



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:42 PM UTC

PDB ID : 1JNH / pdb_00001jnh
Title : Crystal Structure of Fab-Estradiol Complexes
Authors : Monnet, C.; Bettsworth, F.; Stura, E.A.; Le Du, M.-H.; Menez, R.; Derrien, L.; Zinn-Justin, S.; Gilquin, B.; Sibai, G.; Battail-Poirot, N.; Jolivet, M.; Menez, A.; Arnaud, M.; Ducancel, F.; Charbonnier, J.B.
Deposited on : 2001-07-24
Resolution : 2.85 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:

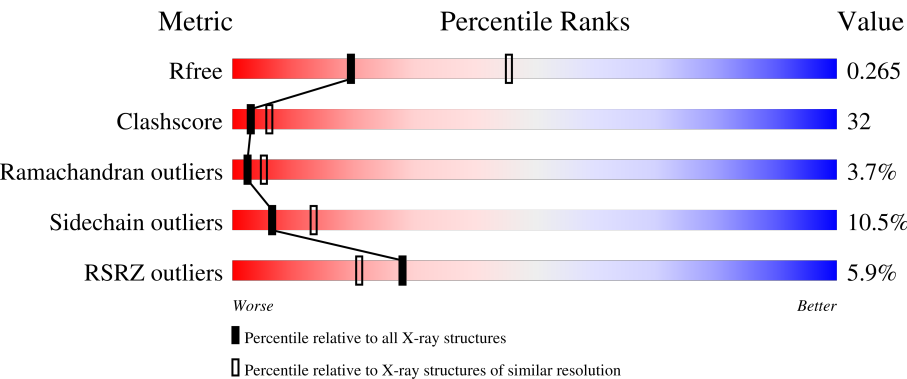
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	212	4% 52%40%5%..
1	C	212	11% 44%45%8%..
1	E	212	13% 40%49%9%..
1	G	212	3% 52%39%7%.

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Mol	Chain	Length	Quality of chain
2	B	218	2%47%43%8%•
2	D	218	4%44%45%7%••
2	F	218	6%49%42%7%•
2	H	218	3%49%41%7%••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12882 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.

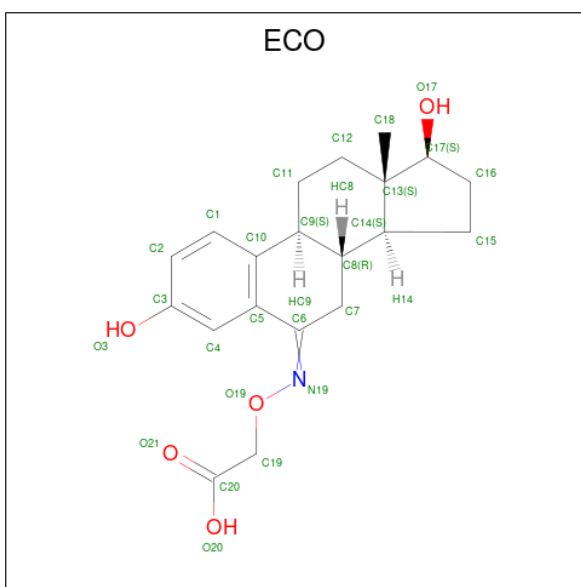
- Molecule 1 is a protein called monoclonal anti-estradiol 10G6D6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1567	979	262	321	5			
1	C	208	Total	C	N	O	S	0	0	0
			1567	979	262	321	5			
1	E	208	Total	C	N	O	S	0	0	0
			1567	979	262	321	5			
1	G	208	Total	C	N	O	S	0	0	0
			1567	979	262	321	5			

- Molecule 2 is a protein called monoclonal anti-estradiol 10G6D6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1614	1021	267	319	7			
2	D	214	Total	C	N	O	S	0	0	0
			1614	1021	267	319	7			
2	F	214	Total	C	N	O	S	0	0	0
			1614	1021	267	319	7			
2	H	214	Total	C	N	O	S	0	0	0
			1614	1021	267	319	7			

- Molecule 3 is ESTRADIOL-6 CARBOXYL-METHYL-OXIME (CCD ID: ECO) (formula: $C_{20}H_{25}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			26	20	1	5		
3	D	1	Total	C	N	O	0	0
			26	20	1	5		
3	F	1	Total	C	N	O	0	0
			26	20	1	5		
3	H	1	Total	C	N	O	0	0
			26	20	1	5		

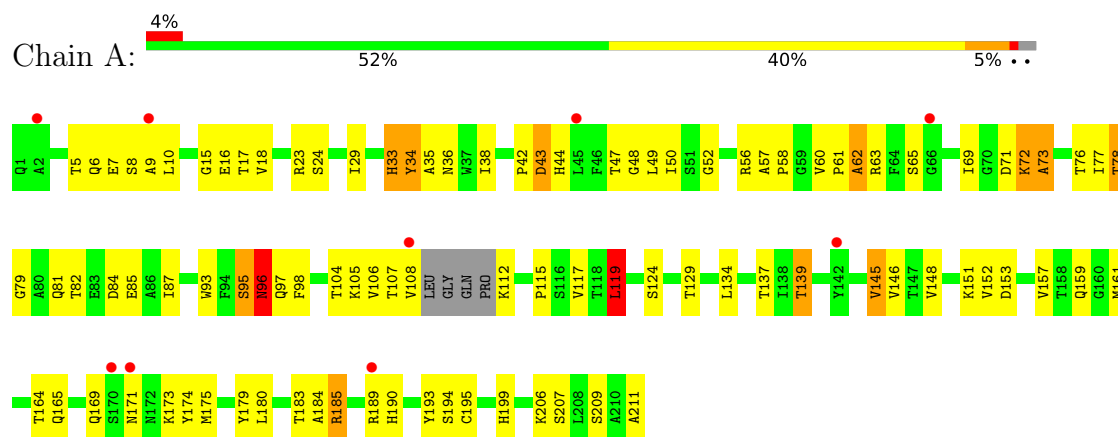
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	6	Total	O	0	0
			6	6		
4	C	3	Total	O	0	0
			3	3		
4	D	10	Total	O	0	0
			10	10		
4	E	6	Total	O	0	0
			6	6		
4	F	4	Total	O	0	0
			4	4		
4	G	8	Total	O	0	0
			8	8		
4	H	10	Total	O	0	0
			10	10		

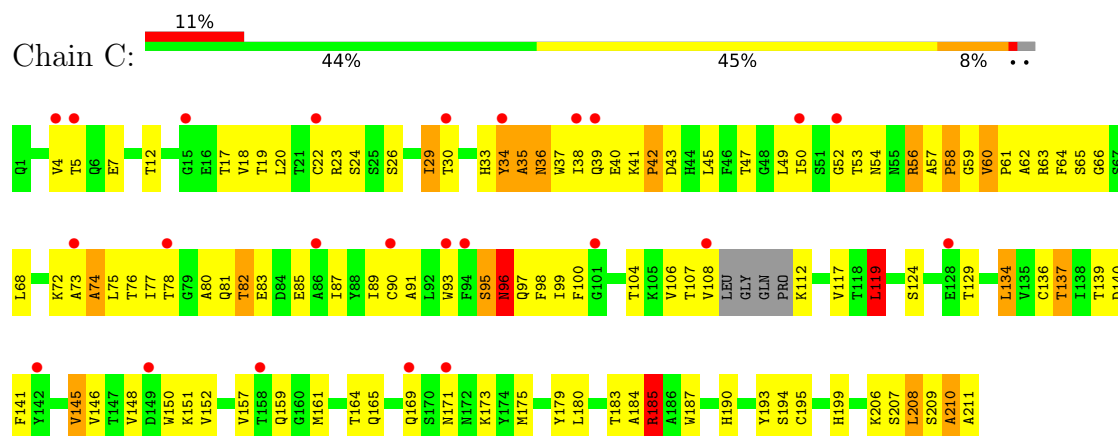
3 Residue-property plots [i](#)

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.

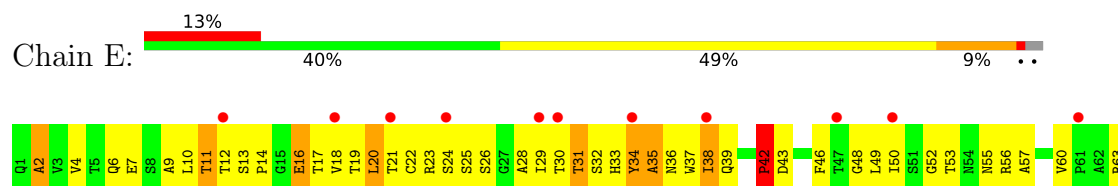
- Molecule 1: monoclonal anti-estradiol 10G6D6 Fab light chain

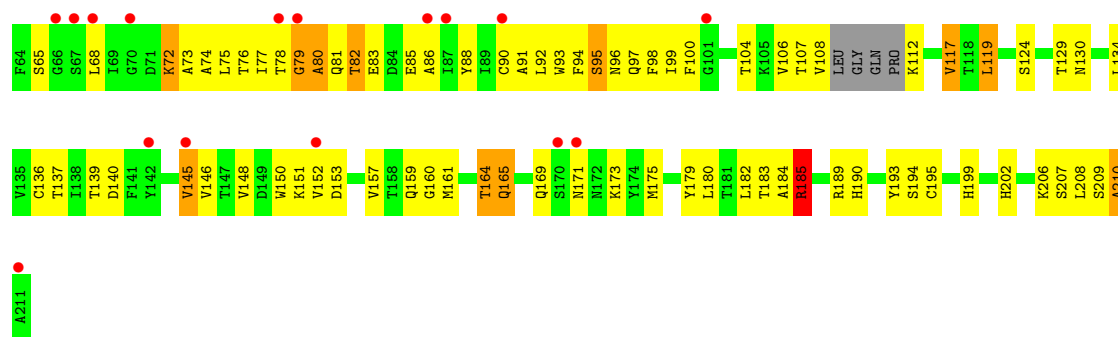


- Molecule 1: monoclonal anti-estradiol 10G6D6 Fab light chain

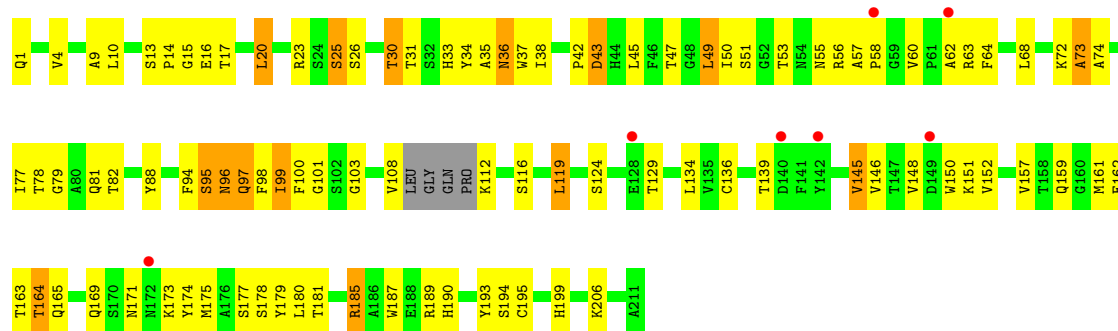


- Molecule 1: monoclonal anti-estradiol 10G6D6 Fab light chain

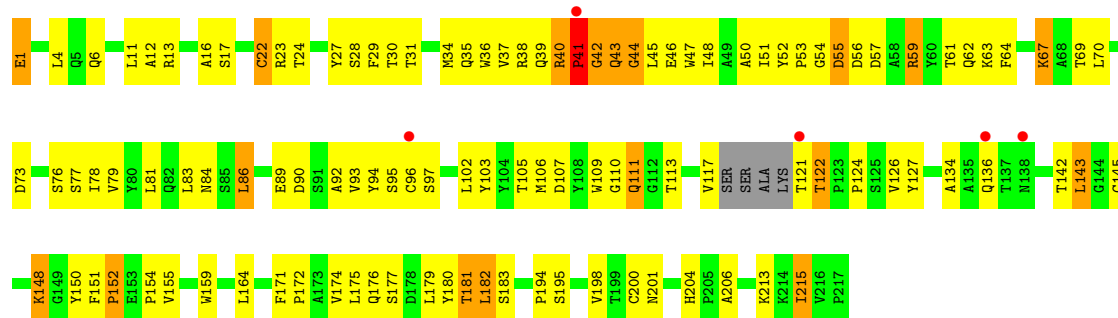




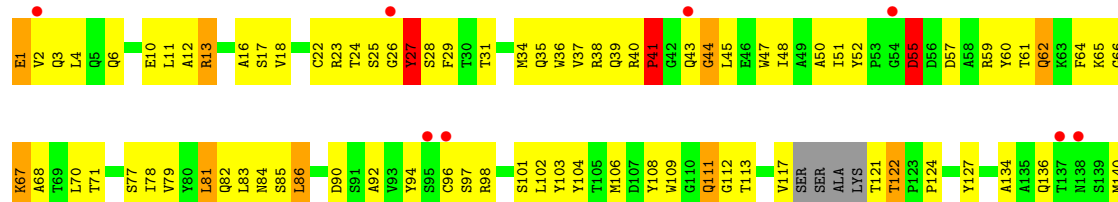
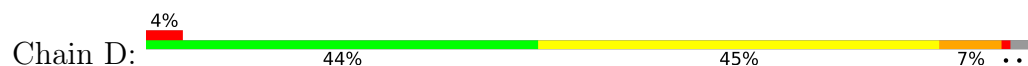
• Molecule 1: monoclonal anti-estradiol 10G6D6 Fab light chain

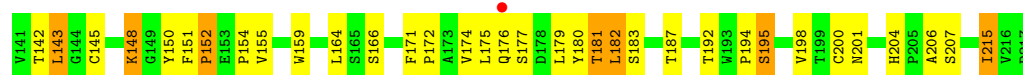


• Molecule 2: monoclonal anti-estradiol 10G6D6 Fab heavy chain

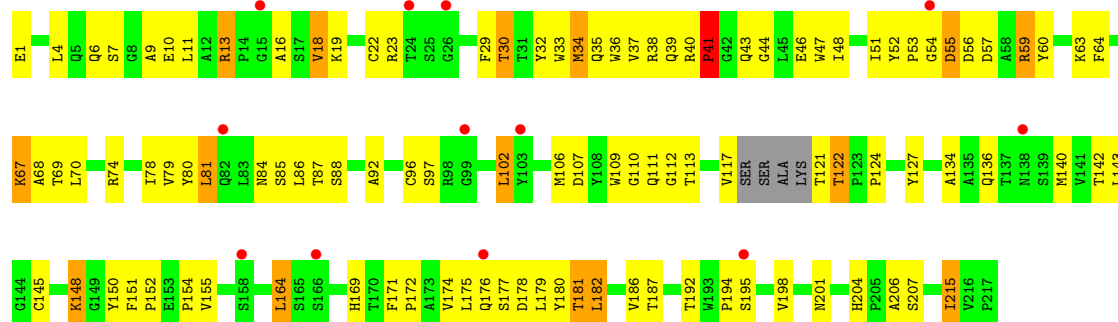


• Molecule 2: monoclonal anti-estradiol 10G6D6 Fab heavy chain

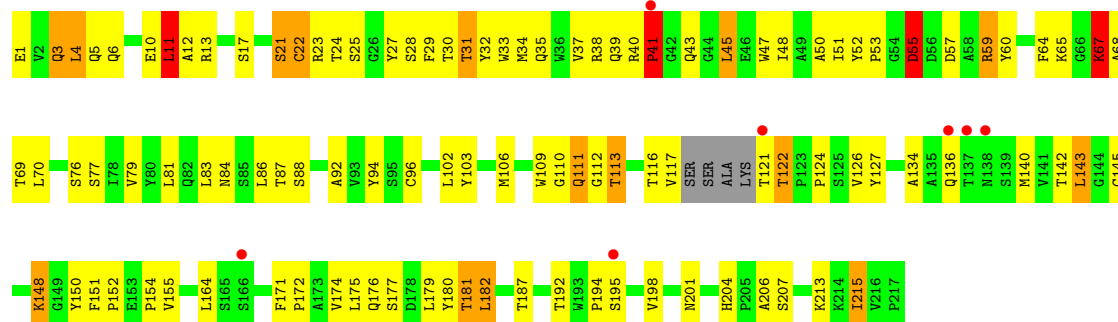




- Molecule 2: monoclonal anti-estradiol 10G6D6 Fab heavy chain



- Molecule 2: monoclonal anti-estradiol 10G6D6 Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.20Å 192.90Å 71.12Å 90.00° 92.93° 90.00°	Depositor
Resolution (Å)	40.00 – 2.85 40.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	83.3 (40.00-2.85) 90.7 (40.00-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.253 0.217 , 0.265	Depositor DCC
R_{free} test set	2742 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 88.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.053 for h,-k,-l 0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12882	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.07% 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: ECO

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	0.51	0/1601	0.97	4/2185 (0.2%)
1	C	0.51	1/1601 (0.1%)	0.96	7/2185 (0.3%)
1	E	0.49	0/1601	0.95	5/2185 (0.2%)
1	G	0.55	0/1601	0.97	2/2185 (0.1%)
2	B	0.52	0/1656	1.00	5/2266 (0.2%)
2	D	0.58	1/1656 (0.1%)	0.98	5/2266 (0.2%)
2	F	0.52	0/1656	0.95	6/2266 (0.3%)
2	H	0.54	0/1656	1.01	8/2266 (0.4%)
All	All	0.53	2/13028 (0.0%)	0.97	42/17804 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	137	THR	CA-CB	5.25	1.59	1.53
2	D	136	GLN	CA-CB	5.24	1.60	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	43	GLN	N-CA-C	8.34	124.70	112.94
2	D	148	LYS	N-CA-C	7.51	122.08	109.76
2	B	148	LYS	N-CA-C	7.50	122.05	109.76
2	H	148	LYS	N-CA-C	7.31	121.74	109.76
2	B	40	ARG	CA-C-N	6.85	128.41	119.84
2	B	40	ARG	C-N-CA	6.85	128.41	119.84
2	F	148	LYS	N-CA-C	6.81	120.93	109.76
1	A	139	THR	N-CA-C	6.48	118.00	108.86
2	D	136	GLN	N-CA-C	-6.45	99.39	109.25
2	H	45	LEU	N-CA-C	6.44	119.31	110.24
1	E	139	THR	N-CA-C	6.41	117.90	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	THR	N-CA-C	6.31	117.76	108.86
2	H	11	LEU	N-CA-C	-6.16	99.67	109.59
1	G	139	THR	N-CA-C	6.15	117.53	108.86
1	C	60	VAL	CA-C-N	6.13	126.09	119.78
1	C	60	VAL	C-N-CA	6.13	126.09	119.78
2	F	136	GLN	N-CA-C	-5.82	100.34	109.25
2	B	136	GLN	N-CA-C	-5.80	100.38	109.25
2	H	30	THR	N-CA-C	5.77	118.79	111.69
2	F	192	THR	N-CA-C	5.64	117.43	111.28
2	F	63	LYS	N-CA-C	5.52	116.97	111.07
1	C	119	LEU	CA-CB-CG	5.50	135.54	116.30
2	H	136	GLN	N-CA-C	-5.42	100.96	109.25
2	F	30	THR	N-CA-C	5.41	116.86	111.07
1	G	73	ALA	N-CA-C	-5.34	101.83	110.32
1	A	73	ALA	N-CA-C	-5.28	100.30	108.90
1	E	140	ASP	N-CA-C	5.26	118.85	111.90
2	D	192	THR	N-CA-C	5.26	117.70	111.33
1	E	99	ILE	N-CA-C	-5.21	100.83	108.85
1	A	33	HIS	N-CA-C	-5.20	106.62	113.17
1	A	119	LEU	CA-CB-CG	5.19	134.47	116.30
1	E	82	THR	N-CA-C	-5.18	106.22	112.54
2	H	192	THR	N-CA-C	5.17	116.91	111.28
1	E	165	GLN	N-CA-C	-5.12	103.08	110.40
1	C	140	ASP	N-CA-C	5.12	118.79	112.24
1	C	74	ALA	N-CA-C	5.11	117.75	109.06
2	B	43	GLN	N-CA-C	5.11	119.67	111.81
2	D	67	LYS	N-CA-C	5.04	117.74	111.24
2	F	102	LEU	N-CA-C	-5.03	107.11	113.20
1	C	82	THR	N-CA-C	-5.03	105.90	112.23
2	H	21	SER	N-CA-C	5.02	117.33	108.75
2	D	97	SER	N-CA-C	5.01	115.92	108.86

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	1567	0	1514	90	0
1	C	1567	0	1514	118	0
1	E	1567	0	1514	129	0
1	G	1567	0	1514	83	0
2	B	1614	0	1551	90	0
2	D	1614	0	1551	121	0
2	F	1614	0	1551	106	0
2	H	1614	0	1551	107	0
3	B	26	0	24	3	0
3	D	26	0	24	3	0
3	F	26	0	24	3	0
3	H	26	0	24	5	0
4	A	7	0	0	1	0
4	B	6	0	0	0	0
4	C	3	0	0	0	0
4	D	10	0	0	2	0
4	E	6	0	0	1	0
4	F	4	0	0	0	0
4	G	8	0	0	3	0
4	H	10	0	0	1	0
All	All	12882	0	12356	798	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 32.

All (798) 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)
2:F:6:GLN:HB2	2:F:111:GLN:HE22	1.23	1.02
2:D:34:MET:HE3	2:D:79:VAL:HB	1.44	1.00
2:H:34:MET:HE3	2:H:79:VAL:HB	1.45	0.99
1:E:68:LEU:HD23	1:E:73:ALA:HB2	1.49	0.94
2:F:124:PRO:HB3	2:F:150:TYR:HB3	1.50	0.94
1:A:24:SER:H	1:A:29:ILE:HD11	1.32	0.93
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.51	0.92
2:D:124:PRO:HB3	2:D:150:TYR:HB3	1.50	0.92
2:B:111:GLN:H	2:B:111:GLN:NE2	1.68	0.91
2:B:34:MET:HE3	2:B:79:VAL:HB	1.53	0.91
2:D:17:SER:HB2	4:D:361:HOH:O	1.69	0.91
2:D:111:GLN:H	2:D:111:GLN:NE2	1.68	0.91
2:B:124:PRO:HB3	2:B:150:TYR:HB3	1.52	0.90
1:G:185:ARG:HA	1:G:185:ARG:NH1	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:SER:H	1:C:29:ILE:HD11	1.36	0.89
1:C:185:ARG:NH1	1:C:185:ARG:HA	1.87	0.89
1:A:185:ARG:NH1	1:A:185:ARG:HA	1.88	0.88
1:A:87:ILE:HG12	1:A:105:LYS:HG2	1.54	0.87
1:E:160:GLY:H	2:H:1:GLU:CD	1.83	0.87
2:D:111:GLN:H	2:D:111:GLN:HE21	1.18	0.87
2:F:6:GLN:HB2	2:F:111:GLN:NE2	1.90	0.86
1:C:49:LEU:HA	1:C:60:VAL:HG21	1.58	0.85
2:H:52:TYR:HD2	2:H:55:ASP:HB2	1.41	0.85
2:D:38:ARG:HB2	2:D:48:ILE:HD11	1.58	0.85
1:C:91:ALA:HB2	1:C:100:PHE:CD2	2.12	0.85
2:B:35:GLN:HG2	2:B:47:TRP:CH2	2.11	0.84
1:C:37:TRP:CZ3	1:C:90:CYS:HB3	2.12	0.84
1:C:85:GLU:HG3	1:C:107:THR:HA	1.59	0.83
1:E:185:ARG:HA	1:E:185:ARG:NH1	1.94	0.81
1:C:95:SER:O	1:C:96:ASN:HB3	1.80	0.81
2:F:35:GLN:HG2	2:F:47:TRP:CH2	2.15	0.81
2:H:17:SER:HA	2:H:86:LEU:CD2	2.11	0.81
1:E:65:SER:HB2	1:E:76:THR:HB	1.61	0.80
2:D:40:ARG:HD3	2:D:43:GLN:NE2	1.97	0.80
1:C:39:GLN:HB2	1:C:49:LEU:HD11	1.64	0.80
1:G:36:ASN:HD22	1:G:37:TRP:N	1.79	0.79
1:E:20:LEU:HD23	1:E:104:THR:HG21	1.62	0.79
2:B:40:ARG:O	2:B:42:GLY:N	2.16	0.78
1:A:134:LEU:HB2	1:A:180:LEU:HB3	1.66	0.78
1:C:134:LEU:HB2	1:C:180:LEU:HB3	1.67	0.77
2:D:34:MET:CE	2:D:79:VAL:HB	2.15	0.76
2:F:6:GLN:CB	2:F:111:GLN:HE22	1.97	0.76
2:B:6:GLN:HE21	2:B:110:GLY:HA3	1.49	0.76
2:B:37:VAL:HG11	2:B:45:LEU:HB3	1.66	0.76
1:A:72:LYS:HB2	1:A:72:LYS:NZ	2.01	0.76
1:G:185:ARG:HA	1:G:185:ARG:CZ	2.16	0.75
1:A:17:THR:HA	1:A:77:ILE:O	1.86	0.75
1:G:181:THR:HG23	4:G:213:HOH:O	1.87	0.74
2:F:30:THR:HB	2:F:54:GLY:HA3	1.66	0.74
1:A:63:ARG:NH2	1:A:81:GLN:HG3	2.02	0.74
2:D:35:GLN:HG2	2:D:47:TRP:CH2	2.22	0.74
2:F:34:MET:HE3	2:F:79:VAL:HB	1.69	0.74
1:C:23:ARG:CZ	1:C:72:LYS:HD3	2.18	0.73
1:E:134:LEU:HB2	1:E:180:LEU:HB3	1.68	0.73
1:C:159:GLN:CD	1:C:159:GLN:H	1.96	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:THR:HG22	2:F:88:SER:N	2.05	0.72
2:H:111:GLN:H	2:H:111:GLN:HE21	1.38	0.72
2:F:48:ILE:HA	2:F:64:PHE:CD2	2.25	0.72
2:D:40:ARG:HG2	2:D:92:ALA:HB2	1.71	0.71
1:E:42:PRO:O	1:E:43:ASP:HB2	1.90	0.71
1:E:159:GLN:H	1:E:159:GLN:CD	1.97	0.71
1:A:48:GLY:HA3	2:B:107:ASP:HA	1.71	0.71
2:D:51:ILE:HB	2:D:70:LEU:HD23	1.70	0.71
1:C:185:ARG:HA	1:C:185:ARG:CZ	2.20	0.71
1:G:134:LEU:HB2	1:G:180:LEU:HB3	1.71	0.70
2:D:26:GLY:O	2:D:27:TYR:HB3	1.92	0.70
1:E:185:ARG:HA	1:E:185:ARG:CZ	2.20	0.70
2:H:40:ARG:HB3	2:H:41:PRO:HD2	1.74	0.70
1:A:159:GLN:CD	1:A:159:GLN:H	1.99	0.70
1:A:185:ARG:HA	1:A:185:ARG:CZ	2.21	0.70
1:E:36:ASN:HD22	1:E:37:TRP:N	1.89	0.70
1:E:20:LEU:HD12	1:E:20:LEU:H	1.57	0.69
1:A:65:SER:OG	1:A:76:THR:HB	1.93	0.69
1:E:48:GLY:HA3	2:F:107:ASP:HA	1.75	0.69
1:E:169:GLN:NE2	1:E:175:MET:HB3	2.08	0.69
2:F:51:ILE:HB	2:F:70:LEU:HD23	1.75	0.69
1:G:159:GLN:H	1:G:159:GLN:CD	1.99	0.69
2:H:60:TYR:HE2	2:H:69:THR:HA	1.58	0.69
1:G:164:THR:HG22	2:H:174:VAL:CG1	2.24	0.68
1:E:95:SER:O	1:E:96:ASN:HB3	1.92	0.68
2:D:12:ALA:O	2:D:117:VAL:HA	1.94	0.68
1:G:38:ILE:HD13	2:H:109:TRP:CZ2	2.28	0.68
1:E:57:ALA:HB3	1:E:60:VAL:CG2	2.24	0.67
1:C:81:GLN:O	1:C:108:VAL:HG21	1.93	0.67
1:A:24:SER:N	1:A:29:ILE:HD11	2.09	0.67
1:C:18:VAL:HG22	1:C:19:THR:H	1.60	0.67
1:C:38:ILE:HB	1:C:89:ILE:HG13	1.77	0.67
1:E:86:ALA:O	1:E:106:VAL:HB	1.93	0.67
1:C:23:ARG:NH1	1:C:72:LYS:HD3	2.10	0.67
1:C:85:GLU:HG3	1:C:106:VAL:O	1.94	0.67
1:C:169:GLN:NE2	1:C:175:MET:HB3	2.10	0.66
2:B:57:ASP:OD2	2:B:59:ARG:NH1	2.28	0.66
2:B:48:ILE:HA	2:B:64:PHE:CD2	2.30	0.66
2:B:30:THR:HB	2:B:54:GLY:HA3	1.76	0.66
1:G:171:ASN:OD1	1:G:173:LYS:HB2	1.96	0.66
1:C:29:ILE:HD13	1:C:72:LYS:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:TRP:HD1	1:C:50:ILE:HB	1.59	0.66
2:H:22:CYS:HB3	2:H:34:MET:HE1	1.78	0.66
1:C:171:ASN:OD1	1:C:173:LYS:HB2	1.96	0.66
1:E:20:LEU:HD23	1:E:104:THR:CG2	2.26	0.66
1:E:171:ASN:OD1	1:E:173:LYS:HB2	1.96	0.66
2:D:4:LEU:CD2	2:D:24:THR:HG22	2.25	0.65
2:F:57:ASP:OD2	2:F:59:ARG:NH1	2.29	0.65
1:G:206:LYS:HD3	2:H:134:ALA:HB1	1.78	0.65
2:F:6:GLN:NE2	2:F:112:GLY:HA2	2.11	0.65
1:A:23:ARG:NH2	1:A:72:LYS:HD3	2.11	0.65
2:H:111:GLN:H	2:H:111:GLN:NE2	1.94	0.65
1:A:164:THR:HG22	2:B:174:VAL:CG1	2.27	0.65
2:D:3:GLN:HG3	2:D:25:SER:HB3	1.78	0.65
1:G:23:ARG:HH22	1:G:72:LYS:CE	2.08	0.65
1:E:2:ALA:HB2	1:E:26:SER:HB3	1.79	0.65
1:G:98:PHE:HB2	2:H:47:TRP:CE3	2.32	0.65
2:H:51:ILE:O	2:H:53:PRO:HD3	1.96	0.65
2:B:37:VAL:CG1	2:B:45:LEU:HB3	2.27	0.64
1:G:169:GLN:NE2	1:G:175:MET:HB3	2.11	0.64
2:D:48:ILE:HA	2:D:64:PHE:CD2	2.32	0.64
2:D:40:ARG:HB3	2:D:41:PRO:HD2	1.78	0.64
2:F:39:GLN:O	2:F:92:ALA:HB1	1.98	0.64
1:G:23:ARG:HH22	1:G:72:LYS:HE2	1.61	0.64
2:D:198:VAL:O	2:D:215:ILE:HG23	1.97	0.64
2:D:6:GLN:NE2	2:D:112:GLY:HA2	2.13	0.63
2:H:12:ALA:O	2:H:117:VAL:HA	1.97	0.63
2:H:17:SER:HA	2:H:86:LEU:HD23	1.80	0.63
1:A:82:THR:HA	1:A:108:VAL:HG11	1.80	0.63
1:E:85:GLU:HG3	1:E:107:THR:HA	1.79	0.63
1:E:68:LEU:HA	1:E:73:ALA:HA	1.81	0.63
2:H:57:ASP:OD2	2:H:59:ARG:NH1	2.32	0.63
2:F:4:LEU:HD12	2:F:109:TRP:HA	1.80	0.63
1:C:29:ILE:HD12	1:C:29:ILE:N	2.14	0.63
2:H:34:MET:CE	2:H:79:VAL:HB	2.26	0.63
1:A:169:GLN:NE2	1:A:175:MET:HB3	2.13	0.63
2:F:37:VAL:HG13	2:F:46:GLU:O	1.98	0.63
2:B:17:SER:HA	2:B:86:LEU:HD22	1.79	0.62
2:D:39:GLN:O	2:D:92:ALA:HB1	1.98	0.62
2:D:40:ARG:HD3	2:D:43:GLN:HE22	1.63	0.62
2:B:182:LEU:C	2:B:182:LEU:HD23	2.24	0.62
2:D:215:ILE:HG13	2:D:215:ILE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:182:LEU:HD23	2:F:182:LEU:C	2.24	0.62
1:E:20:LEU:HD12	1:E:20:LEU:N	2.14	0.62
2:B:62:GLN:OE1	2:F:59:ARG:HD2	1.99	0.62
1:G:38:ILE:HD13	2:H:109:TRP:HZ2	1.64	0.62
1:G:36:ASN:HD22	1:G:36:ASN:C	2.05	0.62
1:C:7:GLU:OE2	1:C:20:LEU:HA	2.00	0.61
1:C:37:TRP:CE2	1:C:75:LEU:HB2	2.35	0.61
1:A:57:ALA:HB1	1:A:58:PRO:HD2	1.82	0.61
1:A:206:LYS:HD3	2:B:134:ALA:HB1	1.80	0.61
1:C:164:THR:HG22	2:D:174:VAL:CG1	2.30	0.61
1:A:63:ARG:CZ	1:A:81:GLN:HG3	2.31	0.61
1:G:35:ALA:HB3	1:G:53:THR:HA	1.80	0.61
1:C:83:GLU:C	1:C:85:GLU:H	2.09	0.61
2:B:4:LEU:HG	2:B:24:THR:HG22	1.83	0.61
2:H:182:LEU:HD23	2:H:182:LEU:C	2.25	0.61
2:B:35:GLN:HG2	2:B:47:TRP:HH2	1.62	0.61
2:D:6:GLN:OE1	2:D:113:THR:HG23	2.01	0.61
1:A:18:VAL:HG12	1:A:77:ILE:HB	1.82	0.60
2:D:70:LEU:HD12	2:D:70:LEU:N	2.16	0.60
2:F:198:VAL:O	2:F:215:ILE:HG23	2.02	0.60
1:A:85:GLU:HG3	1:A:107:THR:HA	1.84	0.60
1:E:7:GLU:O	1:E:104:THR:HG23	2.01	0.60
1:E:53:THR:CG2	1:E:68:LEU:HG	2.32	0.60
1:C:24:SER:N	1:C:29:ILE:HD11	2.14	0.60
1:G:96:ASN:O	1:G:97:GLN:HB3	2.01	0.60
1:A:42:PRO:O	1:A:43:ASP:HB2	2.01	0.60
2:H:31:THR:HA	2:H:52:TYR:OH	2.01	0.60
2:D:59:ARG:HG2	2:D:59:ARG:HH11	1.67	0.60
2:F:40:ARG:O	2:F:41:PRO:C	2.45	0.60
1:C:65:SER:O	1:C:75:LEU:HD12	2.01	0.60
1:E:96:ASN:HA	3:F:353:ECO:C3	2.33	0.59
1:G:164:THR:HG22	2:H:174:VAL:HG12	1.83	0.59
1:A:8:SER:HB3	2:D:166:SER:OG	2.02	0.59
1:A:50:ILE:HD13	1:A:56:ARG:HA	1.83	0.59
2:B:24:THR:HG1	2:B:29:PHE:HD1	1.48	0.59
2:H:6:GLN:HG2	2:H:22:CYS:SG	2.42	0.59
2:H:127:TYR:HE2	2:H:148:LYS:HE2	1.65	0.59
2:D:6:GLN:HB3	2:D:113:THR:CG2	2.32	0.59
2:B:215:ILE:HG13	2:B:215:ILE:O	2.02	0.59
2:F:16:ALA:O	2:F:86:LEU:HD23	2.02	0.59
1:G:94:PHE:O	1:G:95:SER:O	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:THR:HG22	2:B:174:VAL:HG12	1.82	0.59
2:B:152:PRO:O	2:B:204:HIS:HE1	1.86	0.59
1:C:209:SER:O	1:C:211:ALA:N	2.36	0.59
2:F:23:ARG:HG2	2:F:78:ILE:HG12	1.85	0.59
2:H:17:SER:HA	2:H:86:LEU:HD21	1.84	0.59
1:C:42:PRO:O	1:C:43:ASP:HB2	2.01	0.59
2:D:182:LEU:C	2:D:182:LEU:HD23	2.27	0.59
1:E:57:ALA:HB3	1:E:60:VAL:HG21	1.83	0.59
1:A:72:LYS:HB2	1:A:72:LYS:HZ3	1.65	0.59
2:B:46:GLU:OE1	2:B:63:LYS:HE2	2.02	0.59
2:H:171:PHE:HB3	2:H:172:PRO:HD2	1.84	0.59
1:C:18:VAL:HG22	1:C:19:THR:N	2.17	0.59
2:D:29:PHE:CD2	2:D:77:SER:HA	2.38	0.59
2:B:23:ARG:HB3	2:B:78:ILE:HG12	1.84	0.59
1:E:17:THR:HG23	1:E:78:THR:HA	1.85	0.59
2:B:111:GLN:NE2	2:B:111:GLN:N	2.47	0.58
2:F:10:GLU:HG2	2:F:18:VAL:CG1	2.33	0.58
2:D:39:GLN:C	2:D:92:ALA:HB1	2.29	0.58
2:B:43:GLN:O	2:B:44:GLY:O	2.20	0.58
2:F:51:ILE:CG2	2:F:70:LEU:HD23	2.34	0.58
2:H:198:VAL:O	2:H:215:ILE:HG23	2.04	0.58
2:B:40:ARG:HB3	2:B:41:PRO:HD2	1.85	0.58
2:B:31:THR:HA	2:B:52:TYR:OH	2.03	0.58
1:C:85:GLU:CG	1:C:107:THR:HA	2.33	0.58
2:F:19:LYS:HE2	2:F:80:TYR:CD2	2.38	0.58
1:C:17:THR:HA	1:C:77:ILE:O	2.03	0.58
2:D:2:VAL:HB	2:D:108:TYR:CE1	2.39	0.58
1:A:171:ASN:OD1	1:A:173:LYS:HB2	2.04	0.58
2:D:2:VAL:HB	2:D:108:TYR:CD1	2.37	0.58
2:D:6:GLN:HE22	2:D:112:GLY:HA2	1.68	0.58
1:C:34:TYR:HB3	1:C:52:GLY:HA2	1.85	0.57
1:E:36:ASN:HD22	1:E:37:TRP:H	1.51	0.57
2:F:152:PRO:O	2:F:204:HIS:HE1	1.87	0.57
1:E:53:THR:HG21	1:E:68:LEU:HG	1.86	0.57
2:F:124:PRO:CB	2:F:150:TYR:HB3	2.31	0.57
1:G:20:LEU:N	1:G:20:LEU:HD12	2.19	0.57
1:G:82:THR:HA	1:G:108:VAL:HG11	1.85	0.57
2:B:127:TYR:HE2	2:B:148:LYS:HE2	1.68	0.57
2:B:198:VAL:O	2:B:215:ILE:HG23	2.03	0.57
1:E:18:VAL:HG22	1:E:19:THR:N	2.20	0.57
1:A:56:ARG:NE	1:A:62:ALA:HA	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:352:ECO:C7	3:D:352:ECO:H192	2.34	0.57
2:F:87:THR:CG2	2:F:88:SER:N	2.68	0.57
2:D:18:VAL:HG22	2:D:86:LEU:HD21	1.86	0.57
1:A:29:ILE:HD12	1:A:29:ILE:N	2.20	0.57
2:B:1:GLU:O	2:B:1:GLU:CD	2.48	0.57
2:B:54:GLY:O	2:B:55:ASP:HB2	2.04	0.56
2:B:37:VAL:HG12	2:B:38:ARG:N	2.20	0.56
1:G:42:PRO:O	1:G:43:ASP:HB2	2.05	0.56
1:G:56:ARG:HD3	1:G:60:VAL:O	2.05	0.56
2:F:127:TYR:HE2	2:F:148:LYS:HE2	1.68	0.56
1:E:30:THR:C	1:E:32:SER:H	2.13	0.56
2:D:1:GLU:O	2:D:26:GLY:HA3	2.06	0.56
2:H:87:THR:O	2:H:88:SER:C	2.49	0.56
2:D:64:PHE:HB3	2:D:68:ALA:HB3	1.87	0.56
1:A:24:SER:HB3	1:A:29:ILE:HD11	1.88	0.56
2:F:171:PHE:HB3	2:F:172:PRO:HD2	1.86	0.56
1:E:37:TRP:CE2	1:E:75:LEU:HB2	2.40	0.56
1:G:146:VAL:HG12	1:G:199:HIS:HB2	1.88	0.55
1:C:187:TRP:CZ2	1:C:210:ALA:HA	2.41	0.55
2:D:48:ILE:HG12	2:D:64:PHE:CE2	2.41	0.55
2:H:60:TYR:CE2	2:H:69:THR:HA	2.41	0.55
2:H:124:PRO:CB	2:H:150:TYR:HB3	2.33	0.55
1:E:81:GLN:O	1:E:108:VAL:HG11	2.07	0.55
1:E:88:TYR:CE2	1:E:106:VAL:HG21	2.42	0.55
1:G:15:GLY:O	1:G:79:GLY:HA2	2.07	0.55
2:H:175:LEU:HD13	2:H:180:TYR:CE1	2.41	0.55
1:E:14:PRO:HA	1:E:80:ALA:O	2.06	0.55
1:E:152:VAL:HG22	1:E:193:TYR:CD2	2.42	0.55
1:A:152:VAL:HG22	1:A:193:TYR:CD2	2.42	0.55
1:E:11:THR:HG22	1:E:107:THR:HB	1.87	0.55
1:E:31:THR:HG22	1:E:31:THR:O	2.07	0.55
2:H:143:LEU:HD22	2:H:143:LEU:H	1.72	0.55
1:E:20:LEU:O	1:E:74:ALA:HB1	2.07	0.54
1:G:56:ARG:NH1	1:G:56:ARG:HB2	2.22	0.54
1:G:152:VAL:HG12	1:G:190:HIS:CD2	2.42	0.54
2:D:51:ILE:HB	2:D:70:LEU:CD2	2.37	0.54
2:D:83:LEU:HD11	2:D:94:TYR:CE2	2.43	0.54
1:E:38:ILE:HD12	1:E:38:ILE:N	2.22	0.54
2:H:152:PRO:O	2:H:204:HIS:HE1	1.90	0.54
1:C:95:SER:O	1:C:96:ASN:CB	2.52	0.54
1:E:68:LEU:HD23	1:E:73:ALA:CB	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:TYR:CE1	2:B:155:VAL:HG13	2.42	0.54
2:H:81:LEU:HD13	2:H:81:LEU:C	2.32	0.54
2:B:111:GLN:H	2:B:111:GLN:HE21	1.51	0.54
2:F:38:ARG:HB3	2:F:48:ILE:HD11	1.90	0.54
1:G:50:ILE:HD13	1:G:56:ARG:HA	1.88	0.54
1:C:72:LYS:HB2	1:C:72:LYS:NZ	2.22	0.54
2:F:215:ILE:O	2:F:215:ILE:HG13	2.07	0.54
2:F:40:ARG:HA	2:F:92:ALA:HB2	1.88	0.54
2:F:87:THR:HG22	2:F:88:SER:H	1.73	0.54
1:C:152:VAL:HG22	1:C:193:TYR:CD2	2.43	0.54
2:H:70:LEU:HD11	2:H:81:LEU:HD23	1.90	0.54
2:D:13:ARG:N	2:D:13:ARG:HD2	2.23	0.53
2:D:152:PRO:O	2:D:204:HIS:HE1	1.91	0.53
1:E:164:THR:CB	2:F:172:PRO:HG2	2.38	0.53
1:A:9:ALA:O	1:A:10:LEU:HD23	2.07	0.53
2:D:127:TYR:HE2	2:D:148:LYS:HE2	1.72	0.53
1:E:28:ALA:C	1:E:29:ILE:HD12	2.32	0.53
1:G:169:GLN:CD	1:G:175:MET:HE3	2.33	0.53
2:H:40:ARG:O	2:H:41:PRO:C	2.51	0.53
1:A:63:ARG:HD3	1:A:79:GLY:O	2.07	0.53
1:E:50:ILE:HD13	1:E:56:ARG:HA	1.90	0.53
2:F:52:TYR:CD2	2:F:55:ASP:HB2	2.44	0.53
1:E:57:ALA:HB3	1:E:60:VAL:HG23	1.89	0.53
2:H:35:GLN:HG2	2:H:47:TRP:CH2	2.43	0.53
1:A:112:LYS:HD3	1:A:112:LYS:C	2.34	0.53
1:C:40:GLU:HB3	1:C:87:ILE:HB	1.91	0.53
2:D:17:SER:HA	2:D:86:LEU:CD2	2.38	0.53
1:G:30:THR:HG23	1:G:33:HIS:CE1	2.43	0.53
2:H:11:LEU:HD22	2:H:116:THR:HB	1.91	0.53
2:B:176:GLN:OE1	2:B:181:THR:HG21	2.09	0.53
1:E:29:ILE:HD12	1:E:29:ILE:N	2.23	0.53
2:H:6:GLN:NE2	2:H:112:GLY:H	2.07	0.53
2:D:29:PHE:CE2	2:D:77:SER:HA	2.44	0.53
1:E:37:TRP:CZ3	1:E:90:CYS:HB3	2.44	0.53
1:E:82:THR:HA	1:E:108:VAL:HG11	1.91	0.53
2:F:51:ILE:CB	2:F:70:LEU:HD23	2.38	0.53
2:F:52:TYR:HD2	2:F:55:ASP:HB2	1.73	0.53
2:D:67:LYS:HG3	2:D:68:ALA:H	1.73	0.53
2:F:36:TRP:CE3	2:F:81:LEU:HD12	2.44	0.53
2:F:86:LEU:HB3	2:F:117:VAL:HG21	1.91	0.53
1:A:151:LYS:HB2	1:A:194:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:LEU:HD13	2:B:180:TYR:CE1	2.44	0.52
2:D:35:GLN:HG2	2:D:47:TRP:HH2	1.69	0.52
2:D:176:GLN:OE1	2:D:181:THR:HG21	2.09	0.52
1:E:39:GLN:O	1:E:46:PHE:HA	2.08	0.52
1:C:56:ARG:NH2	1:C:64:PHE:O	2.43	0.52
2:D:40:ARG:O	2:D:41:PRO:C	2.52	0.52
1:A:38:ILE:HD13	2:B:109:TRP:CZ2	2.44	0.52
3:H:354:ECO:H192	3:H:354:ECO:C7	2.40	0.52
1:C:82:THR:HA	1:C:108:VAL:HB	1.91	0.52
1:E:34:TYR:O	1:E:35:ALA:C	2.52	0.52
1:C:119:LEU:HD21	1:C:195:CYS:HB3	1.91	0.52
2:D:34:MET:HB3	2:D:51:ILE:HG22	1.92	0.52
2:D:111:GLN:NE2	2:D:111:GLN:N	2.50	0.52
2:F:6:GLN:NE2	2:F:112:GLY:N	2.58	0.52
2:H:176:GLN:O	2:H:177:SER:HB2	2.09	0.52
2:F:6:GLN:HE22	2:F:112:GLY:HA2	1.75	0.52
1:G:34:TYR:HE2	2:H:103:TYR:CE1	2.27	0.52
2:H:57:ASP:OD1	2:H:59:ARG:HD2	2.09	0.52
2:H:150:TYR:CE1	2:H:155:VAL:HG13	2.45	0.52
1:C:97:GLN:O	1:C:97:GLN:HG3	2.10	0.52
2:D:28:SER:OG	2:D:31:THR:OG1	2.23	0.52
1:E:91:ALA:HB2	1:E:100:PHE:CE2	2.44	0.52
2:F:40:ARG:HA	2:F:92:ALA:CB	2.40	0.52
1:C:37:TRP:CD1	1:C:50:ILE:HB	2.43	0.52
1:E:52:GLY:O	1:E:53:THR:HB	2.09	0.52
2:F:6:GLN:NE2	2:F:112:GLY:CA	2.73	0.52
1:G:116:SER:HA	4:G:215:HOH:O	2.09	0.52
1:A:7:GLU:O	1:A:104:THR:HA	2.10	0.52
1:A:85:GLU:HG3	1:A:106:VAL:O	2.10	0.52
1:E:24:SER:H	1:E:29:ILE:HD11	1.74	0.52
2:D:36:TRP:CE3	2:D:81:LEU:HD12	2.45	0.51
1:E:2:ALA:HB3	1:E:94:PHE:CE1	2.44	0.51
1:A:38:ILE:HD13	2:B:109:TRP:HZ2	1.74	0.51
2:B:143:LEU:HD22	2:B:143:LEU:H	1.75	0.51
1:C:161:MET:HA	1:C:179:TYR:O	2.10	0.51
2:D:16:ALA:O	2:D:86:LEU:HD22	2.10	0.51
2:F:175:LEU:HD13	2:F:180:TYR:CE1	2.45	0.51
2:B:29:PHE:CE2	2:B:53:PRO:HB3	2.46	0.51
1:E:4:VAL:HG22	1:E:92:LEU:HD12	1.92	0.51
1:G:152:VAL:HG22	1:G:193:TYR:CD2	2.46	0.51
1:A:98:PHE:HB2	2:B:47:TRP:CE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ARG:HH21	1:C:62:ALA:CA	2.24	0.51
1:E:36:ASN:HA	1:E:50:ILE:O	2.10	0.51
2:F:176:GLN:OE1	2:F:181:THR:HG21	2.10	0.51
2:B:124:PRO:CB	2:B:150:TYR:HB3	2.33	0.51
3:B:351:ECO:H192	3:B:351:ECO:C7	2.40	0.51
1:C:98:PHE:HB2	2:D:47:TRP:CE3	2.45	0.51
2:D:64:PHE:C	2:D:66:GLY:N	2.66	0.51
1:E:112:LYS:HD3	1:E:112:LYS:C	2.35	0.51
1:E:202:HIS:HE1	4:E:213:HOH:O	1.92	0.51
2:B:67:LYS:HE3	2:B:90:ASP:OD2	2.10	0.51
1:C:164:THR:HG22	2:D:174:VAL:HG12	1.93	0.51
1:E:151:LYS:HB2	1:E:194:SER:HB3	1.92	0.51
2:F:140:MET:HE3	2:F:187:THR:HG22	1.92	0.51
1:G:57:ALA:HB3	1:G:60:VAL:CG2	2.40	0.51
1:C:152:VAL:HG13	1:C:193:TYR:CE2	2.46	0.51
2:F:176:GLN:O	2:F:177:SER:HB2	2.09	0.51
1:G:13:SER:O	1:G:14:PRO:C	2.53	0.51
1:G:57:ALA:HB3	1:G:60:VAL:HG21	1.93	0.51
1:C:57:ALA:HB3	1:C:60:VAL:HG23	1.92	0.51
2:D:111:GLN:HE21	2:D:111:GLN:N	1.96	0.51
2:H:6:GLN:HA	2:H:21:SER:O	2.10	0.51
1:C:53:THR:CG2	1:C:68:LEU:HG	2.40	0.51
2:D:61:THR:O	2:D:62:GLN:C	2.52	0.51
2:D:67:LYS:HG3	2:D:68:ALA:N	2.26	0.51
1:G:100:PHE:CG	2:H:45:LEU:HB2	2.46	0.51
2:F:22:CYS:HB3	2:F:34:MET:HE1	1.93	0.50
1:C:56:ARG:HH21	1:C:62:ALA:HA	1.76	0.50
1:G:23:ARG:HH11	1:G:23:ARG:HB2	1.76	0.50
1:G:112:LYS:HD3	1:G:112:LYS:C	2.36	0.50
1:C:23:ARG:HH11	1:C:23:ARG:HB2	1.76	0.50
2:D:171:PHE:HB3	2:D:172:PRO:HD2	1.92	0.50
2:D:194:PRO:O	2:D:195:SER:C	2.54	0.50
1:E:82:THR:HA	1:E:108:VAL:CG1	2.41	0.50
1:E:164:THR:HB	2:F:172:PRO:HG2	1.93	0.50
2:H:40:ARG:HA	2:H:92:ALA:HB2	1.92	0.50
2:D:70:LEU:N	2:D:70:LEU:CD1	2.74	0.50
1:E:152:VAL:HG13	1:E:193:TYR:CE2	2.47	0.50
2:H:176:GLN:OE1	2:H:181:THR:HG21	2.11	0.50
1:A:29:ILE:HD13	1:A:71:ASP:O	2.10	0.50
1:C:152:VAL:HG22	1:C:193:TYR:HD2	1.77	0.50
1:E:9:ALA:O	1:E:10:LEU:HD23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:THR:HG23	1:E:75:LEU:O	2.11	0.50
1:A:161:MET:HA	1:A:179:TYR:O	2.11	0.50
2:B:40:ARG:C	2:B:42:GLY:H	2.19	0.50
1:C:33:HIS:O	1:C:34:TYR:C	2.55	0.50
1:C:81:GLN:O	1:C:108:VAL:HG11	2.12	0.50
1:E:94:PHE:O	1:E:95:SER:O	2.30	0.50
1:E:152:VAL:HG12	1:E:190:HIS:CD2	2.47	0.50
2:F:40:ARG:HB3	2:F:41:PRO:HD2	1.94	0.50
2:F:122:THR:HG21	2:F:179:LEU:HD21	1.94	0.50
1:G:30:THR:OG1	1:G:31:THR:N	2.44	0.50
1:E:91:ALA:HB2	1:E:100:PHE:CD2	2.47	0.50
2:F:87:THR:CG2	2:F:88:SER:H	2.25	0.50
2:F:152:PRO:HD2	2:F:206:ALA:CB	2.42	0.50
2:H:6:GLN:HE21	2:H:110:GLY:HA3	1.76	0.50
1:A:24:SER:CB	1:A:29:ILE:HD11	2.42	0.50
2:B:176:GLN:O	2:B:177:SER:HB2	2.11	0.50
2:B:52:TYR:HD2	2:B:55:ASP:HB3	1.77	0.49
1:A:63:ARG:HB2	1:A:78:THR:O	2.11	0.49
1:C:209:SER:C	1:C:211:ALA:N	2.68	0.49
1:E:164:THR:HG22	2:F:174:VAL:CG1	2.42	0.49
2:F:36:TRP:CD2	2:F:81:LEU:HD12	2.47	0.49
2:H:64:PHE:O	2:H:65:LYS:C	2.54	0.49
2:B:152:PRO:HD2	2:B:206:ALA:CB	2.43	0.49
2:F:6:GLN:NE2	2:F:112:GLY:H	2.10	0.49
2:B:97:SER:HB3	2:B:109:TRP:CD2	2.47	0.49
1:C:23:ARG:NH2	1:C:72:LYS:HD3	2.26	0.49
1:C:146:VAL:HG12	1:C:199:HIS:HB2	1.95	0.49
2:H:194:PRO:O	2:H:195:SER:C	2.55	0.49
2:H:215:ILE:HG13	2:H:215:ILE:O	2.11	0.49
1:A:87:ILE:HG12	1:A:105:LYS:CG	2.37	0.49
2:B:194:PRO:O	2:B:195:SER:C	2.56	0.49
1:E:98:PHE:HD1	2:F:47:TRP:CZ3	2.31	0.49
1:E:189:ARG:O	1:E:189:ARG:HG2	2.13	0.49
1:G:17:THR:HG23	1:G:78:THR:HA	1.92	0.49
2:F:122:THR:HG23	2:F:151:PHE:HB3	1.94	0.49
1:G:189:ARG:HG2	1:G:189:ARG:O	2.13	0.49
1:C:206:LYS:HD3	2:D:134:ALA:HB1	1.93	0.49
2:D:176:GLN:O	2:D:177:SER:HB2	2.12	0.49
1:E:29:ILE:HG22	1:E:68:LEU:HD21	1.95	0.49
2:H:67:LYS:HG3	2:H:68:ALA:H	1.78	0.49
2:F:4:LEU:CD1	2:F:97:SER:HA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:178:ASP:OD1	2:H:28:SER:HB2	2.13	0.49
2:H:37:VAL:HG11	2:H:45:LEU:HB3	1.94	0.49
2:B:17:SER:HB3	2:B:84:ASN:HA	1.95	0.49
2:D:27:TYR:C	2:D:27:TYR:HD2	2.21	0.49
1:E:119:LEU:HD21	1:E:195:CYS:HB3	1.94	0.49
1:A:7:GLU:O	1:A:104:THR:HG23	2.13	0.48
2:B:171:PHE:HB3	2:B:172:PRO:HD2	1.94	0.48
1:C:49:LEU:HA	1:C:60:VAL:CG2	2.37	0.48
2:H:70:LEU:N	2:H:70:LEU:HD12	2.28	0.48
1:E:4:VAL:HG11	1:E:22:CYS:SG	2.53	0.48
1:G:25:SER:O	1:G:26:SER:C	2.56	0.48
2:H:3:GLN:C	2:H:4:LEU:HD23	2.38	0.48
1:C:112:LYS:HD3	1:C:112:LYS:C	2.38	0.48
2:D:27:TYR:C	2:D:27:TYR:CD2	2.91	0.48
1:A:129:THR:HG22	1:A:129:THR:O	2.13	0.48
2:B:36:TRP:CD1	2:B:70:LEU:HD11	2.49	0.48
2:D:1:GLU:HA	2:D:1:GLU:OE1	2.13	0.48
1:E:146:VAL:HG12	1:E:199:HIS:HB2	1.96	0.48
2:F:60:TYR:CE2	2:F:69:THR:HA	2.48	0.48
1:G:96:ASN:HA	3:H:354:ECO:C3	2.44	0.48
1:C:56:ARG:HH21	1:C:62:ALA:C	2.21	0.48
1:E:7:GLU:N	1:E:7:GLU:OE1	2.46	0.48
2:H:22:CYS:HB3	2:H:34:MET:CE	2.43	0.48
2:H:52:TYR:CD2	2:H:55:ASP:HB2	2.33	0.48
2:H:60:TYR:N	2:H:60:TYR:CD1	2.81	0.48
2:H:152:PRO:HD2	2:H:206:ALA:CB	2.43	0.48
1:A:169:GLN:CD	1:A:175:MET:HE3	2.38	0.48
2:B:111:GLN:N	2:B:111:GLN:HE21	2.10	0.48
1:C:93:TRP:HA	1:C:93:TRP:CE3	2.48	0.48
1:C:137:THR:HB	2:D:171:PHE:CZ	2.48	0.48
2:D:84:ASN:O	2:D:85:SER:C	2.56	0.48
1:E:18:VAL:HG12	1:E:77:ILE:HB	1.94	0.48
1:E:19:THR:HA	1:E:75:LEU:O	2.13	0.48
1:G:96:ASN:HA	3:H:354:ECO:C2	2.43	0.48
1:A:85:GLU:OE1	1:A:107:THR:HG23	2.13	0.48
1:G:17:THR:HG23	1:G:77:ILE:O	2.14	0.48
2:H:27:TYR:HD2	2:H:32:TYR:CD2	2.32	0.48
2:F:35:GLN:HG2	2:F:47:TRP:HH2	1.75	0.48
2:B:111:GLN:H	2:B:111:GLN:CD	2.22	0.48
1:E:81:GLN:HB3	1:E:83:GLU:HG2	1.96	0.48
2:F:78:ILE:HG22	2:F:79:VAL:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:MET:HE3	2:F:187:THR:CG2	2.44	0.48
1:C:12:THR:O	1:C:108:VAL:HA	2.14	0.48
2:B:24:THR:HG21	2:B:27:TYR:OH	2.14	0.47
2:D:17:SER:HA	2:D:86:LEU:HD22	1.94	0.47
2:D:52:TYR:HD2	2:D:55:ASP:HB2	1.79	0.47
2:D:64:PHE:O	2:D:66:GLY:N	2.47	0.47
2:F:48:ILE:HG23	2:F:64:PHE:CG	2.49	0.47
1:C:29:ILE:HD12	1:C:29:ILE:H	1.78	0.47
1:C:91:ALA:HA	1:C:99:ILE:O	2.13	0.47
1:C:152:VAL:HG12	1:C:190:HIS:CD2	2.49	0.47
1:C:169:GLN:CD	1:C:175:MET:HE3	2.38	0.47
2:D:35:GLN:HE22	2:D:98:ARG:C	2.21	0.47
2:D:124:PRO:CB	2:D:150:TYR:HB3	2.33	0.47
1:E:24:SER:HB2	1:E:92:LEU:CD1	2.44	0.47
1:G:151:LYS:HB2	1:G:194:SER:HB3	1.95	0.47
2:H:48:ILE:HA	2:H:64:PHE:CD2	2.49	0.47
1:C:39:GLN:CB	1:C:49:LEU:HD11	2.39	0.47
2:F:60:TYR:HE2	2:F:68:ALA:O	1.97	0.47
1:G:152:VAL:CG2	1:G:157:VAL:HG11	2.44	0.47
2:H:29:PHE:CE2	2:H:53:PRO:HB3	2.49	0.47
2:H:57:ASP:CG	2:H:59:ARG:HH11	2.21	0.47
1:A:189:ARG:O	1:A:189:ARG:HG2	2.15	0.47
2:F:150:TYR:CE1	2:F:155:VAL:HG13	2.49	0.47
2:H:122:THR:HG21	2:H:179:LEU:HD21	1.96	0.47
2:F:4:LEU:HB2	2:F:109:TRP:O	2.15	0.47
2:F:34:MET:HG2	2:F:79:VAL:HG21	1.96	0.47
2:F:174:VAL:CG2	2:F:181:THR:HG23	2.44	0.47
1:C:30:THR:C	1:C:68:LEU:HD11	2.40	0.47
1:C:209:SER:O	1:C:210:ALA:C	2.58	0.47
2:D:26:GLY:O	2:D:27:TYR:CB	2.62	0.47
1:E:183:THR:O	1:E:184:ALA:C	2.58	0.47
4:A:217:HOH:O	2:B:44:GLY:HA2	2.15	0.47
2:D:152:PRO:HD2	2:D:206:ALA:CB	2.45	0.47
2:F:51:ILE:HB	2:F:70:LEU:CD2	2.43	0.47
1:G:38:ILE:CD1	2:H:109:TRP:HZ2	2.27	0.47
1:G:134:LEU:HD11	1:G:187:TRP:CZ3	2.50	0.47
1:G:152:VAL:CG1	1:G:190:HIS:CD2	2.98	0.47
2:H:39:GLN:O	2:H:92:ALA:HB1	2.14	0.47
2:H:83:LEU:HD11	2:H:94:TYR:CE2	2.50	0.47
1:E:137:THR:HB	2:F:171:PHE:CZ	2.50	0.47
2:F:40:ARG:HD3	2:F:43:GLN:NE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:GLY:C	1:G:103:GLY:H	2.23	0.47
1:A:119:LEU:HD21	1:A:195:CYS:HB3	1.95	0.47
1:G:34:TYR:O	1:G:35:ALA:C	2.57	0.47
1:A:95:SER:O	1:A:96:ASN:CB	2.63	0.47
2:H:6:GLN:OE1	2:H:113:THR:HG22	2.14	0.47
2:B:51:ILE:HB	2:B:70:LEU:HD23	1.97	0.46
1:C:194:SER:HB2	1:C:207:SER:OG	2.14	0.46
2:F:7:SER:O	2:F:113:THR:HG22	2.15	0.46
2:F:194:PRO:O	2:F:195:SER:C	2.58	0.46
1:A:152:VAL:CG2	1:A:157:VAL:HG11	2.45	0.46
2:F:4:LEU:HD12	2:F:109:TRP:CA	2.46	0.46
2:F:67:LYS:NZ	2:F:84:ASN:O	2.48	0.46
1:E:206:LYS:HD3	2:F:134:ALA:HB1	1.97	0.46
2:B:122:THR:HG23	2:B:151:PHE:HB3	1.97	0.46
2:H:34:MET:O	2:H:50:ALA:HA	2.16	0.46
2:H:122:THR:HG23	2:H:151:PHE:HB3	1.98	0.46
1:A:52:GLY:CA	2:B:103:TYR:HA	2.46	0.46
1:C:57:ALA:HB1	1:C:58:PRO:HD2	1.96	0.46
2:D:34:MET:O	2:D:50:ALA:HA	2.16	0.46
2:D:143:LEU:HD22	2:D:143:LEU:H	1.80	0.46
1:C:152:VAL:CG2	1:C:157:VAL:HG11	2.45	0.46
1:E:12:THR:OG1	1:E:13:SER:N	2.48	0.46
1:E:68:LEU:CD2	1:E:73:ALA:HB2	2.34	0.46
2:D:57:ASP:CG	2:D:59:ARG:HE	2.22	0.46
2:F:68:ALA:O	2:F:69:THR:HG23	2.16	0.46
1:G:20:LEU:O	1:G:74:ALA:HB1	2.15	0.46
2:H:126:VAL:O	2:H:213:LYS:HE3	2.16	0.46
1:A:145:VAL:HG13	1:A:145:VAL:O	2.16	0.46
1:C:20:LEU:HD23	1:C:104:THR:HB	1.98	0.46
2:F:53:PRO:O	2:F:55:ASP:N	2.42	0.46
1:G:23:ARG:HH12	1:G:72:LYS:HE3	1.81	0.46
2:B:22:CYS:HB3	2:B:34:MET:HE1	1.97	0.45
2:B:37:VAL:CG1	2:B:38:ARG:N	2.80	0.45
1:C:93:TRP:CD1	2:D:102:LEU:HD13	2.50	0.45
2:D:175:LEU:HD13	2:D:180:TYR:CE1	2.51	0.45
2:H:67:LYS:NZ	2:H:84:ASN:O	2.49	0.45
1:C:30:THR:HA	1:C:68:LEU:HD13	1.98	0.45
1:E:160:GLY:N	2:H:1:GLU:CD	2.64	0.45
1:G:119:LEU:HD21	1:G:195:CYS:HB3	1.96	0.45
2:H:70:LEU:N	2:H:70:LEU:CD1	2.79	0.45
1:A:152:VAL:HG13	1:A:193:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ARG:NH2	1:C:62:ALA:O	2.48	0.45
2:F:60:TYR:N	2:F:60:TYR:CD1	2.83	0.45
2:D:40:ARG:HB3	2:D:41:PRO:CD	2.43	0.45
1:E:14:PRO:HG3	1:E:108:VAL:HG12	1.98	0.45
1:E:193:TYR:O	1:E:207:SER:HA	2.16	0.45
1:G:56:ARG:HE	1:G:62:ALA:HA	1.82	0.45
1:A:15:GLY:O	1:A:79:GLY:HA2	2.16	0.45
1:A:23:ARG:HB2	1:A:23:ARG:HH11	1.82	0.45
2:D:122:THR:HG23	2:D:151:PHE:HB3	1.98	0.45
1:E:36:ASN:ND2	1:E:50:ILE:O	2.50	0.45
1:C:193:TYR:O	1:C:207:SER:HA	2.17	0.45
2:D:204:HIS:HD2	2:D:207:SER:OG	1.99	0.45
1:E:129:THR:HG22	1:E:129:THR:O	2.17	0.45
2:F:164:LEU:HD23	2:F:186:VAL:HG21	1.97	0.45
1:G:63:ARG:CZ	1:G:81:GLN:HG2	2.46	0.45
2:B:55:ASP:O	2:B:57:ASP:N	2.50	0.45
1:C:41:LYS:O	1:C:42:PRO:C	2.60	0.45
1:C:53:THR:HG21	1:C:68:LEU:HG	1.97	0.45
1:C:183:THR:O	1:C:184:ALA:C	2.60	0.45
1:E:152:VAL:CG1	1:E:190:HIS:CD2	2.99	0.45
1:E:169:GLN:CD	1:E:175:MET:HE3	2.42	0.45
2:H:29:PHE:CD1	2:H:77:SER:HA	2.51	0.45
2:H:29:PHE:CZ	2:H:79:VAL:HG23	2.52	0.45
2:H:69:THR:C	2:H:70:LEU:HD12	2.42	0.45
1:C:129:THR:HG22	1:C:129:THR:O	2.17	0.45
2:D:40:ARG:CG	2:D:92:ALA:HB2	2.43	0.45
2:D:60:TYR:CE2	2:D:70:LEU:HD13	2.52	0.45
1:C:37:TRP:HB2	1:C:50:ILE:H	1.81	0.45
2:F:111:GLN:NE2	2:F:112:GLY:H	2.13	0.45
1:A:72:LYS:HB2	1:A:72:LYS:HZ2	1.80	0.44
2:F:6:GLN:HB3	2:F:113:THR:CG2	2.46	0.44
1:G:9:ALA:O	1:G:10:LEU:HD23	2.17	0.44
1:G:152:VAL:HG13	1:G:193:TYR:CE2	2.52	0.44
1:G:161:MET:HA	1:G:179:TYR:O	2.17	0.44
2:B:73:ASP:OD2	2:B:76:SER:OG	2.32	0.44
2:B:83:LEU:HD11	2:B:94:TYR:CE2	2.53	0.44
1:E:6:GLN:HG2	1:E:21:THR:O	2.17	0.44
2:F:18:VAL:HG23	2:F:86:LEU:HD21	1.99	0.44
2:F:34:MET:HE3	2:F:79:VAL:CB	2.43	0.44
2:F:204:HIS:HD2	2:F:207:SER:OG	2.01	0.44
1:G:56:ARG:NE	1:G:62:ALA:HA	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:THR:HG22	1:A:6:GLN:N	2.33	0.44
2:B:34:MET:O	2:B:50:ALA:HA	2.17	0.44
1:C:83:GLU:C	1:C:85:GLU:N	2.71	0.44
1:E:29:ILE:HG23	1:E:33:HIS:CG	2.53	0.44
1:E:152:VAL:HG22	1:E:193:TYR:HD2	1.82	0.44
1:G:129:THR:HG22	1:G:129:THR:O	2.17	0.44
1:A:44:HIS:NE2	2:B:93:VAL:HG21	2.33	0.44
1:C:66:GLY:HA2	1:C:74:ALA:O	2.17	0.44
2:D:55:ASP:OD1	2:H:65:LYS:HE3	2.18	0.44
1:E:2:ALA:HB3	1:E:94:PHE:HE1	1.82	0.44
1:E:96:ASN:OD1	1:E:97:GLN:HG2	2.16	0.44
2:F:6:GLN:HE21	2:F:110:GLY:C	2.25	0.44
2:F:32:TYR:O	2:F:53:PRO:HD2	2.18	0.44
1:G:56:ARG:NH1	1:G:56:ARG:CB	2.79	0.44
1:A:29:ILE:HG21	1:A:73:ALA:HB2	2.00	0.44
1:A:33:HIS:O	1:A:34:TYR:C	2.59	0.44
2:H:40:ARG:HA	2:H:92:ALA:CB	2.48	0.44
2:H:102:LEU:HD23	3:H:354:ECO:H181	2.00	0.44
2:H:140:MET:HE3	2:H:187:THR:CG2	2.48	0.44
2:B:126:VAL:O	2:B:213:LYS:HE3	2.17	0.44
2:D:59:ARG:HG2	2:D:59:ARG:NH1	2.30	0.44
1:G:49:LEU:HD21	1:G:88:TYR:HE1	1.81	0.44
1:C:61:PRO:HB3	1:C:63:ARG:NH1	2.33	0.44
1:C:179:TYR:OH	2:D:183:SER:HB2	2.18	0.44
1:E:152:VAL:CG2	1:E:157:VAL:HG11	2.48	0.44
2:H:5:GLN:O	2:H:23:ARG:HG2	2.18	0.44
2:B:12:ALA:O	2:B:117:VAL:HA	2.17	0.44
2:B:17:SER:HB2	2:B:83:LEU:O	2.18	0.44
1:E:208:LEU:HD12	1:E:208:LEU:O	2.17	0.44
1:E:209:SER:O	1:E:210:ALA:C	2.61	0.44
2:F:40:ARG:HD3	2:F:43:GLN:HE22	1.83	0.44
1:G:145:VAL:HG13	1:G:145:VAL:O	2.18	0.44
2:H:33:TRP:CD1	3:H:354:ECO:H161	2.53	0.44
1:A:24:SER:HB3	1:A:29:ILE:CD1	2.48	0.44
1:A:57:ALA:O	1:A:60:VAL:HG23	2.18	0.43
1:A:96:ASN:HB2	3:B:351:ECO:O3	2.18	0.43
1:C:145:VAL:O	1:C:145:VAL:HG13	2.18	0.43
2:H:143:LEU:HD22	2:H:143:LEU:N	2.33	0.43
1:A:63:ARG:NE	1:A:84:ASP:OD2	2.51	0.43
1:A:95:SER:O	1:A:96:ASN:HB3	2.17	0.43
2:B:34:MET:HE3	2:B:79:VAL:CB	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:PHE:HE1	1:C:175:MET:HA	1.83	0.43
1:E:50:ILE:HA	1:E:55:ASN:O	2.19	0.43
2:H:29:PHE:CG	2:H:77:SER:HA	2.53	0.43
1:C:136:CYS:HB2	1:C:150:TRP:CZ2	2.53	0.43
2:D:27:TYR:HE1	2:D:98:ARG:HD3	1.82	0.43
2:B:61:THR:O	2:B:62:GLN:C	2.60	0.43
1:C:164:THR:CB	2:D:172:PRO:HG2	2.48	0.43
2:D:34:MET:HE2	2:D:79:VAL:CG2	2.47	0.43
2:F:10:GLU:HG2	2:F:18:VAL:HG12	2.00	0.43
2:B:159:TRP:CZ3	2:B:200:CYS:HB3	2.53	0.43
2:D:159:TRP:CZ3	2:D:200:CYS:HB3	2.54	0.43
2:F:29:PHE:CE2	2:F:74:ARG:HA	2.53	0.43
2:H:81:LEU:HD11	2:H:83:LEU:HD21	1.99	0.43
1:A:34:TYR:O	1:A:35:ALA:C	2.62	0.43
2:D:23:ARG:HB3	2:D:78:ILE:HG12	1.99	0.43
2:D:64:PHE:O	2:D:65:LYS:C	2.61	0.43
1:G:64:PHE:CE1	1:G:77:ILE:HG12	2.53	0.43
1:G:164:THR:CG2	1:G:177:SER:OG	2.66	0.43
2:B:39:GLN:O	2:B:92:ALA:HB1	2.18	0.43
2:H:32:TYR:O	2:H:53:PRO:HD2	2.19	0.43
2:H:140:MET:HE3	2:H:187:THR:HG22	1.99	0.43
2:H:174:VAL:CG2	2:H:181:THR:HG23	2.49	0.43
2:B:38:ARG:HB3	2:B:48:ILE:HD11	1.99	0.43
2:B:143:LEU:HD22	2:B:143:LEU:N	2.33	0.43
2:D:52:TYR:HB3	2:D:57:ASP:HB3	1.99	0.43
3:D:352:ECO:H192	3:D:352:ECO:HC71	2.01	0.43
2:H:11:LEU:HD13	2:H:12:ALA:N	2.34	0.43
1:A:152:VAL:HG22	1:A:193:TYR:HD2	1.81	0.43
1:A:152:VAL:HG12	1:A:190:HIS:CD2	2.54	0.43
2:D:27:TYR:CD1	2:D:98:ARG:NH1	2.86	0.43
2:F:111:GLN:NE2	2:F:112:GLY:N	2.66	0.43
1:A:63:ARG:CZ	1:A:81:GLN:CG	2.96	0.43
1:A:146:VAL:HG12	1:A:199:HIS:HB2	2.01	0.43
2:B:24:THR:OG1	2:B:29:PHE:HD1	2.02	0.43
1:C:209:SER:C	1:C:211:ALA:H	2.27	0.43
1:G:57:ALA:HB1	1:G:58:PRO:HD2	1.99	0.43
1:G:68:LEU:HD23	1:G:73:ALA:HA	2.01	0.43
1:G:152:VAL:HG22	1:G:193:TYR:HD2	1.84	0.43
2:H:70:LEU:CD1	2:H:81:LEU:HD23	2.48	0.43
1:E:161:MET:HA	1:E:179:TYR:O	2.19	0.42
2:F:60:TYR:OH	2:F:69:THR:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:ARG:NH2	1:G:72:LYS:CE	2.79	0.42
1:A:61:PRO:O	1:A:63:ARG:N	2.52	0.42
1:A:93:TRP:HE3	1:A:98:PHE:CE1	2.37	0.42
2:B:36:TRP:NE1	2:B:70:LEU:HD11	2.33	0.42
1:E:88:TYR:HE2	1:E:106:VAL:HG21	1.83	0.42
2:F:10:GLU:HG2	2:F:18:VAL:HG11	2.00	0.42
4:G:217:HOH:O	2:H:171:PHE:HB2	2.19	0.42
2:B:23:ARG:HA	2:B:77:SER:O	2.19	0.42
1:C:63:ARG:HB2	1:C:78:THR:O	2.19	0.42
2:D:60:TYR:HE2	2:D:70:LEU:HD13	1.85	0.42
1:E:36:ASN:OD1	2:F:106:MET:HE3	2.19	0.42
1:E:49:LEU:HD12	1:E:49:LEU:HA	1.84	0.42
1:C:18:VAL:CG1	1:C:77:ILE:HD12	2.49	0.42
2:D:62:GLN:OE1	2:D:62:GLN:HA	2.19	0.42
1:E:130:ASN:HD22	1:E:130:ASN:HA	1.66	0.42
1:C:20:LEU:N	1:C:20:LEU:HD12	2.34	0.42
1:C:57:ALA:HB3	1:C:60:VAL:CG2	2.50	0.42
2:F:33:TRP:O	2:F:34:MET:HB2	2.20	0.42
1:A:115:PRO:HA	1:A:139:THR:O	2.20	0.42
2:B:48:ILE:HG12	2:B:64:PHE:CE2	2.54	0.42
2:B:122:THR:HG21	2:B:179:LEU:HD21	2.01	0.42
1:C:96:ASN:HA	3:D:352:ECO:C3	2.49	0.42
2:D:140:MET:HE3	2:D:187:THR:HG22	2.01	0.42
1:E:53:THR:HG23	1:E:68:LEU:HG	2.02	0.42
1:C:4:VAL:HG12	1:C:5:THR:N	2.34	0.42
1:C:19:THR:HA	1:C:75:LEU:O	2.19	0.42
2:D:103:TYR:C	2:D:104:TYR:CD1	2.98	0.42
1:E:72:LYS:HD3	1:E:72:LYS:N	2.35	0.42
1:A:137:THR:HB	2:B:171:PHE:CZ	2.54	0.42
1:A:174:TYR:CD1	1:A:174:TYR:N	2.88	0.42
2:B:51:ILE:O	2:B:53:PRO:HD3	2.20	0.42
1:C:22:CYS:HB3	1:C:73:ALA:HB3	2.01	0.42
1:C:56:ARG:NH2	1:C:62:ALA:C	2.78	0.42
1:C:93:TRP:NE1	2:D:102:LEU:CD1	2.83	0.42
1:C:208:LEU:HD12	1:C:208:LEU:O	2.19	0.42
1:E:79:GLY:O	1:E:80:ALA:C	2.63	0.42
2:H:45:LEU:HG	4:H:357:HOH:O	2.19	0.42
1:C:34:TYR:O	1:C:35:ALA:C	2.63	0.42
1:E:4:VAL:HA	1:E:23:ARG:O	2.20	0.42
1:E:96:ASN:HA	3:F:353:ECO:C2	2.49	0.42
1:G:51:SER:O	1:G:55:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:TYR:CD1	1:G:174:TYR:N	2.87	0.42
2:B:34:MET:HG2	2:B:79:VAL:HG11	2.01	0.42
1:C:36:ASN:CG	2:D:106:MET:HE3	2.45	0.42
2:D:27:TYR:CE1	2:D:98:ARG:HD3	2.55	0.42
2:D:122:THR:HG21	2:D:179:LEU:HD21	2.01	0.42
1:E:136:CYS:HB2	1:E:150:TRP:CZ2	2.55	0.42
2:F:84:ASN:O	2:F:85:SER:C	2.62	0.42
1:A:69:ILE:O	1:A:72:LYS:NZ	2.53	0.41
2:H:175:LEU:HD13	2:H:180:TYR:CZ	2.55	0.41
1:A:183:THR:O	1:A:184:ALA:C	2.64	0.41
1:A:193:TYR:O	1:A:207:SER:HA	2.20	0.41
1:C:141:PHE:CE1	1:C:175:MET:HA	2.55	0.41
2:D:37:VAL:CG1	2:D:45:LEU:HB3	2.51	0.41
1:E:2:ALA:HB1	1:E:26:SER:H	1.85	0.41
2:H:37:VAL:CG1	2:H:45:LEU:HB3	2.51	0.41
1:A:34:TYR:CD1	2:B:102:LEU:HD13	2.55	0.41
2:B:105:THR:O	2:B:106:MET:HB2	2.20	0.41
1:C:151:LYS:HB2	1:C:194:SER:HB3	2.02	0.41
2:D:86:LEU:HD12	2:D:90:ASP:CB	2.50	0.41
2:D:150:TYR:CE1	2:D:155:VAL:HG13	2.55	0.41
1:G:56:ARG:CB	1:G:56:ARG:HH11	2.32	0.41
3:B:351:ECO:O3	2:F:56:ASP:HB2	2.19	0.41
1:C:30:THR:HA	1:C:68:LEU:CD1	2.51	0.41
1:C:134:LEU:HD11	1:C:187:TRP:CZ3	2.54	0.41
1:E:38:ILE:CG2	1:E:46:PHE:HB3	2.50	0.41
2:D:48:ILE:HA	2:D:64:PHE:CE2	2.55	0.41
1:E:16:GLU:HB3	1:E:17:THR:H	1.74	0.41
2:F:13:ARG:CA	2:F:13:ARG:HE	2.34	0.41
2:F:33:TRP:HB3	2:F:34:MET:H	1.58	0.41
1:A:61:PRO:C	1:A:63:ARG:N	2.79	0.41
1:E:6:GLN:HB3	1:E:7:GLU:H	1.57	0.41
1:E:175:MET:HE1	2:F:169:HIS:ND1	2.35	0.41
1:C:164:THR:HB	2:D:172:PRO:HG2	2.02	0.41
2:H:204:HIS:HD2	2:H:207:SER:OG	2.04	0.41
1:A:6:GLN:HB3	1:A:104:THR:OG1	2.20	0.41
1:C:152:VAL:CG1	1:C:190:HIS:CD2	3.03	0.41
2:D:22:CYS:O	2:D:34:MET:HE1	2.21	0.41
2:D:174:VAL:CG2	2:D:181:THR:HG23	2.51	0.41
1:E:29:ILE:O	1:E:68:LEU:HD22	2.21	0.41
1:G:136:CYS:HB2	1:G:150:TRP:CZ2	2.56	0.41
2:H:38:ARG:O	2:H:38:ARG:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:LEU:HB3	2:H:215:ILE:HG12	2.03	0.41
1:A:152:VAL:O	1:A:153:ASP:HB2	2.20	0.41
2:B:4:LEU:O	2:B:110:GLY:HA2	2.20	0.41
1:C:12:THR:HG23	1:C:108:VAL:HG22	2.02	0.41
1:C:93:TRP:HA	1:C:93:TRP:HE3	1.85	0.41
2:D:81:LEU:CD2	2:D:82:GLN:N	2.84	0.41
1:E:34:TYR:HB3	2:F:102:LEU:O	2.21	0.41
3:F:353:ECO:C7	3:F:353:ECO:H192	2.51	0.41
1:G:36:ASN:C	1:G:36:ASN:ND2	2.77	0.41
1:G:36:ASN:OD1	2:H:106:MET:HE3	2.21	0.41
2:H:4:LEU:HA	2:H:23:ARG:O	2.21	0.41
2:D:28:SER:HB2	2:D:31:THR:HG23	2.02	0.41
2:D:55:ASP:OD2	2:H:60:TYR:N	2.54	0.41
1:E:117:VAL:HG11	1:E:206:LYS:HB2	2.02	0.41
1:A:23:ARG:NH1	1:A:23:ARG:CB	2.84	0.40
1:A:209:SER:C	1:A:211:ALA:N	2.79	0.40
1:C:18:VAL:HG12	1:C:77:ILE:HB	2.02	0.40
2:D:44:GLY:N	4:D:354:HOH:O	2.54	0.40
2:D:64:PHE:C	2:D:66:GLY:H	2.29	0.40
1:E:29:ILE:O	1:E:68:LEU:HD13	2.21	0.40
1:A:179:TYR:OH	2:B:183:SER:HB2	2.21	0.40
2:D:11:LEU:C	2:D:11:LEU:HD13	2.46	0.40
1:E:29:ILE:HD13	1:E:72:LYS:HA	2.02	0.40
1:E:93:TRP:NE1	1:E:95:SER:HA	2.36	0.40
1:E:145:VAL:O	1:E:145:VAL:HG13	2.21	0.40
2:F:37:VAL:CG1	2:F:46:GLU:O	2.66	0.40
2:B:55:ASP:O	2:B:55:ASP:OD2	2.39	0.40
2:D:101:SER:C	2:D:103:TYR:H	2.29	0.40
1:E:2:ALA:HA	1:E:25:SER:HB3	2.04	0.40
1:E:18:VAL:HG22	1:E:19:THR:H	1.85	0.40
1:E:63:ARG:CZ	1:E:81:GLN:HG3	2.51	0.40
1:E:152:VAL:O	1:E:153:ASP:HB2	2.20	0.40
2:F:6:GLN:HE21	2:F:110:GLY:HA3	1.87	0.40
1:G:1:GLN:HB3	1:G:99:ILE:HD11	2.03	0.40
1:G:4:VAL:HG23	1:G:99:ILE:HG22	2.03	0.40
1:G:56:ARG:HB2	1:G:56:ARG:CZ	2.51	0.40
2:H:4:LEU:HD22	2:H:24:THR:HG22	2.02	0.40
2:H:67:LYS:NZ	2:H:67:LYS:HB3	2.37	0.40
1:G:163:THR:HA	1:G:178:SER:HA	2.04	0.40
2:H:76:SER:O	2:H:77:SER:HB2	2.21	0.40
2:H:174:VAL:HG22	2:H:181:THR:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASN:O	1:A:97:GLN:HB3	2.20	0.40
1:A:194:SER:HB2	1:A:207:SER:OG	2.21	0.40
1:C:38:ILE:HD13	2:D:109:TRP:CZ2	2.56	0.40
1:E:30:THR:C	1:E:32:SER:N	2.79	0.40
1:E:182:LEU:HD11	1:E:193:TYR:CE2	2.56	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	204/212 (96%)	180 (88%)	17 (8%)	7 (3%)	3	6
1	C	204/212 (96%)	174 (85%)	17 (8%)	13 (6%)	1	1
1	E	204/212 (96%)	167 (82%)	24 (12%)	13 (6%)	1	1
1	G	204/212 (96%)	179 (88%)	19 (9%)	6 (3%)	3	8
2	B	210/218 (96%)	180 (86%)	23 (11%)	7 (3%)	3	7
2	D	210/218 (96%)	179 (85%)	25 (12%)	6 (3%)	3	8
2	F	210/218 (96%)	184 (88%)	21 (10%)	5 (2%)	4	10
2	H	210/218 (96%)	183 (87%)	23 (11%)	4 (2%)	6	14
All	All	1656/1720 (96%)	1426 (86%)	169 (10%)	61 (4%)	2	5

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	95	SER
2	B	41	PRO
2	B	55	ASP
2	B	56	ASP

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Mol	Chain	Res	Type
1	C	145	VAL
2	D	41	PRO
1	E	95	SER
2	F	41	PRO
1	G	95	SER
1	G	145	VAL
2	H	41	PRO
1	A	145	VAL
2	B	44	GLY
1	C	54	ASN
1	C	95	SER
1	C	96	ASN
1	C	210	ALA
2	D	44	GLY
2	D	55	ASP
1	E	2	ALA
1	E	16	GLU
1	E	35	ALA
1	E	145	VAL
2	F	9	ALA
2	F	34	MET
2	F	55	ASP
2	H	55	ASP
1	A	62	ALA
2	B	42	GLY
2	D	27	TYR
1	E	80	ALA
1	E	164	THR
2	H	25	SER
2	H	67	LYS
1	A	34	TYR
2	B	16	ALA
1	C	80	ALA
1	E	34	TYR
1	E	210	ALA
1	G	16	GLU
1	G	43	ASP
1	C	35	ALA
1	C	58	PRO
1	C	59	GLY
1	C	185	ARG
2	D	62	GLN

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Mol	Chain	Res	Type
2	D	195	SER
1	E	31	THR
1	E	185	ARG
2	F	44	GLY
1	G	97	GLN
1	G	164	THR
1	A	43	ASP
1	A	96	ASN
2	B	28	SER
1	C	26	SER
1	C	34	TYR
1	C	42	PRO
1	E	42	PRO
1	E	79	GLY

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	176/180 (98%)	164 (93%)	12 (7%)	14	30
1	C	176/180 (98%)	161 (92%)	15 (8%)	10	22
1	E	176/180 (98%)	165 (94%)	11 (6%)	16	34
1	G	176/180 (98%)	161 (92%)	15 (8%)	10	22
2	B	178/187 (95%)	151 (85%)	27 (15%)	3	5
2	D	178/187 (95%)	155 (87%)	23 (13%)	4	7
2	F	178/187 (95%)	158 (89%)	20 (11%)	6	11
2	H	178/187 (95%)	153 (86%)	25 (14%)	3	6
All	All	1416/1468 (96%)	1268 (90%)	148 (10%)	6	13

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASN

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Mol	Chain	Res	Type
1	A	47	THR
1	A	49	LEU
1	A	72	LYS
1	A	78	THR
1	A	96	ASN
1	A	117	VAL
1	A	119	LEU
1	A	124	SER
1	A	148	VAL
1	A	165	GLN
1	A	185	ARG
2	B	1	GLU
2	B	11	LEU
2	B	13	ARG
2	B	22	CYS
2	B	41	PRO
2	B	59	ARG
2	B	67	LYS
2	B	69	THR
2	B	81	LEU
2	B	86	LEU
2	B	89	GLU
2	B	95	SER
2	B	96	CYS
2	B	111	GLN
2	B	113	THR
2	B	121	THR
2	B	122	THR
2	B	142	THR
2	B	143	LEU
2	B	145	CYS
2	B	152	PRO
2	B	154	PRO
2	B	164	LEU
2	B	181	THR
2	B	182	LEU
2	B	201	ASN
2	B	215	ILE
1	C	29	ILE
1	C	36	ASN
1	C	45	LEU
1	C	47	THR

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Mol	Chain	Res	Type
1	C	56	ARG
1	C	76	THR
1	C	96	ASN
1	C	117	VAL
1	C	119	LEU
1	C	124	SER
1	C	134	LEU
1	C	148	VAL
1	C	165	GLN
1	C	185	ARG
1	C	208	LEU
2	D	1	GLU
2	D	10	GLU
2	D	13	ARG
2	D	27	TYR
2	D	41	PRO
2	D	55	ASP
2	D	71	THR
2	D	81	LEU
2	D	86	LEU
2	D	96	CYS
2	D	111	GLN
2	D	121	THR
2	D	122	THR
2	D	142	THR
2	D	143	LEU
2	D	145	CYS
2	D	152	PRO
2	D	154	PRO
2	D	164	LEU
2	D	181	THR
2	D	182	LEU
2	D	201	ASN
2	D	215	ILE
1	E	11	THR
1	E	20	LEU
1	E	38	ILE
1	E	42	PRO
1	E	72	LYS
1	E	117	VAL
1	E	119	LEU
1	E	124	SER

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Mol	Chain	Res	Type
1	E	148	VAL
1	E	165	GLN
1	E	185	ARG
2	F	1	GLU
2	F	11	LEU
2	F	13	ARG
2	F	18	VAL
2	F	41	PRO
2	F	59	ARG
2	F	67	LYS
2	F	81	LEU
2	F	96	CYS
2	F	121	THR
2	F	122	THR
2	F	142	THR
2	F	143	LEU
2	F	145	CYS
2	F	154	PRO
2	F	164	LEU
2	F	181	THR
2	F	182	LEU
2	F	201	ASN
2	F	215	ILE
1	G	20	LEU
1	G	25	SER
1	G	30	THR
1	G	36	ASN
1	G	45	LEU
1	G	47	THR
1	G	49	LEU
1	G	96	ASN
1	G	99	ILE
1	G	119	LEU
1	G	124	SER
1	G	148	VAL
1	G	162	GLU
1	G	165	GLN
1	G	185	ARG
2	H	3	GLN
2	H	4	LEU
2	H	10	GLU
2	H	11	LEU

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Mol	Chain	Res	Type
2	H	13	ARG
2	H	22	CYS
2	H	31	THR
2	H	41	PRO
2	H	55	ASP
2	H	59	ARG
2	H	67	LYS
2	H	96	CYS
2	H	111	GLN
2	H	113	THR
2	H	121	THR
2	H	122	THR
2	H	142	THR
2	H	143	LEU
2	H	145	CYS
2	H	154	PRO
2	H	164	LEU
2	H	181	THR
2	H	182	LEU
2	H	201	ASN
2	H	215	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	6	GLN
1	A	96	ASN
1	A	97	GLN
1	A	130	ASN
1	A	202	HIS
2	B	3	GLN
2	B	6	GLN
2	B	39	GLN
2	B	43	GLN
2	B	82	GLN
2	B	84	ASN
2	B	111	GLN
2	B	204	HIS
1	C	1	GLN
1	C	36	ASN
1	C	39	GLN

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Mol	Chain	Res	Type
1	C	44	HIS
1	C	54	ASN
1	C	97	GLN
1	C	130	ASN
2	D	5	GLN
2	D	6	GLN
2	D	35	GLN
2	D	43	GLN
2	D	82	GLN
2	D	111	GLN
2	D	176	GLN
2	D	204	HIS
1	E	6	GLN
1	E	36	ASN
1	E	130	ASN
1	E	202	HIS
2	F	3	GLN
2	F	6	GLN
2	F	35	GLN
2	F	43	GLN
2	F	111	GLN
2	F	204	HIS
1	G	1	GLN
1	G	36	ASN
1	G	96	ASN
1	G	130	ASN
2	H	3	GLN
2	H	6	GLN
2	H	39	GLN
2	H	43	GLN
2	H	62	GLN
2	H	82	GLN
2	H	111	GLN
2	H	204	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	ECO	B	351	-	29,29,29	3.71	16 (55%)	41,44,44	3.54	9 (21%)
3	ECO	F	353	-	29,29,29	4.01	18 (62%)	41,44,44	3.58	9 (21%)
3	ECO	D	352	-	29,29,29	3.85	16 (55%)	41,44,44	3.53	9 (21%)
3	ECO	H	354	-	29,29,29	3.71	19 (65%)	41,44,44	3.53	10 (24%)

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	ECO	B	351	-	-	4/6/49/49	0/4/4/4
3	ECO	F	353	-	-	5/6/49/49	0/4/4/4
3	ECO	D	352	-	-	5/6/49/49	0/4/4/4
3	ECO	H	354	-	-	4/6/49/49	0/4/4/4

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	351	ECO	C6-N19	11.91	1.38	1.28
3	F	353	ECO	C6-N19	11.53	1.38	1.28
3	D	352	ECO	C6-N19	11.40	1.38	1.28
3	H	354	ECO	C6-N19	10.63	1.37	1.28
3	F	353	ECO	C5-C10	8.52	1.49	1.40
3	D	352	ECO	C5-C10	8.41	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	354	ECO	C5-C10	8.34	1.49	1.40
3	B	351	ECO	C5-C10	7.74	1.49	1.40
3	F	353	ECO	C9-C8	6.12	1.61	1.54
3	F	353	ECO	C1-C10	5.94	1.47	1.39
3	D	352	ECO	C1-C10	5.82	1.46	1.39
3	D	352	ECO	C9-C8	5.46	1.60	1.54
3	H	354	ECO	C9-C8	5.37	1.60	1.54
3	B	351	ECO	C9-C8	5.24	1.60	1.54
3	H	354	ECO	C1-C10	5.08	1.45	1.39
3	B	351	ECO	C1-C10	4.66	1.45	1.39
3	H	354	ECO	C13-C14	4.20	1.62	1.55
3	F	353	ECO	C5-C6	4.09	1.56	1.47
3	D	352	ECO	C18-C13	4.08	1.61	1.54
3	F	353	ECO	C4-C5	4.06	1.46	1.39
3	D	352	ECO	C4-C5	4.03	1.46	1.39
3	F	353	ECO	C18-C13	4.00	1.60	1.54
3	H	354	ECO	C4-C5	3.97	1.46	1.39
3	D	352	ECO	C5-C6	3.94	1.56	1.47
3	D	352	ECO	C4-C3	3.94	1.45	1.39
3	D	352	ECO	O19-N19	3.90	1.49	1.42
3	H	354	ECO	C5-C6	3.79	1.55	1.47
3	F	353	ECO	C13-C14	3.75	1.61	1.55
3	B	351	ECO	C13-C14	3.71	1.61	1.55
3	F	353	ECO	O19-N19	3.66	1.48	1.42
3	B	351	ECO	O19-N19	3.63	1.48	1.42
3	B	351	ECO	C18-C13	3.62	1.60	1.54
3	B	351	ECO	C11-C9	3.59	1.58	1.53
3	F	353	ECO	C7-C6	3.56	1.59	1.50
3	F	353	ECO	C8-C14	3.55	1.60	1.53
3	B	351	ECO	C5-C6	3.54	1.55	1.47
3	H	354	ECO	C18-C13	3.52	1.60	1.54
3	B	351	ECO	C4-C5	3.52	1.45	1.39
3	B	351	ECO	C8-C14	3.49	1.60	1.53
3	F	353	ECO	C4-C3	3.48	1.44	1.39
3	D	352	ECO	C8-C14	3.48	1.60	1.53
3	F	353	ECO	C11-C9	3.43	1.58	1.53
3	D	352	ECO	C13-C14	3.36	1.61	1.55
3	D	352	ECO	C7-C6	3.36	1.59	1.50
3	F	353	ECO	C2-C1	3.36	1.44	1.38
3	B	351	ECO	C7-C6	3.35	1.59	1.50
3	H	354	ECO	C8-C14	3.35	1.59	1.53
3	F	353	ECO	C10-C9	3.29	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	354	ECO	C7-C6	3.28	1.59	1.50
3	F	353	ECO	C2-C3	3.26	1.45	1.39
3	H	354	ECO	C11-C9	3.13	1.58	1.53
3	B	351	ECO	C4-C3	3.11	1.43	1.39
3	H	354	ECO	C4-C3	3.05	1.43	1.39
3	D	352	ECO	C2-C1	3.02	1.43	1.38
3	H	354	ECO	O19-N19	2.99	1.47	1.42
3	D	352	ECO	C2-C3	2.93	1.44	1.39
3	H	354	ECO	C2-C1	2.84	1.43	1.38
3	H	354	ECO	C2-C3	2.72	1.44	1.39
3	D	352	ECO	C10-C9	2.66	1.56	1.52
3	D	352	ECO	C11-C9	2.64	1.57	1.53
3	B	351	ECO	C2-C1	2.55	1.42	1.38
3	B	351	ECO	C2-C3	2.48	1.43	1.39
3	H	354	ECO	C10-C9	2.46	1.55	1.52
3	H	354	ECO	O19-C19	-2.20	1.40	1.42
3	H	354	ECO	C16-C17	2.19	1.58	1.53
3	H	354	ECO	C13-C17	2.13	1.57	1.54
3	F	353	ECO	O19-C19	-2.11	1.40	1.42
3	B	351	ECO	C10-C9	2.06	1.55	1.52
3	F	353	ECO	O17-C17	2.02	1.46	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	353	ECO	C19-O19-N19	15.27	124.40	107.92
3	F	353	ECO	O19-N19-C6	14.87	133.69	111.47
3	D	352	ECO	C19-O19-N19	14.82	123.91	107.92
3	B	351	ECO	O19-N19-C6	14.80	133.58	111.47
3	H	354	ECO	O19-N19-C6	14.70	133.43	111.47
3	H	354	ECO	C19-O19-N19	14.61	123.69	107.92
3	B	351	ECO	C19-O19-N19	14.58	123.65	107.92
3	D	352	ECO	O19-N19-C6	14.12	132.57	111.47
3	D	352	ECO	O19-C19-C20	4.43	118.45	111.75
3	H	354	ECO	O19-C19-C20	4.02	117.83	111.75
3	B	351	ECO	O19-C19-C20	3.68	117.32	111.75
3	D	352	ECO	C15-C14-C13	-3.24	100.03	103.84
3	F	353	ECO	O19-C19-C20	3.06	116.38	111.75
3	B	351	ECO	C15-C14-C13	-2.88	100.45	103.84
3	D	352	ECO	C11-C9-C8	-2.79	107.80	111.45
3	D	352	ECO	O20-C20-O21	-2.74	116.28	123.33
3	F	353	ECO	C15-C14-C13	-2.61	100.78	103.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	354	ECO	C15-C14-C13	-2.58	100.81	103.84
3	B	351	ECO	O20-C20-O21	-2.47	116.99	123.33
3	H	354	ECO	O20-C20-O21	-2.44	117.05	123.33
3	F	353	ECO	C13-C14-C8	-2.41	110.99	114.41
3	B	351	ECO	C11-C9-C8	-2.40	108.31	111.45
3	B	351	ECO	C10-C5-C6	2.26	122.65	118.58
3	H	354	ECO	C11-C9-C8	-2.26	108.50	111.45
3	D	352	ECO	O21-C20-C19	-2.24	112.66	121.99
3	D	352	ECO	C16-C17-C13	2.24	106.29	104.52
3	H	354	ECO	O21-C20-C19	-2.24	112.67	121.99
3	F	353	ECO	O21-C20-C19	-2.23	112.69	121.99
3	B	351	ECO	O21-C20-C19	-2.22	112.77	121.99
3	F	353	ECO	C11-C9-C8	-2.21	108.56	111.45
3	F	353	ECO	O20-C20-O21	-2.21	117.65	123.33
3	H	354	ECO	C18-C13-C14	2.20	115.66	111.68
3	H	354	ECO	C16-C17-C13	2.19	106.25	104.52
3	H	354	ECO	C10-C5-C6	2.18	122.50	118.58
3	B	351	ECO	C16-C17-C13	2.16	106.22	104.52
3	D	352	ECO	C13-C14-C8	-2.01	111.56	114.41
3	F	353	ECO	C16-C17-C13	2.00	106.10	104.52

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	351	ECO	C5-C6-N19-O19
3	B	351	ECO	C6-N19-O19-C19
3	D	352	ECO	C5-C6-N19-O19
3	D	352	ECO	C6-N19-O19-C19
3	F	353	ECO	C5-C6-N19-O19
3	F	353	ECO	C6-N19-O19-C19
3	H	354	ECO	C5-C6-N19-O19
3	H	354	ECO	C6-N19-O19-C19
3	F	353	ECO	O19-C19-C20-O20
3	B	351	ECO	O19-C19-C20-O20
3	F	353	ECO	O19-C19-C20-O21
3	D	352	ECO	O19-C19-C20-O20
3	D	352	ECO	O19-C19-C20-O21
3	H	354	ECO	O19-C19-C20-O20
3	D	352	ECO	C20-C19-O19-N19
3	B	351	ECO	C20-C19-O19-N19
3	F	353	ECO	C20-C19-O19-N19

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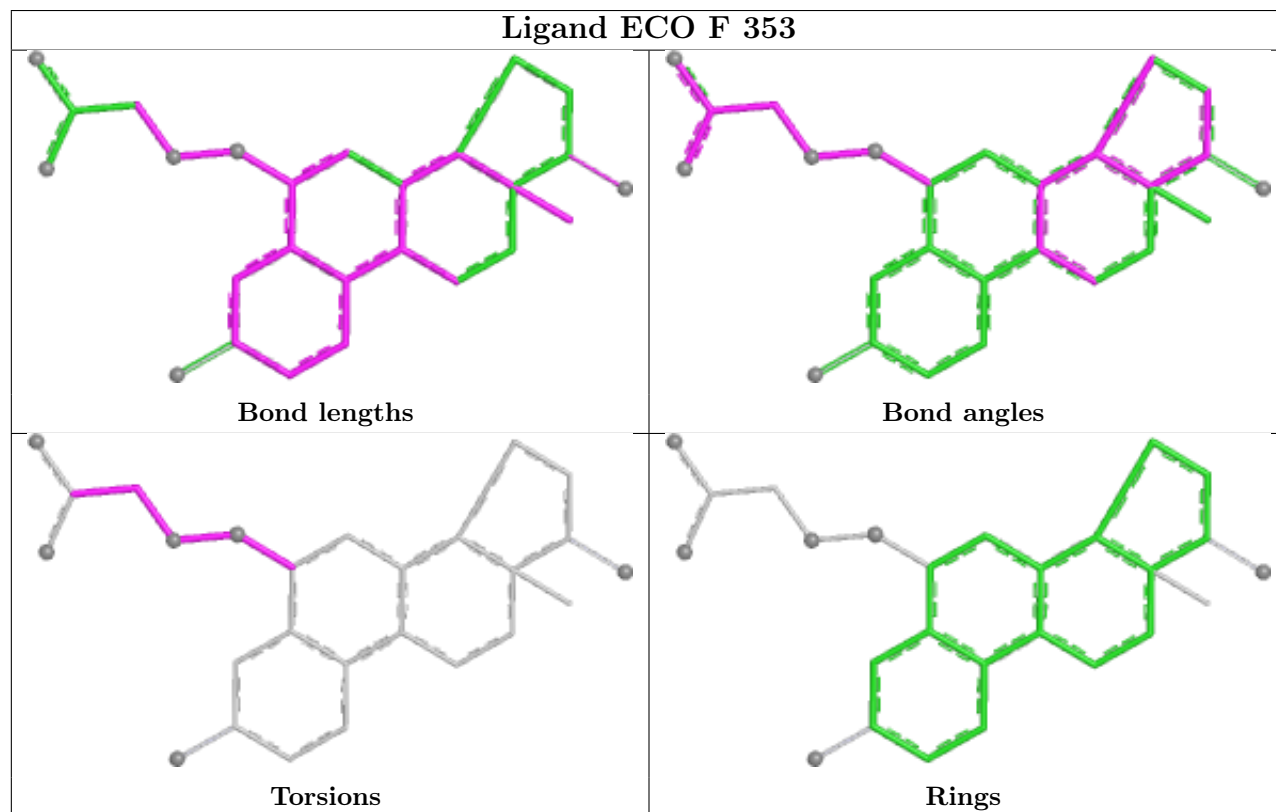
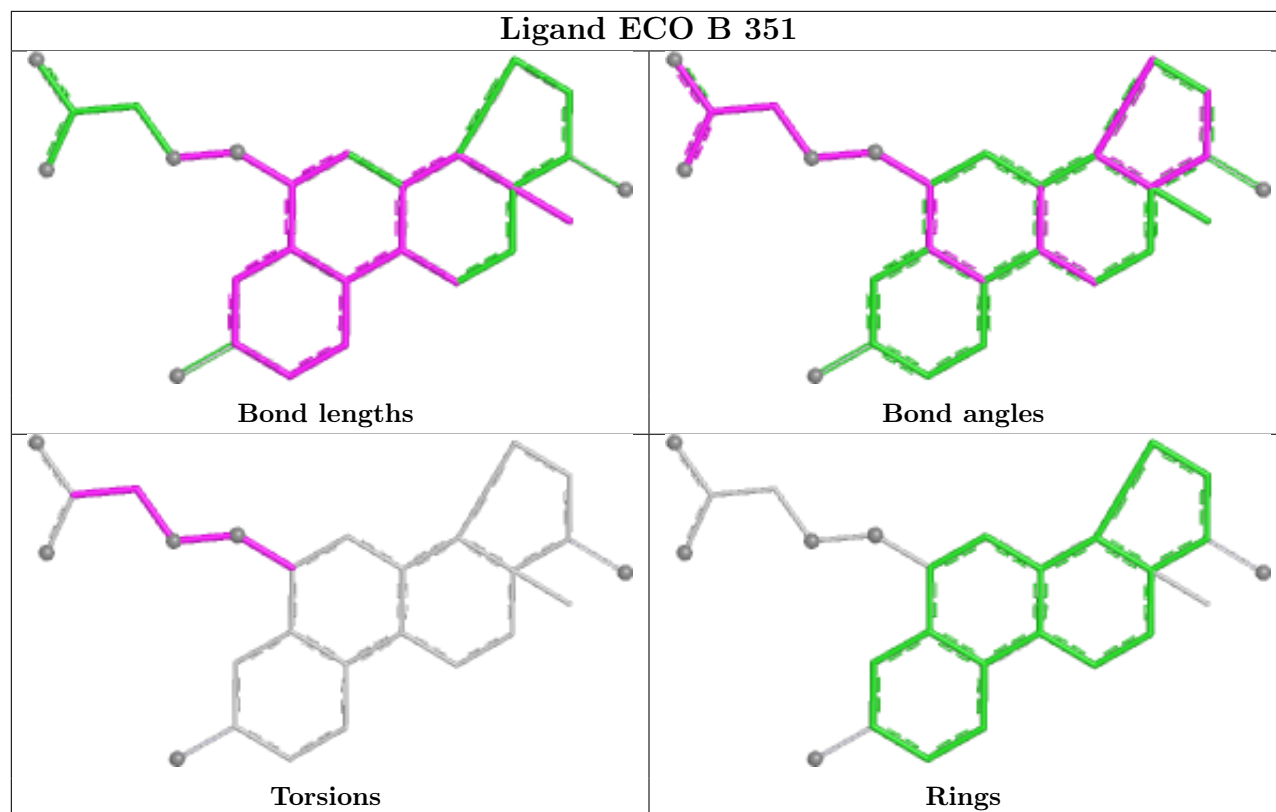
Mol	Chain	Res	Type	Atoms
3	H	354	ECO	C20-C19-O19-N19

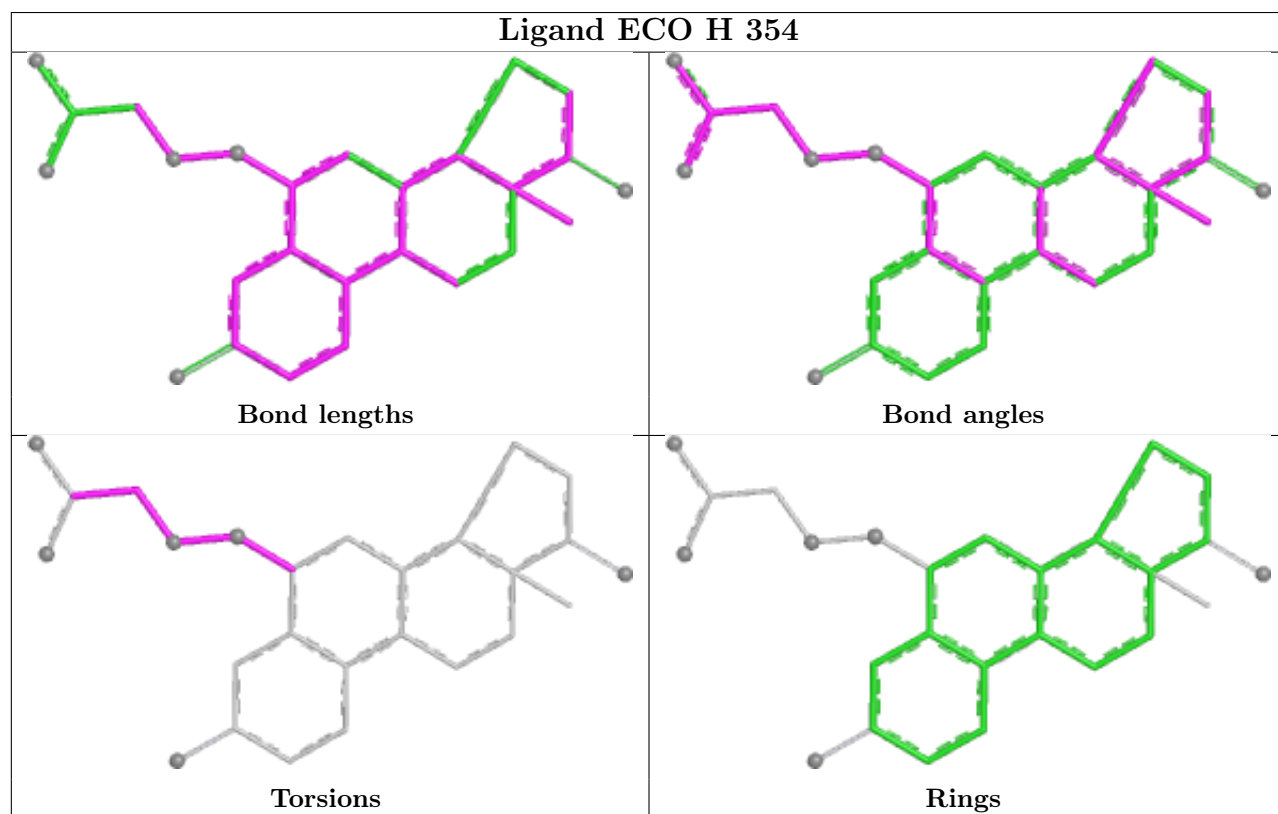
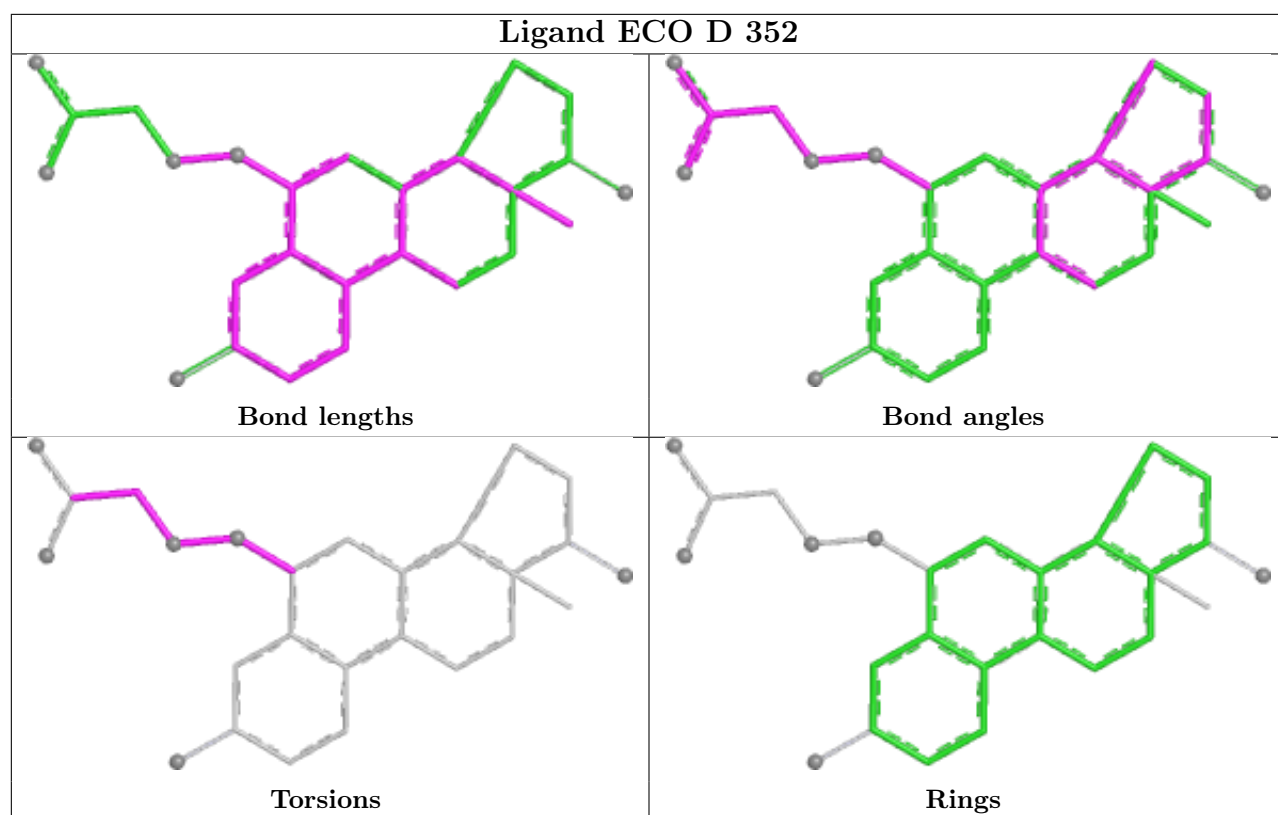
There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	351	ECO	3	0
3	F	353	ECO	3	0
3	D	352	ECO	3	0
3	H	354	ECO	5	0

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





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	208/212 (98%)	0.31	9 (4%) 40 31	15, 55, 103, 150	0
1	C	208/212 (98%)	0.72	24 (11%) 9 7	11, 74, 123, 155	0
1	E	208/212 (98%)	0.82	27 (12%) 7 5	11, 82, 138, 191	0
1	G	208/212 (98%)	0.14	7 (3%) 48 38	17, 46, 101, 148	0
2	B	214/218 (98%)	0.13	5 (2%) 61 52	18, 45, 90, 117	0
2	D	214/218 (98%)	0.16	9 (4%) 40 32	13, 47, 98, 134	0
2	F	214/218 (98%)	0.26	12 (5%) 30 22	12, 51, 105, 156	0
2	H	214/218 (98%)	0.05	7 (3%) 49 40	13, 40, 88, 129	0
All	All	1688/1720 (98%)	0.32	100 (5%) 28 21	11, 51, 116, 191	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	66	GLY	7.3
1	C	90	CYS	5.0
2	D	96	CYS	4.3
1	G	142	TYR	4.2
2	B	136	GLN	4.1
1	E	90	CYS	4.1
1	G	172	ASN	3.9
2	H	136	GLN	3.9
1	A	189	ARG	3.7
1	C	142	TYR	3.6
1	E	24	SER	3.5
2	F	54	GLY	3.3
2	H	138	ASN	3.3
2	H	195	SER	3.3
1	A	2	ALA	3.2
2	F	176	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	96	CYS	3.1
1	C	108	VAL	3.1
1	E	152	VAL	3.1
1	E	145	VAL	3.1
1	E	211	ALA	3.1
2	B	41	PRO	3.1
1	E	67	SER	3.0
2	D	138	ASN	3.0
1	E	171	ASN	3.0
1	C	169	GLN	3.0
1	A	108	VAL	2.9
1	A	171	ASN	2.9
2	F	26	GLY	2.8
1	E	38	ILE	2.8
1	E	86	ALA	2.7
1	C	86	ALA	2.7
1	C	94	PHE	2.7
1	A	66	GLY	2.7
1	C	158	THR	2.7
2	D	54	GLY	2.7
1	C	73	ALA	2.7
1	A	142	TYR	2.6
1	E	101	GLY	2.6
1	E	21	THR	2.6
2	D	43	GLN	2.6
2	F	24	THR	2.5
2	H	41	PRO	2.5
1	E	29	ILE	2.5
2	F	99	GLY	2.5
1	E	18	VAL	2.5
2	D	2	VAL	2.5
2	H	166	SER	2.5
1	C	128	GLU	2.5
1	C	78	THR	2.5
1	C	22	CYS	2.5
1	C	149	ASP	2.4
1	G	62	ALA	2.4
1	C	171	ASN	2.4
1	E	87	ILE	2.4
2	F	195	SER	2.4
1	A	9	ALA	2.4
1	C	5	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	78	THR	2.4
1	A	170	SER	2.4
2	F	166	SER	2.4
1	C	15	GLY	2.3
1	C	93	TRP	2.3
2	D	137	THR	2.3
1	E	61	PRO	2.3
1	C	101	GLY	2.3
1	G	140	ASP	2.3
1	G	128	GLU	2.3
1	E	34	TYR	2.3
2	B	138	ASN	2.2
1	E	68	LEU	2.2
1	C	39	GLN	2.2
1	E	170	SER	2.2
1	C	50	ILE	2.2
2	D	176	GLN	2.2
1	C	4	VAL	2.2
1	E	47	THR	2.2
1	G	149	ASP	2.2
1	G	58	PRO	2.2
1	E	30	THR	2.2
2	F	15	GLY	2.2
2	F	82	GLN	2.2
1	C	52	GLY	2.2
1	E	142	TYR	2.2
1	C	38	ILE	2.1
2	H	137	THR	2.1
1	A	45	LEU	2.1
2	F	103	TYR	2.1
2	F	158	SER	2.1
2	B	121	THR	2.1
2	D	95	SER	2.1
1	C	30	THR	2.1
2	H	121	THR	2.1
2	F	138	ASN	2.1
1	E	12	THR	2.1
1	E	70	GLY	2.0
1	E	50	ILE	2.0
1	C	34	TYR	2.0
1	E	79	GLY	2.0
2	D	26	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](#)

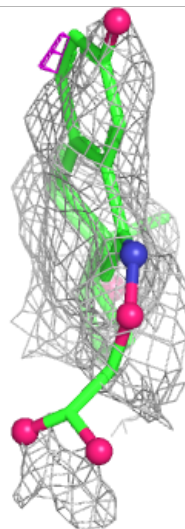
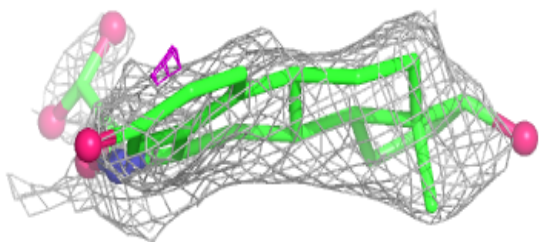
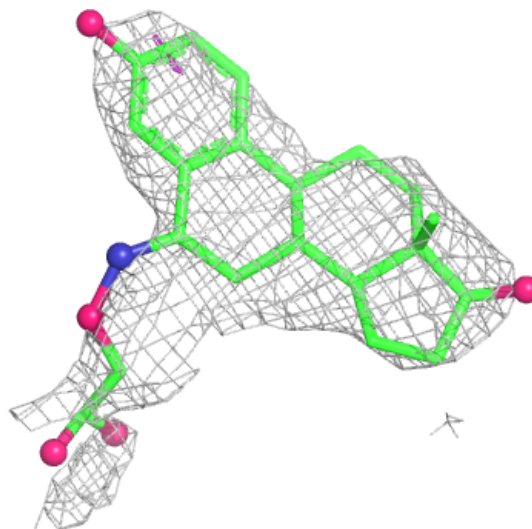
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ECO	F	353	26/26	0.77	0.14	52,53,88,88	0
3	ECO	D	352	26/26	0.81	0.13	52,53,88,88	0
3	ECO	H	354	26/26	0.85	0.16	52,53,88,88	0
3	ECO	B	351	26/26	0.87	0.12	52,53,88,88	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.

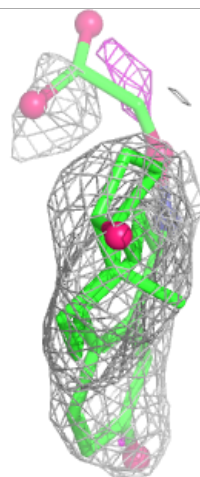
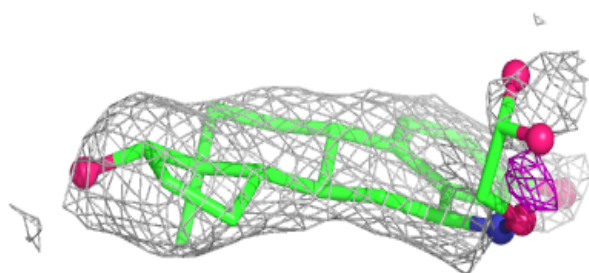
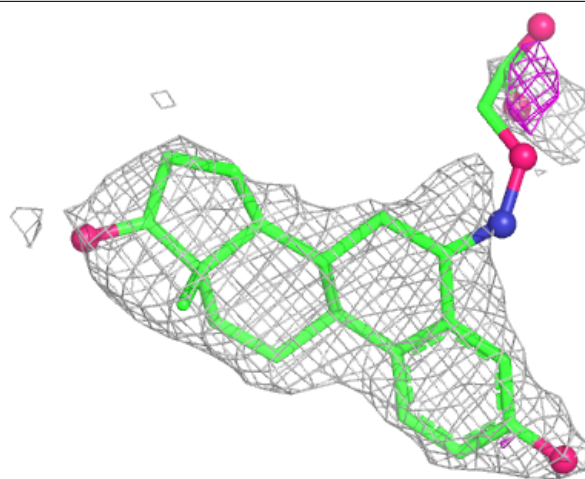
Electron density around ECO F 353:

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



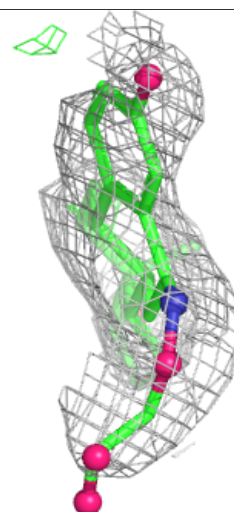
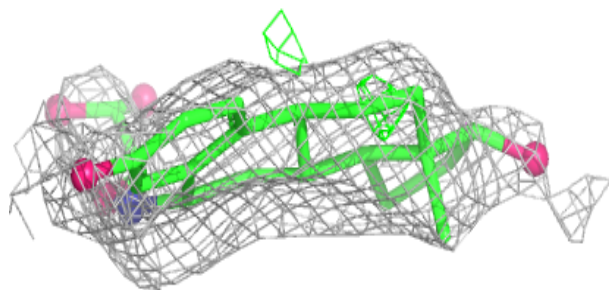
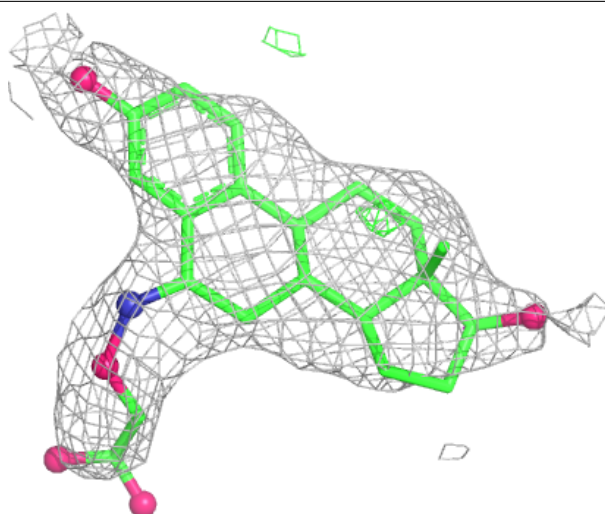
Electron density around ECO D 352:

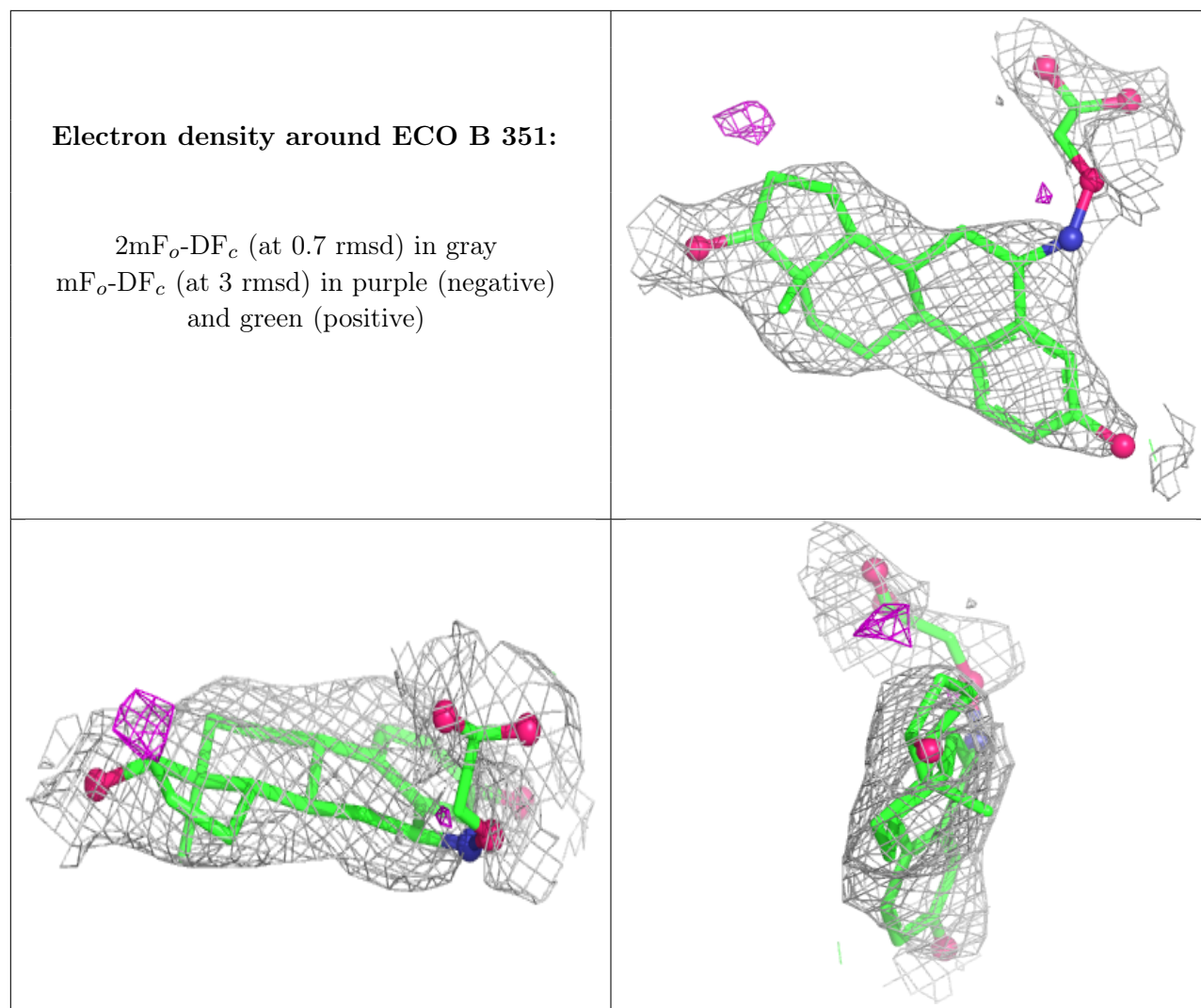
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ECO H 354:

$2mF_o-DF_c$ (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.