
2	B	219/219 (100%)	0.65	28 (12%) 7 6	22, 41, 82, 100	0
2	H	217/219 (99%)	0.52	34 (15%) 5 4	15, 37, 92, 100	0
All	All	869/872 (99%)	0.44	82 (9%) 14 11	15, 38, 76, 100	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	128	SER	6.8
1	A	94	VAL	6.6
2	H	128	SER	6.4
2	H	129	LYS	4.9
2	B	133	GLY	4.8
2	B	131	THR	4.4
1	L	212	GLY	4.4
1	L	94	VAL	4.4
2	H	130	SER	4.3
1	L	7	THR	4.3
2	B	2	VAL	4.3
2	H	132	SER	4.3
2	B	132	SER	4.1
2	B	137	ALA	4.0
2	H	127	SER	4.0
2	H	2	VAL	3.9
2	B	191	THR	3.6
2	H	158	ALA	3.5
1	A	7	THR	3.5
2	H	211	VAL	3.5
2	B	193	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	192	GLN	3.4
2	H	193	THR	3.4
1	A	127	SER	3.3
2	H	197	ASN	3.2
2	H	185	PRO	3.2
2	H	155	ASN	3.1
2	H	188	SER	3.1
2	B	1082	ASN	3.1
2	B	6	GLU	3.0
2	B	27	TYR	3.0
1	L	151	ASP	2.9
2	B	127	SER	2.8
1	L	188	LYS	2.8
2	B	42	GLY	2.8
2	H	195	ILE	2.8
2	H	1	GLN	2.8
2	H	25	SER	2.7
2	B	130	SER	2.7
2	B	188	SER	2.7
2	H	6	GLU	2.7
2	H	26	GLY	2.7
2	H	190	GLY	2.7
1	L	203	SER	2.7
2	H	131	THR	2.7
1	L	205	VAL	2.6
2	H	159	LEU	2.6
2	H	189	LEU	2.6
1	L	1	GLU	2.6
2	H	133	GLY	2.6
1	L	121	SER	2.6
1	A	1	GLU	2.6
2	B	2082	ASN	2.5
2	H	135	THR	2.5
2	B	212	GLU	2.5
2	H	137	ALA	2.5
2	H	186	SER	2.5
1	A	123	GLU	2.4
2	B	28	THR	2.4
2	B	129	LYS	2.4
1	L	125	LEU	2.3
1	A	87	PHE	2.3
2	H	27	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	1	GLN	2.3
2	H	184	VAL	2.3
2	B	10	GLU	2.3
1	A	211	ARG	2.3
2	B	126	PRO	2.3
2	H	125	ALA	2.2
1	L	211	ARG	2.2
2	B	183	THR	2.2
2	B	134	GLY	2.2
2	H	206	LYS	2.2
2	B	136	ALA	2.1
2	B	190	GLY	2.1
2	H	136	ALA	2.1
1	A	70	ASP	2.1
2	B	25	SER	2.1
2	B	201	LYS	2.1
1	L	114	SER	2.1
2	H	208	ASP	2.0
2	H	187	SER	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.

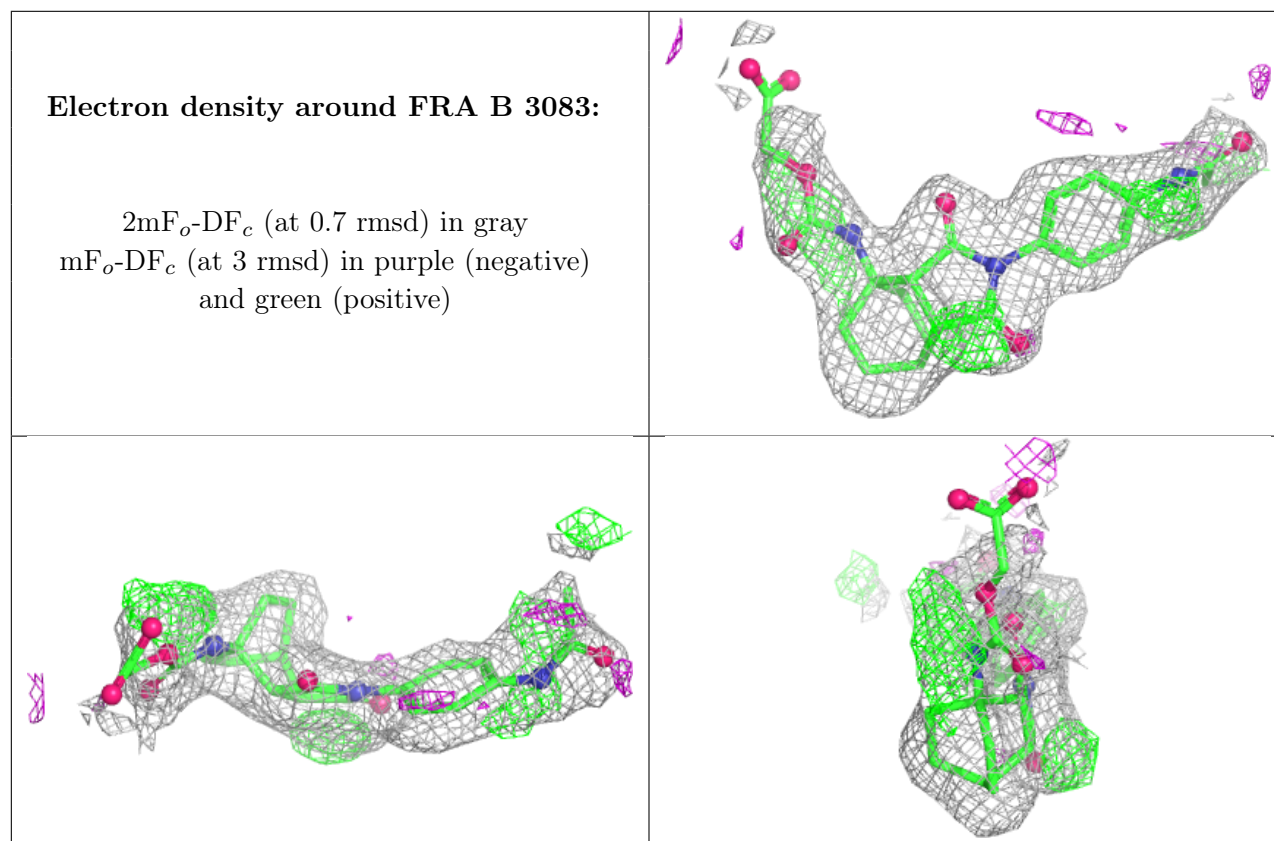
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FRA	B	3083	31/31	0.80	0.19	29,39,90,95	0
4	FRA	H	3083	31/31	0.91	0.12	17,25,87,98	0
3	CD	L	5029	1/1	0.98	0.04	62,62,62,62	0
3	CD	L	5028	1/1	0.99	0.05	37,37,37,37	0

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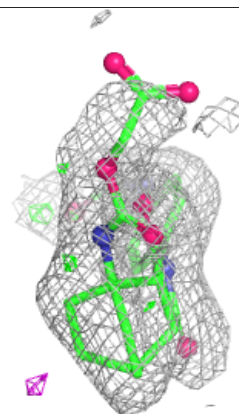
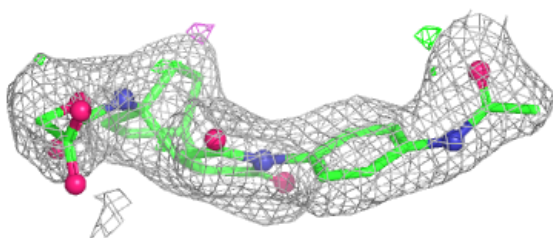
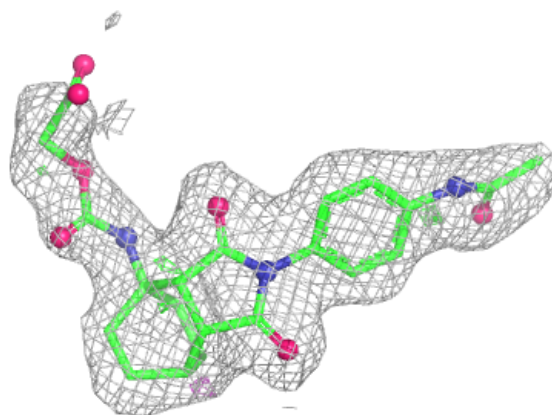
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CD	A	5028	1/1	0.99	0.05	41,41,41,41	0
3	CD	A	5029	1/1	1.00	0.02	41,41,41,41	0

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 FRA H 3083:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.