



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:56 AM UTC

PDB ID : 1FM6 / pdb_00001fm6
Title : THE 2.1 ANGSTROM RESOLUTION CRYSTAL STRUCTURE OF THE HETERODIMER OF THE HUMAN RXRALPHA AND PPARGAMMA LIGAND BINDING DOMAINS RESPECTIVELY BOUND WITH 9-CIS RETINOIC ACID AND ROSIGLITAZONE AND CO-ACTIVATOR PEP-TIDES.
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Deposited on : 2000-08-16
Resolution : 2.10 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

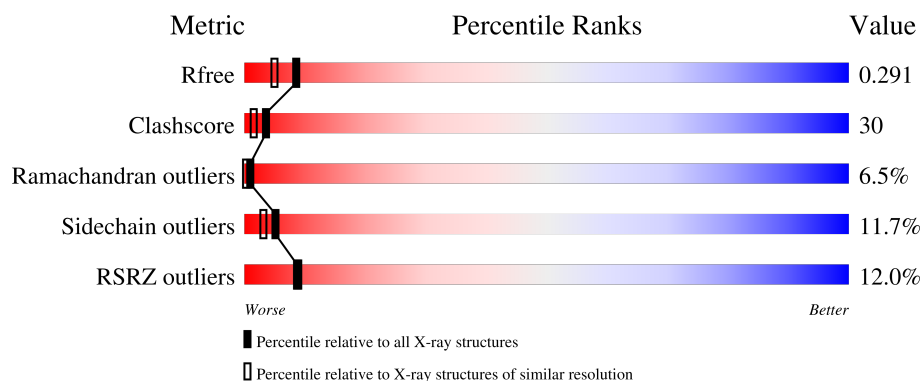
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	238	16% 54% 33% 8% • •
1	U	238	15% 49% 37% 10% • •
2	D	272	8% 59% 30% 9% •

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	X	272	8% 56% 31% 10%
3	B	25	4% 16% 20% 60%
3	E	25	8% 40% 20% 36%
3	V	25	12% 32% 12% 12% 40%
3	Y	25	12% 8% 28% 16% 48%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8838 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 RETINOIC ACID RECEPTOR RXR-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1754	1117	306	321	10			
1	U	232	Total	C	N	O	S	0	0	0
			1754	1117	306	321	10			

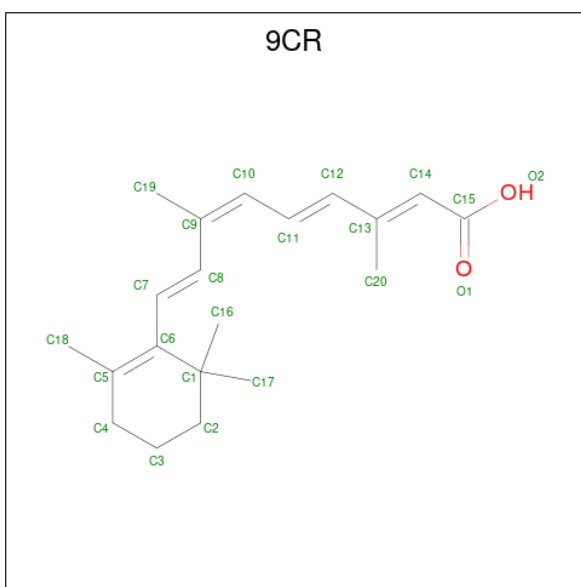
- Molecule 2 is a protein called PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	272	Total	C	N	O	S	0	0	0
			2183	1409	356	408	10			
2	X	272	Total	C	N	O	S	0	0	0
			2142	1377	347	408	10			

- Molecule 3 is a protein called STEROID RECEPTOR COACTIVATOR.

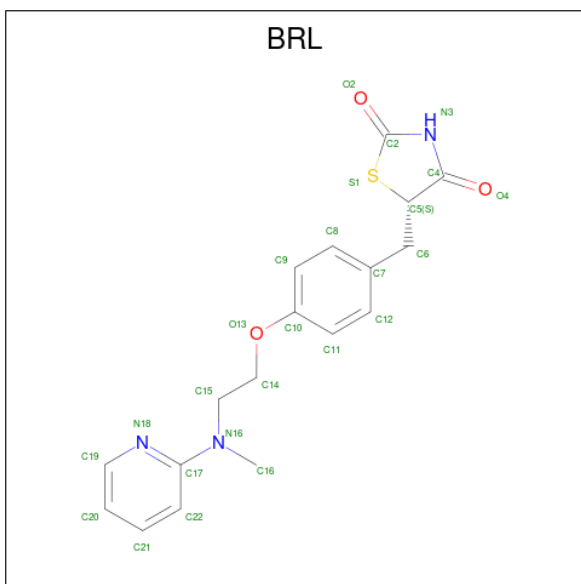
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	10	Total	C	N	O	0	0	0
			86	55	18	13			
3	V	15	Total	C	N	O	0	0	0
			127	79	27	21			
3	E	16	Total	C	N	O	0	0	0
			129	79	27	23			
3	Y	13	Total	C	N	O	0	0	0
			117	73	25	19			

- Molecule 4 is (9cis)-retinoic acid (CCD ID: 9CR) (formula: C₂₀H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	20	2		
4	U	1	Total	C	O	0	0
			22	20	2		

- Molecule 5 is 2,4-THIAZOLIDINEDIONE, 5-[[4-[2-(METHYL-2-PYRIDINYLAMINO)ETHOXY]PHENYL]METHYL]-(9CL) (CCD ID: BRL) (formula: C₁₈H₁₉N₃O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	S	0	0
			25	18	3	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	X	1	Total	C	N	O	S	0	0
			25	18	3	3	1		

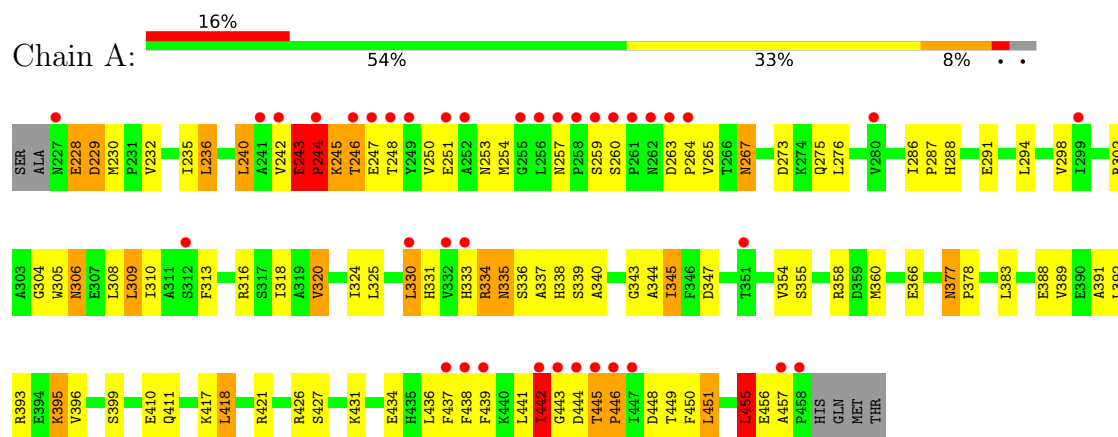
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	64	Total	O	0	0
			64	64		
6	D	151	Total	O	0	0
			151	151		
6	U	79	Total	O	0	0
			79	79		
6	X	132	Total	O	0	0
			132	132		
6	B	3	Total	O	0	0
			3	3		
6	V	8	Total	O	0	0
			8	8		
6	E	9	Total	O	0	0
			9	9		
6	Y	6	Total	O	0	0
			6	6		

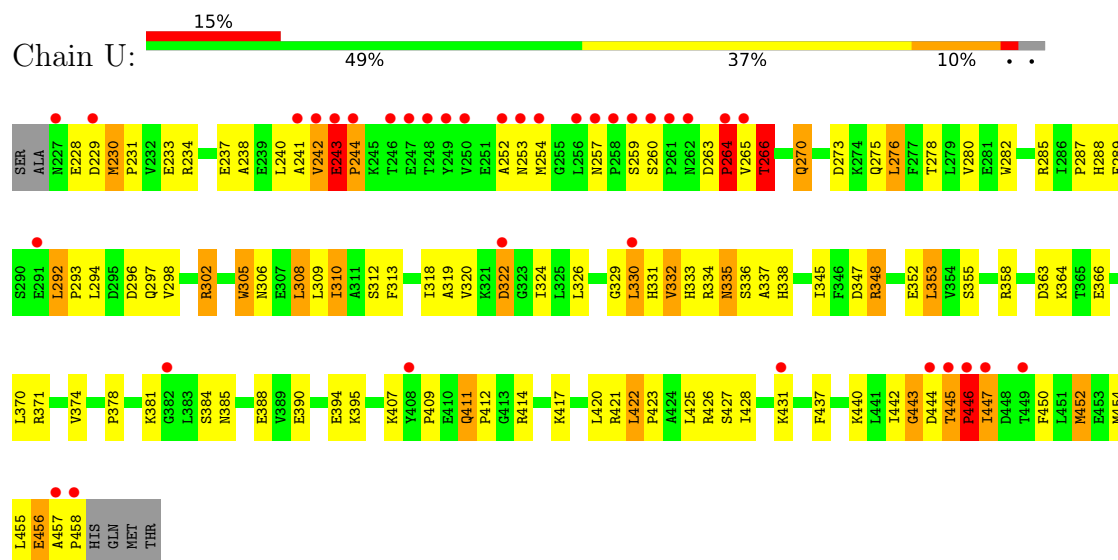
3 Residue-property plots [i](#)

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.

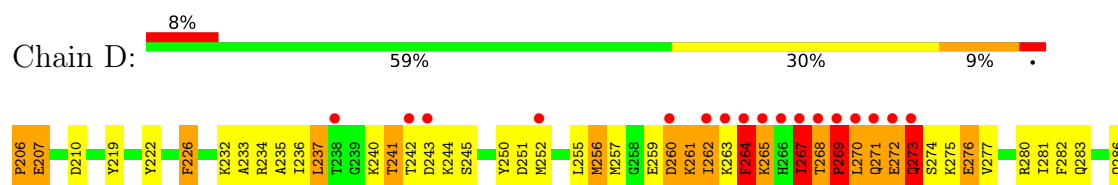
• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

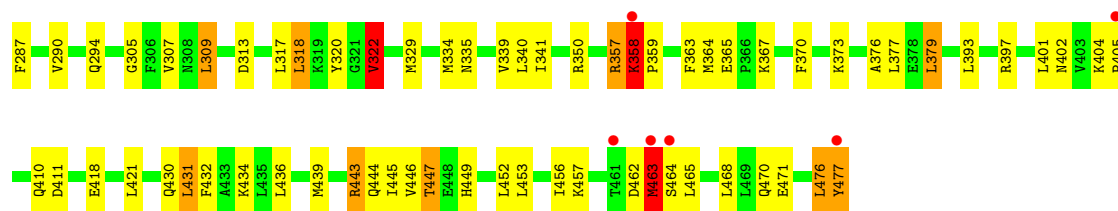


• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

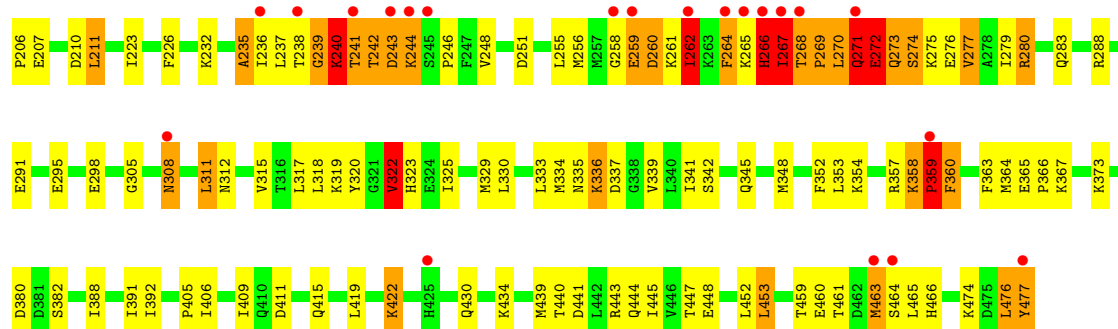


• Molecule 2: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA

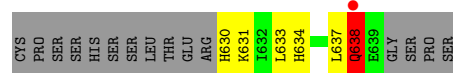




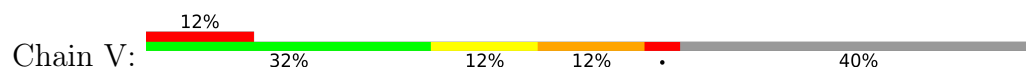
• Molecule 2: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA



• Molecule 3: STEROID RECEPTOR COACTIVATOR



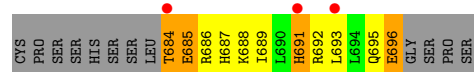
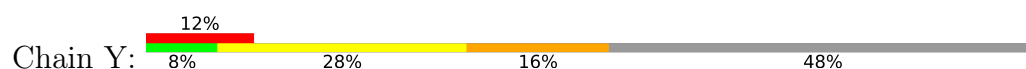
• Molecule 3: STEROID RECEPTOR COACTIVATOR



• Molecule 3: STEROID RECEPTOR COACTIVATOR



• Molecule 3: STEROID RECEPTOR COACTIVATOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.26Å 222.36Å 55.29Å 90.00° 98.59° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.8 (20.00-2.10) 87.7 (20.00-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.10Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.250 , 0.292 0.249 , 0.291	Depositor DCC
R_{free} test set	6068 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8838	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: 9CR, BRL

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	0.44	0/1789	1.16	23/2414 (1.0%)
1	U	0.44	0/1789	1.03	8/2414 (0.3%)
2	D	0.44	0/2221	1.02	13/2992 (0.4%)
2	X	0.41	0/2178	1.04	12/2938 (0.4%)
3	B	0.37	0/87	1.21	2/116 (1.7%)
3	E	0.38	0/131	0.97	0/175
3	V	0.38	0/129	0.87	0/171
3	Y	0.35	0/118	0.92	0/156
All	All	0.43	0/8442	1.06	58/11376 (0.5%)

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	277	VAL	N-CA-C	-12.51	101.28	113.53
2	D	267	ILE	N-CA-C	10.42	117.36	106.21
2	D	264	PHE	N-CA-C	-10.28	99.61	111.03
1	A	243	GLU	C-N-CD	-10.26	98.02	120.60
1	U	456	GLU	N-CA-C	-9.73	100.90	113.17
1	A	264	PRO	N-CA-C	8.77	124.72	114.20
2	X	266	HIS	N-CA-C	8.69	129.30	110.80
1	U	411	GLN	CA-C-N	8.63	128.37	119.56
1	U	411	GLN	C-N-CA	8.63	128.37	119.56
1	A	243	GLU	CA-C-N	8.38	147.12	127.00
1	A	243	GLU	C-N-CA	8.38	147.12	127.00
2	D	261	LYS	N-CA-C	-8.14	101.68	111.69
1	A	411	GLN	CA-C-N	8.10	128.87	119.47
1	A	411	GLN	C-N-CA	8.10	128.87	119.47
1	A	263	ASP	CA-C-N	7.85	128.83	120.12
1	A	263	ASP	C-N-CA	7.85	128.83	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	445	THR	CA-C-N	7.78	129.56	119.84
1	U	445	THR	C-N-CA	7.78	129.56	119.84
1	A	438	PHE	N-CA-C	-7.71	103.19	112.59
1	A	377	ASN	CA-C-N	7.55	127.19	119.56
1	A	377	ASN	C-N-CA	7.55	127.19	119.56
1	A	265	VAL	N-CA-C	-7.40	101.91	112.35
2	D	226	PHE	CA-C-N	7.33	126.87	119.24
2	D	226	PHE	C-N-CA	7.33	126.87	119.24
2	X	260	ASP	N-CA-C	-7.17	103.75	114.64
2	D	358	LYS	CA-C-N	-7.14	112.83	120.47
2	D	358	LYS	C-N-CA	-7.14	112.83	120.47
2	X	360	PHE	N-CA-C	-7.14	104.44	113.72
1	A	439	PHE	N-CA-C	-6.73	106.95	114.62
2	X	322	VAL	N-CA-C	6.59	117.28	110.36
3	B	638	GLN	N-CA-C	6.44	121.28	113.17
2	D	255	LEU	N-CA-C	-6.33	104.30	111.07
2	X	206	PRO	N-CA-CB	6.21	109.83	103.00
2	D	206	PRO	N-CA-CB	6.13	109.74	103.00
1	A	354	VAL	N-CA-C	5.98	116.64	110.36
2	X	262	ILE	N-CA-C	5.97	121.77	109.34
1	U	348	ARG	N-CA-C	-5.82	104.93	111.28
1	U	266	THR	N-CA-C	-5.81	104.55	111.69
2	D	335	ASN	N-CA-C	-5.78	100.98	109.18
1	A	421	ARG	N-CA-C	-5.77	106.08	113.23
2	D	322	VAL	N-CA-C	5.74	116.39	110.36
2	X	235	ALA	N-CA-C	-5.63	104.78	111.03
2	X	337	ASP	N-CA-C	5.54	120.20	113.38
1	A	451	LEU	N-CA-C	-5.53	105.16	111.14
1	A	445	THR	CA-C-N	5.48	126.69	119.84
1	A	445	THR	C-N-CA	5.48	126.69	119.84
2	D	236	ILE	N-CA-C	5.46	115.66	110.53
1	A	251	GLU	N-CA-C	5.36	117.88	111.71
3	B	631	LYS	N-CA-C	5.26	116.70	110.97
1	A	267	ASN	CA-C-N	5.25	127.87	120.42
1	A	267	ASN	C-N-CA	5.25	127.87	120.42
1	U	421	ARG	N-CA-C	-5.20	106.94	113.28
2	X	267	ILE	N-CA-C	5.15	120.06	109.34
1	A	448	ASP	N-CA-C	5.11	116.89	110.24
2	X	466	HIS	CA-C-N	5.11	125.15	119.32
2	X	466	HIS	C-N-CA	5.11	125.15	119.32
1	A	395	LYS	N-CA-C	-5.11	105.71	111.28
2	D	273	GLN	N-CA-C	5.06	121.58	110.80

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	1754	0	1733	81	0
1	U	1754	0	1733	139	0
2	D	2183	0	2243	140	0
2	X	2142	0	2162	109	0
3	B	86	0	86	9	0
3	E	129	0	125	18	0
3	V	127	0	131	13	0
3	Y	117	0	123	19	0
4	A	22	0	27	1	0
4	U	22	0	27	2	0
5	D	25	0	19	4	0
5	X	25	0	19	1	0
6	A	64	0	0	3	0
6	B	3	0	0	0	0
6	D	151	0	0	6	0
6	E	9	0	0	1	0
6	U	79	0	0	10	0
6	V	8	0	0	1	0
6	X	132	0	0	6	0
6	Y	6	0	0	0	0
All	All	8838	0	8428	496	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 30.

All (496) 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:A:335:ASN:HD22	1:A:336:SER:N	1.45	1.12
1:A:267:ASN:HD22	1:A:330:LEU:HD11	1.16	1.10
2:D:262:ILE:HA	2:D:265:LYS:HB2	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:685:GLU:HG2	3:E:686:ARG:H	1.27	0.99
1:U:306:ASN:O	1:U:310:ILE:HG22	1.64	0.95
1:U:289:PHE:O	1:U:292:LEU:HD22	1.66	0.95
2:X:280:ARG:HH11	2:X:280:ARG:HG2	1.29	0.95
1:A:335:ASN:HD22	1:A:336:SER:H	1.14	0.93
1:A:267:ASN:HD22	1:A:330:LEU:CD1	1.85	0.90
2:D:273:GLN:HA	2:D:280:ARG:HD3	1.54	0.90
2:D:261:LYS:HG2	2:D:265:LYS:HE3	1.52	0.89
1:U:345:ILE:HD13	1:U:431:LYS:HD3	1.55	0.87
2:D:268:THR:H	2:D:269:PRO:HD2	1.38	0.86
2:D:270:LEU:HD22	2:D:287:PHE:CG	2.10	0.86
2:D:264:PHE:C	2:D:264:PHE:HD1	1.84	0.86
1:U:454:MET:HE3	3:V:633:LEU:HG	1.58	0.85
1:A:294:LEU:HD11	3:B:638:GLN:HE21	1.43	0.84
1:A:267:ASN:ND2	1:A:330:LEU:HD11	1.92	0.83
2:D:476:LEU:HG	2:D:477:TYR:H	1.44	0.82
2:D:264:PHE:C	2:D:264:PHE:CD1	2.57	0.81
2:D:262:ILE:HD13	2:D:265:LYS:HD2	1.63	0.81
2:D:471:GLU:OE2	3:E:689:ILE:HG22	1.81	0.81
1:U:244:PRO:HD2	6:U:527:HOH:O	1.83	0.79
2:D:271:GLN:HE22	2:D:280:ARG:CG	1.95	0.79
2:D:268:THR:N	2:D:269:PRO:HD2	1.94	0.79
2:D:271:GLN:HG3	2:D:283:GLN:OE1	1.83	0.78
2:X:244:LYS:HE3	2:X:246:PRO:HG3	1.66	0.78
2:D:271:GLN:HE22	2:D:280:ARG:CD	1.96	0.78
1:A:243:GLU:HB2	1:A:244:PRO:O	1.84	0.77
1:U:302:ARG:HH12	1:U:457:ALA:HA	1.49	0.77
3:Y:689:ILE:O	3:Y:692:ARG:HG2	1.84	0.77
2:D:471:GLU:CD	3:E:689:ILE:HG22	2.10	0.77
2:D:240:LYS:O	2:D:241:THR:HG22	1.85	0.76
1:U:243:GLU:HA	1:U:244:PRO:O	1.85	0.76
1:U:276:LEU:HD11	1:U:305:TRP:CD1	2.22	0.75
1:A:383:LEU:HD21	1:A:389:VAL:HG21	1.67	0.75
2:X:238:THR:HG23	2:X:239:GLY:H	1.52	0.75
2:X:238:THR:HG23	2:X:239:GLY:N	2.02	0.75
1:A:230:MET:CE	1:A:235:ILE:HD11	2.17	0.75
1:U:238:ALA:O	1:U:242:VAL:HG22	1.86	0.75
2:D:269:PRO:HB3	2:D:272:GLU:OE2	1.86	0.74
1:U:335:ASN:ND2	1:U:336:SER:H	1.85	0.74
1:U:452:MET:HE3	1:U:452:MET:HA	1.68	0.74
1:U:243:GLU:HB3	1:U:244:PRO:HA	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:457:LYS:HA	2:D:463:MET:HG3	1.70	0.74
2:X:262:ILE:C	2:X:264:PHE:H	1.94	0.74
1:U:335:ASN:HD22	1:U:336:SER:H	1.33	0.73
2:D:271:GLN:HE22	2:D:280:ARG:HG2	1.53	0.73
2:D:443:ARG:HD2	2:D:477:TYR:CE2	2.22	0.73
1:U:310:ILE:HD13	1:U:310:ILE:C	2.13	0.73
3:Y:684:THR:HB	3:Y:685:GLU:OE2	1.89	0.73
1:U:318:ILE:HD12	1:U:319:ALA:N	2.04	0.73
1:U:442:ILE:HD12	1:U:443:GLY:N	2.04	0.72
2:X:269:PRO:HG2	2:X:270:LEU:H	1.53	0.72
2:X:261:LYS:O	2:X:262:ILE:O	2.08	0.72
1:A:417:LYS:HE2	6:A:555:HOH:O	1.90	0.72
3:Y:696:GLU:O	3:Y:696:GLU:HG2	1.90	0.72
1:U:440:LYS:HD2	1:U:452:MET:HE1	1.73	0.71
2:D:268:THR:O	2:D:269:PRO:O	2.07	0.71
2:D:273:GLN:C	2:D:275:LYS:H	1.97	0.71
2:D:206:PRO:HA	6:D:624:HOH:O	1.89	0.71
2:D:273:GLN:HA	2:D:280:ARG:CD	2.21	0.70
2:D:237:LEU:HD12	2:D:237:LEU:H	1.57	0.70
1:A:445:THR:O	1:A:446:PRO:O	2.10	0.69
2:D:357:ARG:HG3	2:D:358:LYS:H	1.56	0.69
1:A:294:LEU:HD11	3:B:638:GLN:NE2	2.08	0.69
2:D:377:LEU:HB2	2:D:379:LEU:CD1	2.22	0.69
2:X:320:TYR:CE1	2:X:476:LEU:HD23	2.28	0.68
1:A:333:HIS:HD2	1:A:335:ASN:ND2	1.91	0.68
2:X:264:PHE:O	2:X:265:LYS:C	2.36	0.68
3:E:686:ARG:HH12	3:E:691:HIS:CD2	2.12	0.68
2:X:411:ASP:HB2	6:X:515:HOH:O	1.92	0.68
2:D:404:LYS:HB3	2:D:405:PRO:HD3	1.75	0.68
2:D:411:ASP:HB2	6:D:556:HOH:O	1.93	0.67
2:X:279:ILE:O	2:X:283:GLN:HG3	1.95	0.67
1:A:230:MET:HE2	1:A:396:VAL:HG22	1.75	0.67
2:X:273:GLN:O	2:X:275:LYS:N	2.28	0.67
2:D:377:LEU:HB2	2:D:379:LEU:HD11	1.76	0.67
3:E:691:HIS:HB3	6:E:408:HOH:O	1.95	0.67
1:U:417:LYS:HE3	6:X:542:HOH:O	1.94	0.67
1:A:320:VAL:HG21	1:A:331:HIS:CE1	2.29	0.66
2:D:262:ILE:CA	2:D:265:LYS:HB2	2.23	0.66
2:D:443:ARG:HD2	2:D:477:TYR:HE2	1.61	0.65
1:A:298:VAL:HG13	3:B:633:LEU:HD12	1.78	0.65
2:D:262:ILE:HA	2:D:265:LYS:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ASN:ND2	1:A:336:SER:H	1.90	0.65
2:X:258:GLY:O	2:X:259:GLU:HG3	1.96	0.65
1:A:437:PHE:HE1	1:A:455:LEU:O	1.79	0.65
2:X:280:ARG:HG2	2:X:280:ARG:NH1	2.04	0.65
2:D:269:PRO:C	2:D:270:LEU:HG	2.21	0.64
1:U:293:PRO:O	1:U:297:GLN:HG3	1.97	0.64
1:U:310:ILE:HD12	1:U:425:LEU:HD12	1.79	0.64
2:D:260:ASP:O	2:D:263:LYS:HB2	1.97	0.64
3:E:685:GLU:CG	3:E:686:ARG:H	2.06	0.64
1:A:335:ASN:HD22	1:A:335:ASN:C	2.05	0.64
2:D:271:GLN:NE2	2:D:280:ARG:HG2	2.12	0.64
1:U:334:ARG:NH1	1:U:347:ASP:OD1	2.31	0.64
1:U:264:PRO:C	1:U:266:THR:H	2.06	0.64
1:U:456:GLU:O	1:U:458:PRO:HD3	1.98	0.64
1:A:335:ASN:ND2	1:A:336:SER:N	2.31	0.64
2:D:357:ARG:HG3	2:D:358:LYS:N	2.13	0.64
2:X:474:LYS:HD3	3:Y:686:ARG:HH21	1.63	0.63
1:A:456:GLU:O	1:A:456:GLU:HG3	1.97	0.63
2:D:358:LYS:HB2	2:D:359:PRO:CD	2.29	0.63
1:U:298:VAL:HG13	3:V:633:LEU:CD1	2.28	0.63
1:A:228:GLU:O	1:A:229:ASP:HB2	1.99	0.63
2:D:262:ILE:HA	2:D:265:LYS:CB	2.25	0.63
2:X:336:LYS:HD2	2:X:336:LYS:H	1.63	0.63
2:D:237:LEU:HD12	2:D:237:LEU:N	2.14	0.62
2:X:311:LEU:HD22	3:Y:691:HIS:CE1	2.35	0.62
3:Y:685:GLU:OE1	3:Y:686:ARG:HG2	1.99	0.62
1:A:273:ASP:OD1	1:A:449:THR:O	2.16	0.62
2:D:468:LEU:HD13	3:E:689:ILE:CG2	2.30	0.62
2:D:358:LYS:CB	2:D:359:PRO:CD	2.77	0.62
1:U:229:ASP:O	1:U:230:MET:HB2	1.98	0.62
2:D:233:ALA:O	2:D:237:LEU:CD1	2.46	0.62
2:D:370:PHE:HB2	2:D:445:ILE:HD11	1.81	0.62
2:D:270:LEU:HD22	2:D:287:PHE:CD1	2.35	0.62
1:A:236:LEU:HD22	1:A:240:LEU:HD22	1.82	0.62
1:U:334:ARG:NH1	1:U:338:HIS:NE2	2.48	0.61
1:U:334:ARG:HG3	1:U:334:ARG:HH11	1.64	0.61
2:X:311:LEU:HD22	3:Y:691:HIS:HE1	1.65	0.61
1:U:447:ILE:HD13	1:U:447:ILE:H	1.66	0.61
6:U:564:HOH:O	2:X:373:LYS:HD3	2.00	0.61
2:D:357:ARG:CG	2:D:358:LYS:H	2.09	0.61
2:X:262:ILE:C	2:X:264:PHE:N	2.57	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:363:PHE:CB	2:X:452:LEU:HD21	2.31	0.61
2:D:271:GLN:CD	2:D:271:GLN:O	2.44	0.61
3:B:634:HIS:CE1	3:B:638:GLN:HE22	2.19	0.61
1:U:242:VAL:HG23	1:U:242:VAL:O	2.01	0.60
2:X:237:LEU:HD13	2:X:335:ASN:HD22	1.66	0.60
1:U:297:GLN:HE21	3:V:637:LEU:HD22	1.65	0.60
2:X:363:PHE:HB3	2:X:452:LEU:HD21	1.83	0.60
2:X:443:ARG:O	2:X:447:THR:HG23	2.02	0.60
1:A:338:HIS:C	1:A:340:ALA:H	2.09	0.60
2:D:443:ARG:O	2:D:447:THR:HG23	2.02	0.60
1:U:422:LEU:HB3	2:X:440:THR:HG21	1.83	0.60
3:E:685:GLU:HG2	3:E:686:ARG:N	2.06	0.60
2:D:379:LEU:N	2:D:379:LEU:HD12	2.17	0.60
2:X:463:MET:O	2:X:464:SER:HB2	2.00	0.59
1:U:423:PRO:HG3	2:X:440:THR:HG22	1.84	0.59
1:U:310:ILE:HA	1:U:313:PHE:CE2	2.38	0.59
1:U:310:ILE:HD12	1:U:425:LEU:CD1	2.32	0.59
1:U:297:GLN:NE2	3:V:637:LEU:HD22	2.17	0.59
1:U:353:LEU:HD22	1:U:428:ILE:HD12	1.85	0.59
2:D:468:LEU:HD13	3:E:689:ILE:HG23	1.85	0.59
1:U:231:PRO:HG2	1:U:234:ARG:HB2	1.84	0.59
1:U:335:ASN:HD22	1:U:335:ASN:N	2.01	0.59
1:U:394:GLU:OE2	2:X:434:LYS:HE2	2.02	0.58
1:U:445:THR:N	1:U:446:PRO:HD3	2.18	0.58
3:V:641:SER:H	3:V:642:PRO:CD	2.16	0.58
3:V:642:PRO:HB2	6:V:269:HOH:O	2.04	0.58
1:U:322:ASP:HB3	1:U:331:HIS:NE2	2.18	0.58
2:X:477:TYR:HD1	2:X:477:TYR:OXT	1.87	0.58
1:U:229:ASP:O	1:U:230:MET:CB	2.52	0.57
1:U:335:ASN:HD22	1:U:336:SER:N	2.02	0.57
2:X:238:THR:CG2	2:X:239:GLY:H	2.16	0.57
2:D:271:GLN:HE22	2:D:280:ARG:HD2	1.69	0.57
1:U:456:GLU:O	1:U:456:GLU:HG3	2.04	0.57
2:X:334:MET:HG2	2:X:339:VAL:HB	1.84	0.57
1:U:302:ARG:NH1	1:U:457:ALA:HA	2.19	0.57
1:U:310:ILE:HD11	1:U:353:LEU:CD2	2.34	0.57
2:X:405:PRO:O	2:X:409:ILE:HG13	2.05	0.57
2:D:244:LYS:HE3	2:D:245:SER:O	2.04	0.57
1:A:243:GLU:HB2	1:A:244:PRO:C	2.29	0.57
1:U:305:TRP:CD1	1:U:305:TRP:C	2.81	0.57
1:U:334:ARG:NH1	1:U:347:ASP:CG	2.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:262:ILE:HD13	2:D:265:LYS:CD	2.34	0.57
1:U:335:ASN:ND2	1:U:336:SER:N	2.53	0.56
1:U:427:SER:HB2	2:X:443:ARG:HG3	1.87	0.56
1:U:457:ALA:HB3	6:U:545:HOH:O	2.05	0.56
1:U:364:LYS:NZ	6:U:508:HOH:O	2.38	0.56
1:U:447:ILE:HD13	1:U:447:ILE:N	2.20	0.56
2:D:379:LEU:HD13	6:D:506:HOH:O	2.05	0.56
1:A:232:VAL:HG23	1:A:399:SER:HB3	1.88	0.56
2:X:422:LYS:O	2:X:422:LYS:HE3	2.06	0.56
2:D:318:LEU:O	2:D:322:VAL:HB	2.05	0.56
2:X:365:GLU:HB3	2:X:366:PRO:HD3	1.87	0.56
1:A:441:LEU:O	1:A:442:ILE:HB	2.04	0.56
1:A:288:HIS:HA	1:A:291:GLU:HG3	1.87	0.56
2:D:241:THR:O	2:D:241:THR:HG23	2.06	0.56
2:D:259:GLU:O	2:D:262:ILE:HG12	2.05	0.56
2:X:259:GLU:CD	2:X:266:HIS:CB	2.79	0.56
2:X:276:GLU:HA	6:X:525:HOH:O	2.05	0.56
2:X:441:ASP:O	2:X:445:ILE:HG12	2.06	0.56
1:U:358:ARG:NH1	6:U:523:HOH:O	2.39	0.55
2:X:317:LEU:HD11	2:X:406:ILE:HD13	1.88	0.55
1:U:242:VAL:HG11	1:U:282:TRP:HB2	1.89	0.55
1:U:298:VAL:HG13	3:V:633:LEU:HD13	1.88	0.55
1:U:264:PRO:O	1:U:266:THR:N	2.35	0.55
2:X:358:LYS:O	2:X:360:PHE:N	2.40	0.55
2:D:430:GLN:O	2:D:434:LYS:HG3	2.06	0.55
1:U:242:VAL:HB	1:U:278:THR:HG22	1.88	0.55
2:X:272:GLU:O	2:X:273:GLN:HB3	2.07	0.55
1:A:243:GLU:HB3	1:A:244:PRO:HB2	1.88	0.55
2:D:465:LEU:HB3	2:D:470:GLN:HG2	1.89	0.55
2:X:476:LEU:HD22	2:X:477:TYR:CD1	2.42	0.55
2:X:238:THR:CG2	2:X:239:GLY:N	2.69	0.55
2:X:269:PRO:O	2:X:272:GLU:HG3	2.07	0.55
1:A:246:THR:O	1:A:248:THR:N	2.38	0.55
1:A:267:ASN:ND2	1:A:330:LEU:CD1	2.61	0.55
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.42	0.55
1:U:310:ILE:HA	1:U:313:PHE:CD2	2.41	0.55
2:D:364:MET:SD	5:D:503:BRL:H11	2.48	0.54
2:X:236:ILE:CG2	2:X:246:PRO:HG2	2.37	0.54
1:U:243:GLU:HB3	1:U:244:PRO:CA	2.37	0.54
2:X:267:ILE:O	2:X:268:THR:OG1	2.23	0.54
2:D:471:GLU:CG	3:E:687:HIS:HA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:231:PRO:HB2	1:U:233:GLU:OE1	2.07	0.54
1:U:241:ALA:O	1:U:243:GLU:N	2.40	0.54
1:A:391:ALA:O	1:A:395:LYS:HG3	2.08	0.54
1:A:426:ARG:NH2	6:A:513:HOH:O	2.41	0.54
2:D:261:LYS:CG	2:D:265:LYS:HE3	2.34	0.53
2:X:244:LYS:HD2	2:X:244:LYS:C	2.32	0.53
1:U:334:ARG:HH12	1:U:347:ASP:CG	2.17	0.53
2:X:325:ILE:HG12	2:X:388:ILE:HG23	1.91	0.53
1:A:242:VAL:O	1:A:243:GLU:O	2.25	0.53
2:X:357:ARG:O	2:X:360:PHE:HB2	2.07	0.53
2:D:260:ASP:HB3	2:D:263:LYS:HD2	1.90	0.53
1:U:318:ILE:HD12	1:U:318:ILE:C	2.33	0.53
1:U:294:LEU:HD12	1:U:294:LEU:O	2.08	0.53
1:A:343:GLY:O	1:A:345:ILE:N	2.42	0.53
2:D:268:THR:N	2:D:269:PRO:CD	2.71	0.53
1:A:306:ASN:H	1:A:306:ASN:HD22	1.55	0.53
1:A:320:VAL:HG22	6:A:537:HOH:O	2.09	0.53
2:D:273:GLN:HB3	2:D:280:ARG:NE	2.24	0.53
2:D:282:PHE:CZ	2:D:286:GLN:NE2	2.77	0.53
2:X:364:MET:SD	5:X:504:BRL:H11	2.49	0.53
2:D:357:ARG:NH1	2:D:358:LYS:HB2	2.24	0.52
1:U:437:PHE:CE1	1:U:455:LEU:O	2.62	0.52
2:D:256:MET:O	2:D:260:ASP:OD2	2.27	0.52
2:D:259:GLU:C	2:D:261:LYS:H	2.17	0.52
3:V:638:GLN:O	3:V:638:GLN:HG3	2.08	0.52
1:A:345:ILE:HG12	1:A:431:LYS:HD2	1.91	0.52
2:D:401:LEU:C	2:D:402:ASN:HD22	2.17	0.52
1:U:444:ASP:O	1:U:445:THR:C	2.52	0.52
2:D:313:ASP:O	2:D:317:LEU:HG	2.10	0.52
2:D:357:ARG:HH11	2:D:358:LYS:HB2	1.74	0.52
1:U:324:ILE:HG12	1:U:332:VAL:HG22	1.92	0.52
2:X:262:ILE:O	2:X:264:PHE:N	2.38	0.52
2:D:262:ILE:HD13	2:D:265:LYS:NZ	2.25	0.52
2:D:462:ASP:O	2:D:463:MET:C	2.51	0.52
2:X:264:PHE:C	2:X:266:HIS:N	2.66	0.52
2:D:273:GLN:CA	2:D:280:ARG:HD3	2.33	0.52
2:D:252:MET:HG3	2:D:277:VAL:HG21	1.92	0.51
1:U:452:MET:HA	1:U:452:MET:CE	2.39	0.51
1:U:390:GLU:O	1:U:394:GLU:HG3	2.10	0.51
2:X:270:LEU:O	2:X:272:GLU:HG2	2.10	0.51
2:X:270:LEU:O	2:X:272:GLU:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:354:LYS:HD2	2:X:365:GLU:OE1	2.11	0.51
2:X:460:GLU:O	2:X:461:THR:C	2.52	0.51
1:U:264:PRO:C	1:U:266:THR:N	2.69	0.51
1:A:437:PHE:CE1	1:A:455:LEU:HG	2.46	0.51
3:E:686:ARG:HA	3:E:686:ARG:NE	2.26	0.51
1:U:334:ARG:O	1:U:338:HIS:HD2	1.93	0.51
1:A:313:PHE:CD1	1:A:313:PHE:C	2.88	0.50
1:U:273:ASP:OD1	1:U:450:PHE:HB3	2.11	0.50
1:U:454:MET:CE	3:V:633:LEU:HG	2.35	0.50
2:X:380:ASP:OD1	2:X:382:SER:OG	2.26	0.50
3:Y:684:THR:O	3:Y:691:HIS:CD2	2.64	0.50
2:X:274:SER:O	2:X:275:LYS:C	2.54	0.50
1:A:298:VAL:HG22	3:B:637:LEU:HD12	1.93	0.50
2:D:273:GLN:C	2:D:275:LYS:N	2.65	0.50
1:U:276:LEU:CD1	1:U:305:TRP:CD1	2.92	0.50
1:U:411:GLN:NE2	1:U:414:ARG:HH11	2.09	0.50
4:U:502:9CR:H19	4:U:502:9CR:H8	1.93	0.50
2:D:233:ALA:O	2:D:237:LEU:HD12	2.11	0.50
2:D:271:GLN:O	2:D:272:GLU:C	2.55	0.50
1:U:378:PRO:HG3	1:U:390:GLU:OE1	2.12	0.50
1:U:310:ILE:CD1	1:U:425:LEU:CD1	2.89	0.50
2:X:336:LYS:H	2:X:336:LYS:CD	2.20	0.50
2:D:237:LEU:H	2:D:237:LEU:CD1	2.22	0.50
2:D:367:LYS:HD2	2:D:367:LYS:N	2.27	0.50
1:U:305:TRP:HZ3	6:U:545:HOH:O	1.95	0.50
2:X:342:SER:CB	2:X:345:GLN:HB2	2.42	0.50
2:D:273:GLN:O	2:D:274:SER:HB2	2.13	0.49
1:U:310:ILE:HD11	1:U:353:LEU:HD23	1.93	0.49
1:U:426:ARG:NH1	6:U:512:HOH:O	2.34	0.49
2:X:251:ASP:HA	2:X:352:PHE:CD1	2.47	0.49
2:D:273:GLN:HB3	2:D:280:ARG:CZ	2.42	0.49
1:U:333:HIS:HB2	1:U:335:ASN:HD21	1.77	0.49
2:D:261:LYS:O	2:D:265:LYS:HG3	2.12	0.49
1:U:345:ILE:HD13	1:U:431:LYS:CD	2.34	0.49
2:X:341:ILE:HD13	2:X:348:MET:HE3	1.94	0.49
3:E:685:GLU:O	3:E:686:ARG:HB3	2.11	0.49
2:D:363:PHE:CZ	2:D:364:MET:HG2	2.48	0.49
1:A:316:ARG:NH1	1:A:325:LEU:O	2.42	0.49
1:A:360:MET:CE	1:A:418:LEU:HD13	2.42	0.49
1:U:292:LEU:C	1:U:292:LEU:HD23	2.38	0.49
1:U:427:SER:HB2	2:X:443:ARG:CG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:268:THR:O	2:X:272:GLU:OE2	2.30	0.48
1:U:326:LEU:HD12	1:U:330:LEU:HB3	1.95	0.48
1:A:445:THR:N	1:A:446:PRO:CD	2.76	0.48
1:A:331:HIS:C	1:A:331:HIS:CD2	2.92	0.48
2:D:270:LEU:O	2:D:271:GLN:HB2	2.12	0.48
2:D:421:LEU:HD22	2:D:431:LEU:HD13	1.94	0.48
1:A:304:GLY:O	1:A:308:LEU:HG	2.13	0.48
1:A:333:HIS:HD2	1:A:335:ASN:CG	2.22	0.48
1:U:407:LYS:C	1:U:409:PRO:HD3	2.38	0.48
2:D:471:GLU:HG2	3:E:687:HIS:HA	1.94	0.48
2:X:240:LYS:O	2:X:241:THR:O	2.32	0.48
2:X:444:GLN:O	2:X:448:GLU:HB2	2.13	0.48
1:U:353:LEU:HD22	1:U:428:ILE:CD1	2.44	0.48
2:X:242:THR:O	2:X:242:THR:OG1	2.32	0.48
1:A:392:LEU:HD23	1:A:395:LYS:HD2	1.96	0.48
1:U:334:ARG:NH1	1:U:347:ASP:OD2	2.44	0.48
1:A:427:SER:HB3	2:D:443:ARG:HG3	1.96	0.48
1:U:335:ASN:ND2	1:U:335:ASN:N	2.62	0.48
2:X:273:GLN:O	2:X:273:GLN:HG3	2.13	0.48
2:D:449:HIS:HE2	5:D:503:BRL:C2	2.27	0.47
1:U:302:ARG:HH22	1:U:457:ALA:N	2.12	0.47
2:X:411:ASP:OD1	2:X:415:GLN:NE2	2.47	0.47
1:U:306:ASN:O	1:U:310:ILE:CG2	2.50	0.47
2:D:307:VAL:HG22	6:D:540:HOH:O	2.14	0.47
2:D:357:ARG:HD2	2:D:358:LYS:HG2	1.96	0.47
1:U:445:THR:O	1:U:446:PRO:O	2.33	0.47
2:X:260:ASP:OD2	2:X:261:LYS:N	2.46	0.47
1:A:441:LEU:O	1:A:442:ILE:CB	2.62	0.47
2:D:267:ILE:O	2:D:267:ILE:HG22	2.14	0.47
2:D:358:LYS:CB	2:D:359:PRO:HD3	2.43	0.47
2:D:363:PHE:CE1	2:D:364:MET:HG2	2.49	0.47
1:A:360:MET:HE1	1:A:418:LEU:HD13	1.96	0.47
2:D:226:PHE:CG	2:D:329:MET:HE1	2.50	0.47
1:U:252:ALA:O	1:U:329:GLY:O	2.33	0.47
2:X:305:GLY:O	2:X:308:ASN:ND2	2.41	0.47
2:D:257:MET:O	2:D:261:LYS:HB2	2.15	0.47
4:A:501:9CR:H19	4:A:501:9CR:H8	1.97	0.47
2:D:207:GLU:O	2:D:210:ASP:HB2	2.15	0.47
1:U:298:VAL:HG22	3:V:633:LEU:HD13	1.96	0.47
2:X:266:HIS:C	2:X:267:ILE:HG13	2.39	0.47
3:B:633:LEU:HD13	3:B:633:LEU:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:692:ARG:HG3	3:Y:693:LEU:N	2.30	0.47
2:X:232:LYS:O	2:X:235:ALA:HB3	2.15	0.46
2:D:286:GLN:NE2	2:D:465:LEU:HD12	2.30	0.46
1:A:243:GLU:CB	1:A:244:PRO:C	2.89	0.46
2:D:373:LYS:O	2:D:376:ALA:HB3	2.16	0.46
2:D:377:LEU:CB	2:D:379:LEU:HD11	2.44	0.46
2:D:462:ASP:OD1	2:D:462:ASP:N	2.42	0.46
1:A:434:GLU:HG3	6:D:626:HOH:O	2.15	0.46
1:A:437:PHE:CE1	1:A:455:LEU:O	2.65	0.46
2:D:237:LEU:HD11	2:D:340:LEU:HD11	1.98	0.46
2:D:358:LYS:HB2	2:D:359:PRO:HD2	1.96	0.46
2:D:477:TYR:CD1	2:D:477:TYR:C	2.93	0.46
1:U:292:LEU:HB2	1:U:293:PRO:HD2	1.98	0.46
1:U:437:PHE:HE1	1:U:455:LEU:O	1.98	0.46
2:D:264:PHE:HD1	2:D:264:PHE:O	1.96	0.46
1:A:338:HIS:HD2	1:A:343:GLY:HA3	1.80	0.46
1:A:451:LEU:O	1:A:455:LEU:HB2	2.15	0.46
2:X:325:ILE:HD11	2:X:392:ILE:HG13	1.97	0.46
2:D:379:LEU:CD1	2:D:379:LEU:N	2.79	0.46
2:X:477:TYR:OXT	2:X:477:TYR:CD1	2.67	0.46
1:U:242:VAL:HB	1:U:278:THR:CG2	2.46	0.46
1:U:228:GLU:O	1:U:228:GLU:CD	2.59	0.45
1:U:287:PRO:O	1:U:288:HIS:HB2	2.16	0.45
1:U:348:ARG:O	1:U:352:GLU:HG3	2.16	0.45
2:D:290:VAL:O	2:D:294:GLN:HG3	2.16	0.45
1:U:280:VAL:HG11	3:V:636:LEU:HB3	1.97	0.45
1:U:334:ARG:HH11	1:U:334:ARG:CG	2.29	0.45
1:A:449:THR:HG22	1:A:450:PHE:H	1.82	0.45
1:U:293:PRO:HB2	1:U:296:ASP:OD2	2.16	0.45
3:Y:685:GLU:CD	3:Y:685:GLU:H	2.24	0.45
2:X:272:GLU:HB2	2:X:273:GLN:H	1.37	0.45
3:V:641:SER:H	3:V:642:PRO:HD2	1.82	0.45
1:A:230:MET:HE3	1:A:235:ILE:HD11	1.96	0.45
2:D:334:MET:HG2	2:D:339:VAL:HB	1.98	0.45
1:U:231:PRO:HG3	1:U:234:ARG:HD3	1.97	0.45
1:A:273:ASP:OD2	1:U:237:GLU:OE2	2.35	0.45
1:A:377:ASN:HA	1:A:393:ARG:NH2	2.32	0.45
1:U:228:GLU:O	1:U:228:GLU:CG	2.64	0.45
1:U:455:LEU:HD23	1:U:455:LEU:HA	1.80	0.45
1:A:449:THR:O	1:A:451:LEU:N	2.43	0.45
2:X:271:GLN:HG3	6:X:563:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:335:ASN:ND2	1:U:335:ASN:H	2.15	0.45
2:D:237:LEU:CD1	2:D:340:LEU:HD11	2.47	0.45
2:D:379:LEU:CD1	2:D:379:LEU:H	2.30	0.45
1:U:363:ASP:OD1	1:U:366:GLU:HG3	2.16	0.45
1:A:228:GLU:O	1:A:229:ASP:CB	2.62	0.44
2:D:242:THR:HG23	2:D:242:THR:O	2.17	0.44
1:U:292:LEU:CD2	1:U:297:GLN:HG2	2.47	0.44
1:U:370:LEU:O	1:U:374:VAL:HG23	2.18	0.44
1:U:333:HIS:HB2	1:U:335:ASN:ND2	2.32	0.44
2:X:319:LYS:NZ	3:Y:687:HIS:HE1	2.16	0.44
1:U:355:SER:HB2	6:U:523:HOH:O	2.18	0.44
2:X:259:GLU:OE1	2:X:266:HIS:CB	2.64	0.44
2:X:312:ASN:CG	3:Y:684:THR:HG23	2.42	0.44
3:E:695:GLN:HE21	3:E:695:GLN:HB3	1.48	0.44
1:U:230:MET:HE1	1:U:287:PRO:O	2.18	0.44
2:X:242:THR:O	2:X:243:ASP:HB3	2.18	0.44
2:X:348:MET:SD	2:X:353:LEU:HD21	2.57	0.44
2:X:391:ILE:HG12	2:X:439:MET:HE3	2.00	0.44
2:D:232:LYS:O	2:D:235:ALA:HB3	2.17	0.44
2:X:288:ARG:O	2:X:288:ARG:NH1	2.49	0.44
1:A:287:PRO:O	1:A:288:HIS:HB2	2.17	0.44
2:D:358:LYS:HB3	2:D:359:PRO:HD3	1.98	0.44
2:D:379:LEU:HD12	2:D:379:LEU:H	1.83	0.44
1:U:305:TRP:CG	1:U:306:ASN:N	2.85	0.43
1:U:445:THR:N	1:U:446:PRO:CD	2.81	0.43
2:X:255:LEU:O	2:X:258:GLY:O	2.36	0.43
1:A:338:HIS:C	1:A:340:ALA:N	2.75	0.43
1:A:377:ASN:HA	1:A:378:PRO:HD3	1.77	0.43
2:X:336:LYS:HD2	2:X:336:LYS:N	2.32	0.43
2:X:453:LEU:HD12	2:X:453:LEU:HA	1.85	0.43
3:E:685:GLU:CG	3:E:686:ARG:N	2.74	0.43
2:X:363:PHE:O	2:X:367:LYS:HD3	2.18	0.43
2:X:477:TYR:HA	6:X:551:HOH:O	2.17	0.43
1:A:294:LEU:HD21	3:B:634:HIS:NE2	2.34	0.43
1:A:318:ILE:HG23	1:A:358:ARG:HB2	2.00	0.43
2:D:233:ALA:O	2:D:237:LEU:HD13	2.18	0.43
2:X:312:ASN:CG	3:Y:684:THR:CG2	2.91	0.43
1:A:343:GLY:O	1:A:344:ALA:HB3	2.19	0.43
1:U:242:VAL:HG11	1:U:282:TRP:CA	2.48	0.43
1:U:411:GLN:HA	1:U:412:PRO:HD2	1.78	0.43
1:A:245:LYS:O	1:A:246:THR:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:436:LEU:O	2:D:439:MET:HB2	2.19	0.43
1:U:313:PHE:CD1	1:U:313:PHE:C	2.96	0.43
1:A:275:GLN:HA	1:A:275:GLN:NE2	2.34	0.43
2:D:305:GLY:O	2:D:309:LEU:HD13	2.18	0.43
1:U:292:LEU:HD21	1:U:297:GLN:HG2	2.00	0.43
1:U:384:SER:O	1:U:385:ASN:HB2	2.18	0.43
1:A:305:TRP:O	1:A:309:LEU:HB2	2.19	0.43
2:D:241:THR:O	2:D:241:THR:CG2	2.67	0.43
2:D:271:GLN:O	2:D:271:GLN:CG	2.67	0.43
1:U:310:ILE:HD11	1:U:353:LEU:HD21	2.01	0.43
2:D:275:LYS:O	2:D:276:GLU:O	2.37	0.43
1:U:335:ASN:C	1:U:337:ALA:N	2.77	0.43
2:X:211:LEU:HB3	2:X:419:LEU:HD23	2.01	0.43
3:B:638:GLN:HE21	3:B:638:GLN:HB3	1.55	0.43
2:D:443:ARG:HA	2:D:443:ARG:HD3	1.87	0.42
1:U:334:ARG:O	1:U:338:HIS:CD2	2.73	0.42
1:U:332:VAL:O	1:U:332:VAL:CG2	2.67	0.42
2:X:342:SER:HB3	2:X:345:GLN:HB2	2.02	0.42
2:X:358:LYS:HA	2:X:359:PRO:HD2	1.85	0.42
2:D:259:GLU:C	2:D:261:LYS:N	2.77	0.42
1:U:312:SER:OG	1:U:371:ARG:CZ	2.67	0.42
1:U:437:PHE:HB3	6:U:577:HOH:O	2.19	0.42
1:U:243:GLU:CB	1:U:244:PRO:HA	2.46	0.42
1:U:308:LEU:HD11	1:U:371:ARG:O	2.19	0.42
2:X:226:PHE:CG	2:X:329:MET:HE1	2.54	0.42
1:A:306:ASN:H	1:A:306:ASN:ND2	2.17	0.42
1:A:334:ARG:O	1:A:337:ALA:HB3	2.19	0.42
2:X:322:VAL:HG12	2:X:323:HIS:N	2.34	0.42
1:A:338:HIS:HD2	1:A:343:GLY:CA	2.32	0.42
1:U:348:ARG:O	1:U:352:GLU:CG	2.68	0.42
2:X:363:PHE:CB	2:X:452:LEU:CD2	2.98	0.42
2:D:320:TYR:CB	2:D:397:ARG:HD2	2.50	0.42
1:U:266:THR:O	1:U:270:GLN:HB2	2.20	0.42
1:U:352:GLU:HG3	1:U:428:ILE:HD11	2.00	0.42
2:X:358:LYS:C	2:X:360:PHE:N	2.78	0.42
1:A:298:VAL:O	1:A:302:ARG:HG3	2.20	0.42
2:D:275:LYS:O	2:D:280:ARG:CG	2.68	0.42
1:U:423:PRO:CG	2:X:440:THR:HG22	2.47	0.42
6:U:533:HOH:O	3:V:630:HIS:HB3	2.20	0.42
3:Y:688:LYS:NZ	3:Y:688:LYS:HB3	2.35	0.42
1:A:443:GLY:O	1:A:444:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:219:TYR:O	2:D:222:TYR:HB3	2.20	0.41
2:D:281:ILE:HG23	5:D:503:BRL:H22	2.02	0.41
2:X:280:ARG:NH1	2:X:280:ARG:CG	2.75	0.41
2:X:342:SER:HB2	2:X:345:GLN:HB2	2.00	0.41
1:A:324:ILE:HG22	1:A:325:LEU:N	2.35	0.41
1:U:276:LEU:HD13	1:U:309:LEU:HD11	2.02	0.41
2:X:260:ASP:OD2	2:X:260:ASP:C	2.62	0.41
3:E:686:ARG:NH1	3:E:686:ARG:O	2.52	0.41
3:Y:686:ARG:CZ	3:Y:686:ARG:HB3	2.49	0.41
2:X:270:LEU:C	2:X:272:GLU:H	2.23	0.41
3:B:634:HIS:HE1	3:B:638:GLN:HE22	1.66	0.41
2:D:341:ILE:HG22	5:D:503:BRL:H152	2.02	0.41
2:D:350:ARG:NH2	2:D:365:GLU:OE2	2.51	0.41
2:D:471:GLU:CD	3:E:687:HIS:HA	2.46	0.41
3:Y:684:THR:CA	3:Y:691:HIS:NE2	2.84	0.41
1:U:345:ILE:CD1	1:U:431:LYS:HD3	2.38	0.41
2:D:457:LYS:NZ	6:D:566:HOH:O	2.54	0.41
1:A:334:ARG:HD2	1:A:347:ASP:OD1	2.21	0.41
1:U:229:ASP:HB3	1:U:395:LYS:HD3	2.03	0.41
3:E:686:ARG:O	3:E:687:HIS:C	2.60	0.41
2:D:393:LEU:O	2:D:410:GLN:HB2	2.21	0.41
3:Y:685:GLU:CD	3:Y:685:GLU:N	2.78	0.41
2:D:401:LEU:C	2:D:402:ASN:ND2	2.78	0.41
1:U:394:GLU:O	2:X:430:GLN:NE2	2.49	0.41
2:X:367:LYS:HD2	2:X:367:LYS:N	2.36	0.41
3:Y:684:THR:N	3:Y:691:HIS:CE1	2.89	0.41
2:D:250:TYR:CD1	2:D:250:TYR:N	2.88	0.41
2:D:418:GLU:HG3	2:D:432:PHE:CG	2.56	0.41
2:D:446:VAL:HG11	2:D:477:TYR:HE1	1.85	0.41
2:X:291:GLU:O	2:X:295:GLU:HG3	2.21	0.41
2:X:358:LYS:O	2:X:359:PRO:C	2.64	0.41
2:X:207:GLU:HB3	2:X:210:ASP:OD2	2.20	0.40
2:X:223:ILE:HD11	6:X:587:HOH:O	2.20	0.40
2:X:264:PHE:O	2:X:266:HIS:CB	2.70	0.40
2:D:367:LYS:HD2	2:D:367:LYS:H	1.84	0.40
2:D:418:GLU:HG3	2:D:432:PHE:CD2	2.56	0.40
1:U:302:ARG:HH22	1:U:456:GLU:C	2.30	0.40
4:U:502:9CR:H8	4:U:502:9CR:H10	1.87	0.40
1:A:366:GLU:HG2	1:A:418:LEU:HD21	2.03	0.40
2:D:452:LEU:O	2:D:456:ILE:HG13	2.22	0.40
2:D:476:LEU:HG	2:D:477:TYR:N	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:684:THR:HB	3:Y:685:GLU:H	1.74	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	230/238 (97%)	191 (83%)	21 (9%)	18 (8%)	1	0
1	U	230/238 (97%)	191 (83%)	24 (10%)	15 (6%)	1	0
2	D	270/272 (99%)	240 (89%)	15 (6%)	15 (6%)	1	0
2	X	270/272 (99%)	235 (87%)	16 (6%)	19 (7%)	1	0
3	B	8/25 (32%)	7 (88%)	1 (12%)	0	100	100
3	E	14/25 (56%)	13 (93%)	1 (7%)	0	100	100
3	V	13/25 (52%)	10 (77%)	2 (15%)	1 (8%)	1	0
3	Y	11/25 (44%)	10 (91%)	1 (9%)	0	100	100
All	All	1046/1120 (93%)	897 (86%)	81 (8%)	68 (6%)	1	0

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	GLU
1	A	244	PRO
1	A	246	THR
1	A	247	GLU
1	A	253	ASN
1	A	254	MET
1	A	257	ASN
1	A	260	SER
1	A	442	ILE

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Mol	Chain	Res	Type
1	A	446	PRO
2	D	265	LYS
2	D	269	PRO
2	D	271	GLN
2	D	273	GLN
2	D	276	GLU
2	D	357	ARG
2	D	358	LYS
2	D	463	MET
1	U	230	MET
1	U	253	ASN
1	U	259	SER
1	U	263	ASP
1	U	264	PRO
1	U	443	GLY
1	U	446	PRO
2	X	240	LYS
2	X	241	THR
2	X	259	GLU
2	X	262	ILE
2	X	270	LEU
2	X	271	GLN
2	X	273	GLN
2	X	274	SER
2	X	359	PRO
1	A	339	SER
2	D	243	ASP
1	U	242	VAL
1	U	322	ASP
2	X	243	ASP
2	X	269	PRO
2	X	272	GLU
1	A	245	LYS
2	D	260	ASP
2	D	464	SER
2	D	476	LEU
1	U	254	MET
2	X	264	PHE
1	A	229	ASP
1	A	259	SER
1	A	334	ARG
1	A	455	LEU

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Mol	Chain	Res	Type
2	D	272	GLU
1	U	243	GLU
1	U	244	PRO
1	U	257	ASN
2	X	266	HIS
2	X	267	ILE
2	X	463	MET
1	A	250	VAL
2	D	241	THR
3	V	641	SER
1	U	265	VAL
2	X	268	THR
2	X	358	LYS
1	A	457	ALA
2	X	239	GLY
2	D	268	THR
1	U	260	SER

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	182/205 (89%)	163 (90%)	19 (10%)	7	4
1	U	182/205 (89%)	157 (86%)	25 (14%)	3	2
2	D	244/245 (100%)	222 (91%)	22 (9%)	9	6
2	X	236/245 (96%)	209 (89%)	27 (11%)	5	3
3	B	9/24 (38%)	7 (78%)	2 (22%)	1	0
3	E	14/24 (58%)	13 (93%)	1 (7%)	13	11
3	V	14/24 (58%)	10 (71%)	4 (29%)	0	0
3	Y	13/24 (54%)	8 (62%)	5 (38%)	0	0
All	All	894/996 (90%)	789 (88%)	105 (12%)	5	3

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	GLU
1	A	236	LEU
1	A	240	LEU
1	A	244	PRO
1	A	276	LEU
1	A	286	ILE
1	A	306	ASN
1	A	309	LEU
1	A	320	VAL
1	A	330	LEU
1	A	335	ASN
1	A	345	ILE
1	A	355	SER
1	A	388	GLU
1	A	410	GLU
1	A	418	LEU
1	A	436	LEU
1	A	442	ILE
1	A	455	LEU
2	D	207	GLU
2	D	234	ARG
2	D	237	LEU
2	D	251	ASP
2	D	256	MET
2	D	262	ILE
2	D	264	PHE
2	D	267	ILE
2	D	269	PRO
2	D	270	LEU
2	D	309	LEU
2	D	318	LEU
2	D	322	VAL
2	D	358	LYS
2	D	379	LEU
2	D	431	LEU
2	D	443	ARG
2	D	444	GLN
2	D	447	THR
2	D	453	LEU
2	D	463	MET
2	D	477	TYR
1	U	240	LEU
1	U	243	GLU

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Mol	Chain	Res	Type
1	U	264	PRO
1	U	266	THR
1	U	270	GLN
1	U	275	GLN
1	U	276	LEU
1	U	285	ARG
1	U	292	LEU
1	U	302	ARG
1	U	305	TRP
1	U	308	LEU
1	U	310	ILE
1	U	320	VAL
1	U	330	LEU
1	U	332	VAL
1	U	335	ASN
1	U	353	LEU
1	U	381	LYS
1	U	388	GLU
1	U	420	LEU
1	U	422	LEU
1	U	446	PRO
1	U	447	ILE
1	U	452	MET
2	X	211	LEU
2	X	240	LYS
2	X	242	THR
2	X	244	LYS
2	X	248	VAL
2	X	256	MET
2	X	267	ILE
2	X	271	GLN
2	X	272	GLU
2	X	277	VAL
2	X	280	ARG
2	X	298	GLU
2	X	308	ASN
2	X	311	LEU
2	X	315	VAL
2	X	318	LEU
2	X	322	VAL
2	X	330	LEU
2	X	333	LEU

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Mol	Chain	Res	Type
2	X	336	LYS
2	X	359	PRO
2	X	422	LYS
2	X	453	LEU
2	X	459	THR
2	X	465	LEU
2	X	476	LEU
2	X	477	TYR
3	B	630	HIS
3	B	638	GLN
3	V	633	LEU
3	V	636	LEU
3	V	638	GLN
3	V	641	SER
3	E	695	GLN
3	Y	684	THR
3	Y	685	GLU
3	Y	691	HIS
3	Y	695	GLN
3	Y	696	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	270	GLN
1	A	288	HIS
1	A	306	ASN
1	A	331	HIS
1	A	333	HIS
1	A	335	ASN
1	A	338	HIS
2	D	253	ASN
2	D	266	HIS
2	D	271	GLN
2	D	402	ASN
2	D	430	GLN
2	D	451	GLN
1	U	270	GLN
1	U	275	GLN
1	U	297	GLN
1	U	333	HIS

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Mol	Chain	Res	Type
1	U	335	ASN
1	U	385	ASN
1	U	406	HIS
1	U	411	GLN
2	X	402	ASN
2	X	415	GLN
2	X	424	ASN
2	X	437	GLN
2	X	451	GLN
3	B	630	HIS
3	B	638	GLN
3	E	695	GLN
3	Y	687	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
4	9CR	U	502	-	22,22,22	3.76	10 (45%)	30,30,30	2.68	12 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BRL	D	503	-	27,27,27	2.71	15 (55%)	36,36,36	2.69	12 (33%)
4	9CR	A	501	-	22,22,22	3.86	10 (45%)	30,30,30	2.49	14 (46%)
5	BRL	X	504	-	27,27,27	2.58	11 (40%)	36,36,36	2.80	11 (30%)

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	9CR	U	502	-	-	6/15/32/32	0/1/1/1
5	BRL	D	503	-	-	2/14/26/26	0/3/3/3
4	9CR	A	501	-	-	6/15/32/32	0/1/1/1
5	BRL	X	504	-	-	0/14/26/26	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	9CR	C1-C6	11.89	1.69	1.53
4	U	502	9CR	C1-C6	10.89	1.67	1.53
4	U	502	9CR	C5-C6	8.90	1.49	1.34
4	A	501	9CR	C5-C6	8.81	1.49	1.34
5	D	503	BRL	C17-N16	7.64	1.56	1.37
5	X	504	BRL	C17-N16	7.35	1.55	1.37
4	U	502	9CR	C16-C1	5.82	1.64	1.53
5	X	504	BRL	C9-C10	4.63	1.47	1.38
5	D	503	BRL	C9-C10	4.57	1.47	1.38
4	A	501	9CR	C16-C1	4.43	1.62	1.53
4	A	501	9CR	C20-C13	3.94	1.58	1.50
4	A	501	9CR	C2-C1	3.87	1.62	1.54
5	D	503	BRL	C2-N3	-3.65	1.32	1.36
5	X	504	BRL	C16-N16	3.63	1.51	1.46
5	X	504	BRL	C2-N3	-3.60	1.32	1.36
4	U	502	9CR	C4-C5	3.59	1.57	1.51
5	D	503	BRL	C5-C4	3.50	1.55	1.52
5	D	503	BRL	C16-N16	3.49	1.51	1.46
4	A	501	9CR	C4-C5	3.32	1.57	1.51
4	U	502	9CR	C2-C1	3.31	1.61	1.54
4	U	502	9CR	C20-C13	3.19	1.57	1.50
5	X	504	BRL	C17-N18	3.15	1.41	1.34
5	D	503	BRL	C22-C17	3.12	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	504	BRL	C22-C17	3.11	1.46	1.39
5	D	503	BRL	C17-N18	3.08	1.40	1.34
4	U	502	9CR	C2-C3	3.00	1.59	1.52
4	A	501	9CR	C2-C3	2.98	1.59	1.52
4	A	501	9CR	C14-C13	2.76	1.39	1.35
4	U	502	9CR	C14-C15	2.74	1.54	1.47
5	X	504	BRL	C12-C7	2.74	1.44	1.38
5	D	503	BRL	C12-C7	2.65	1.44	1.38
4	A	501	9CR	C10-C9	2.58	1.41	1.35
5	D	503	BRL	O13-C10	2.57	1.43	1.37
5	X	504	BRL	O13-C10	2.46	1.43	1.37
5	D	503	BRL	C4-N3	-2.44	1.34	1.37
5	X	504	BRL	C11-C10	2.44	1.43	1.38
4	U	502	9CR	C10-C9	2.44	1.41	1.35
5	D	503	BRL	C8-C7	2.42	1.43	1.38
4	A	501	9CR	C14-C15	2.40	1.53	1.47
5	X	504	BRL	C15-N16	2.28	1.53	1.46
5	X	504	BRL	C8-C7	2.28	1.43	1.38
4	U	502	9CR	C14-C13	2.23	1.38	1.35
5	D	503	BRL	C11-C10	2.19	1.42	1.38
5	D	503	BRL	C12-C11	2.10	1.42	1.38
5	D	503	BRL	C9-C8	2.00	1.42	1.38
5	D	503	BRL	C15-N16	2.00	1.52	1.46

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	504	BRL	C4-N3-C2	-9.25	112.02	118.20
5	X	504	BRL	S1-C2-N3	8.87	116.68	110.44
5	D	503	BRL	S1-C2-N3	8.79	116.62	110.44
5	D	503	BRL	C4-N3-C2	-8.44	112.57	118.20
4	U	502	9CR	C17-C1-C6	6.83	120.96	110.24
4	A	501	9CR	C17-C1-C6	6.67	120.71	110.24
4	U	502	9CR	C16-C1-C6	-6.17	100.57	110.24
4	U	502	9CR	C7-C8-C9	5.68	134.63	126.23
4	A	501	9CR	C7-C8-C9	5.05	133.71	126.23
5	X	504	BRL	C5-C4-N3	4.75	116.01	111.99
5	X	504	BRL	O2-C2-N3	-4.65	121.03	125.76
5	D	503	BRL	C5-C4-N3	4.59	115.88	111.99
5	D	503	BRL	O2-C2-N3	-4.50	121.18	125.76
4	U	502	9CR	C19-C9-C8	4.35	124.73	118.09
4	A	501	9CR	C16-C1-C6	-4.34	103.44	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	9CR	C19-C9-C8	3.90	124.04	118.09
4	A	501	9CR	C19-C9-C10	-3.61	116.96	122.82
5	X	504	BRL	C5-S1-C2	-3.47	90.59	92.77
4	U	502	9CR	C19-C9-C10	-3.41	117.29	122.82
5	X	504	BRL	C6-C5-S1	-3.25	108.53	113.32
4	A	501	9CR	C20-C13-C12	3.14	122.88	118.09
4	U	502	9CR	C2-C1-C6	3.14	114.99	110.44
4	A	501	9CR	C8-C7-C6	3.13	135.37	127.00
4	U	502	9CR	C20-C13-C12	3.06	122.77	118.09
5	D	503	BRL	O4-C4-N3	-3.05	121.33	124.93
5	X	504	BRL	C19-N18-C17	3.03	121.21	116.81
5	D	503	BRL	C5-S1-C2	-2.88	90.96	92.77
5	D	503	BRL	C19-N18-C17	2.84	120.93	116.81
4	U	502	9CR	C8-C7-C6	2.82	134.53	127.00
4	A	501	9CR	C1-C6-C5	-2.80	118.81	122.64
5	D	503	BRL	C22-C17-N18	-2.78	117.97	123.46
5	X	504	BRL	C22-C17-N18	-2.75	118.04	123.46
5	D	503	BRL	O2-C2-S1	-2.67	122.19	124.61
5	X	504	BRL	O2-C2-S1	-2.57	122.29	124.61
4	A	501	9CR	C16-C1-C2	-2.49	99.39	108.95
5	X	504	BRL	O4-C4-N3	-2.45	122.05	124.93
5	D	503	BRL	N18-C17-N16	2.44	120.47	116.62
4	U	502	9CR	C1-C6-C5	-2.41	119.35	122.64
5	D	503	BRL	C6-C5-S1	-2.38	109.82	113.32
5	D	503	BRL	C4-C5-S1	-2.34	103.97	105.93
4	A	501	9CR	C2-C1-C6	2.29	113.77	110.44
4	U	502	9CR	C11-C10-C9	-2.26	124.11	127.28
4	U	502	9CR	C7-C6-C5	2.18	126.59	121.56
4	A	501	9CR	C11-C10-C9	-2.18	124.22	127.28
4	A	501	9CR	O2-C15-C14	2.13	119.74	113.40
4	U	502	9CR	O2-C15-C14	2.11	119.68	113.40
5	X	504	BRL	N18-C17-N16	2.10	119.94	116.62
4	A	501	9CR	C7-C6-C5	2.08	126.35	121.56
4	A	501	9CR	C4-C5-C6	-2.04	119.95	122.70

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	9CR	C5-C6-C7-C8
4	U	502	9CR	C5-C6-C7-C8
4	A	501	9CR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	U	502	9CR	C1-C6-C7-C8
4	A	501	9CR	C13-C14-C15-O1
4	A	501	9CR	C13-C14-C15-O2
4	U	502	9CR	C13-C14-C15-O1
4	U	502	9CR	C13-C14-C15-O2
5	D	503	BRL	C11-C10-O13-C14
5	D	503	BRL	C9-C10-O13-C14
4	A	501	9CR	C11-C10-C9-C19
4	U	502	9CR	C11-C10-C9-C19
4	A	501	9CR	C11-C10-C9-C8
4	U	502	9CR	C11-C10-C9-C8

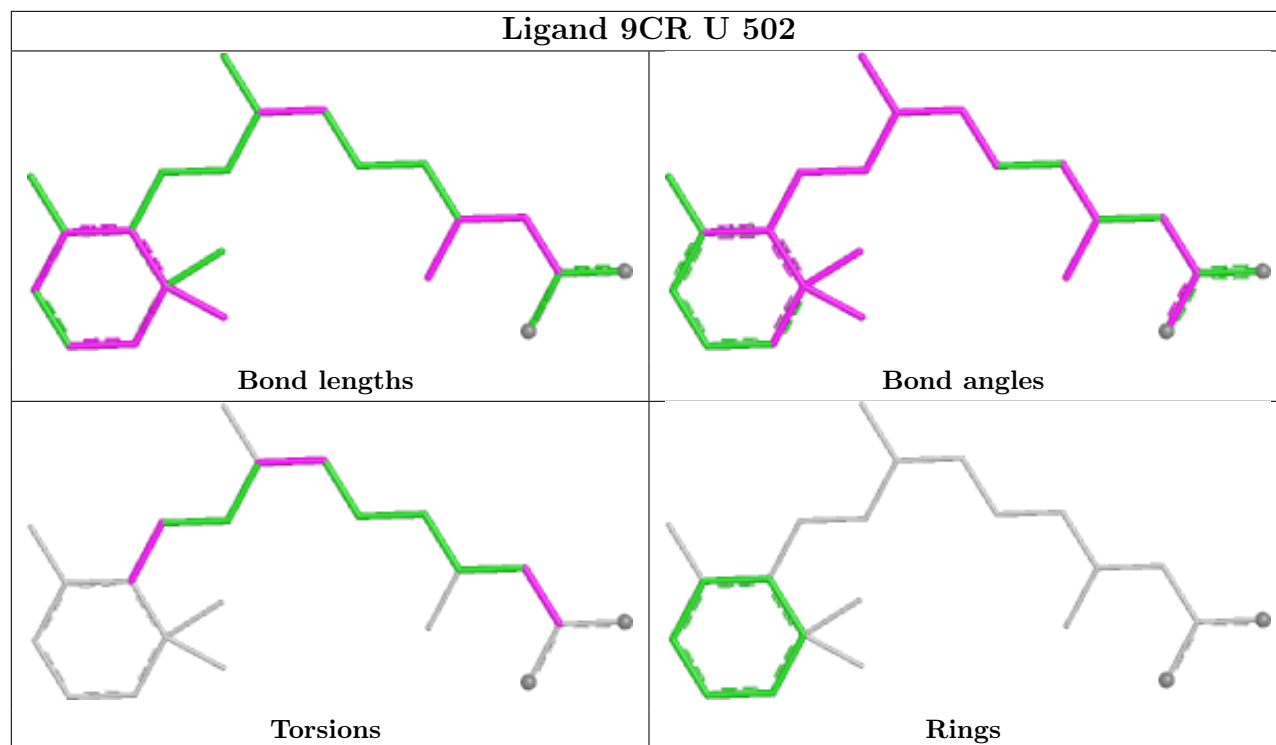
There are no ring outliers.

4 monomers are involved in 8 short contacts:

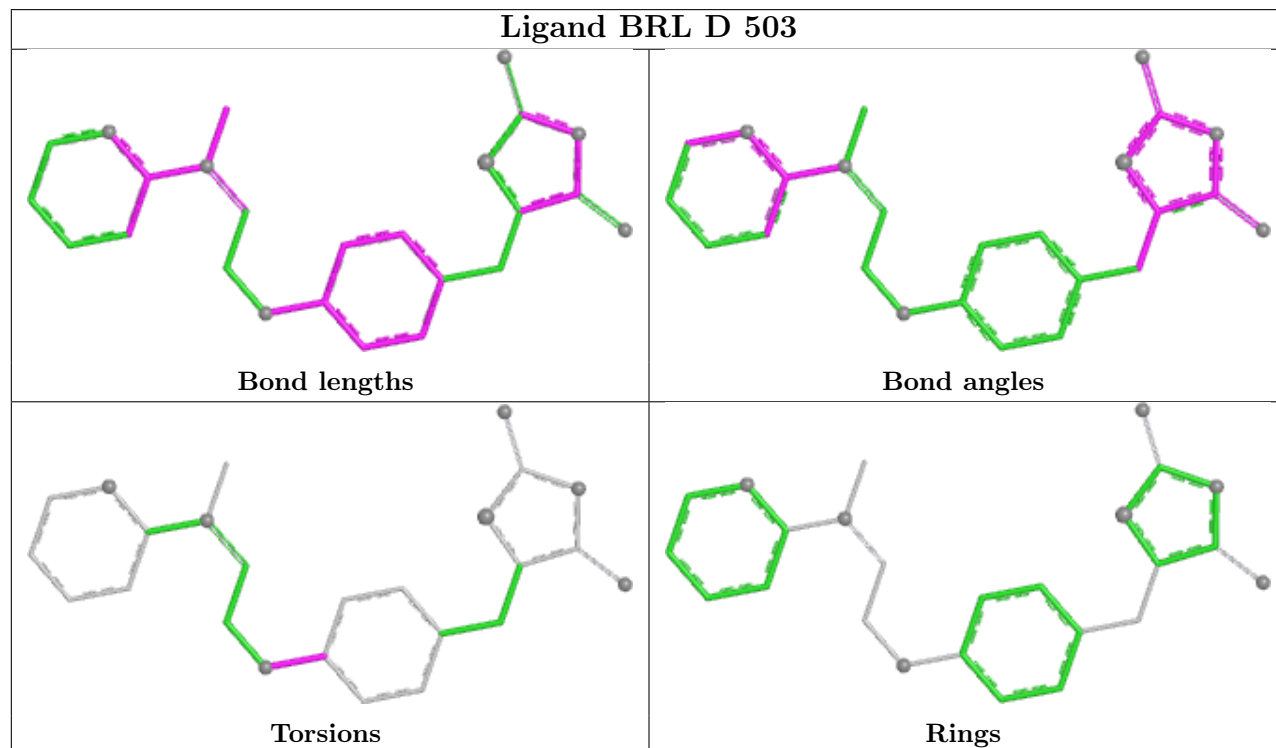
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	502	9CR	2	0
5	D	503	BRL	4	0
4	A	501	9CR	1	0
5	X	504	BRL	1	0

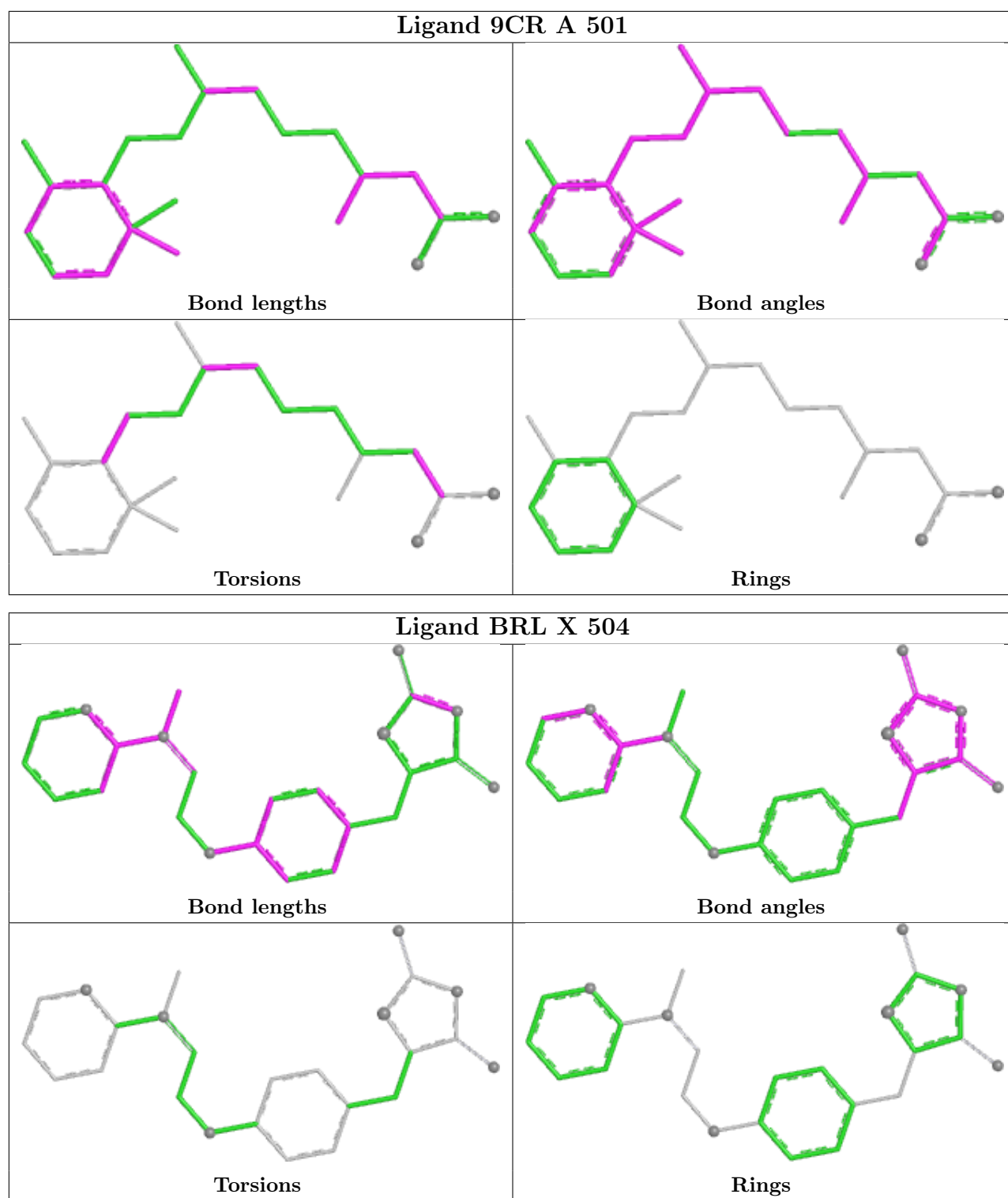
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 9CR U 502



Ligand BRL D 503





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	232/238 (97%)	0.89	38 (16%) 4 4	32, 54, 120, 134	0
1	U	232/238 (97%)	0.82	36 (15%) 5 5	31, 51, 119, 126	0
2	D	272/272 (100%)	0.58	23 (8%) 16 17	31, 46, 93, 119	0
2	X	272/272 (100%)	0.58	21 (7%) 19 21	31, 51, 88, 100	0
3	B	10/25 (40%)	0.99	1 (10%) 12 13	55, 64, 75, 81	0
3	E	16/25 (64%)	1.05	2 (12%) 8 8	53, 63, 81, 86	0
3	V	15/25 (60%)	1.20	3 (20%) 3 3	59, 72, 101, 104	0
3	Y	13/25 (52%)	1.73	3 (23%) 2 2	61, 75, 85, 93	0
All	All	1062/1120 (94%)	0.74	127 (11%) 9 9	31, 51, 99, 134	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	262	ILE	6.9
1	U	259	SER	6.6
2	D	271	GLN	6.5
1	A	249	TYR	5.7
2	D	242	THR	5.6
2	D	270	LEU	5.5
2	D	269	PRO	5.3
1	A	258	PRO	5.2
2	X	264	PHE	5.0
2	D	272	GLU	4.9
1	U	227	ASN	4.9
1	A	252	ALA	4.7
2	D	243	ASP	4.5
1	U	260	SER	4.5
1	U	257	ASN	4.5
1	A	446	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	U	457	ALA	4.4
1	A	261	PRO	4.4
3	Y	691	HIS	4.3
1	U	446	PRO	4.3
2	X	267	ILE	4.1
2	X	238	THR	4.1
1	U	244	PRO	4.1
1	A	248	THR	4.0
1	A	457	ALA	3.9
1	U	252	ALA	3.9
1	U	258	PRO	3.9
1	A	438	PHE	3.9
2	X	262	ILE	3.9
1	A	445	THR	3.8
2	D	477	TYR	3.8
1	A	256	LEU	3.8
2	D	264	PHE	3.7
1	U	445	THR	3.7
3	Y	693	LEU	3.7
2	X	243	ASP	3.6
2	X	268	THR	3.6
1	U	444	ASP	3.4
1	U	250	VAL	3.4
1	A	227	ASN	3.3
1	A	264	PRO	3.3
1	A	443	GLY	3.3
2	X	245	SER	3.3
2	D	464	SER	3.2
1	U	264	PRO	3.2
3	V	642	PRO	3.2
2	D	260	ASP	3.2
2	X	463	MET	3.2
1	U	253	ASN	3.1
1	U	256	LEU	3.1
2	D	267	ILE	3.1
2	D	273	GLN	3.0
1	U	249	TYR	3.0
1	A	255	GLY	3.0
3	Y	684	THR	3.0
1	A	458	PRO	3.0
2	X	258	GLY	2.9
1	U	242	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	265	LYS	2.9
3	E	689	ILE	2.8
1	A	259	SER	2.8
1	U	254	MET	2.8
1	A	244	PRO	2.8
1	A	444	ASP	2.8
2	D	266	HIS	2.7
1	U	247	GLU	2.7
1	A	447	ILE	2.7
1	U	262	ASN	2.7
1	U	248	THR	2.7
3	V	641	SER	2.7
2	D	358	LYS	2.7
2	X	271	GLN	2.6
2	X	359	PRO	2.6
1	A	299	ILE	2.6
2	X	259	GLU	2.6
1	A	333	HIS	2.6
1	A	251	GLU	2.6
3	B	638	GLN	2.5
1	A	280	VAL	2.5
2	X	265	LYS	2.5
1	A	257	ASN	2.5
1	A	312	SER	2.5
2	X	425	HIS	2.5
2	D	238	THR	2.5
2	X	477	TYR	2.4
1	U	458	PRO	2.4
1	U	243	GLU	2.4
2	X	236	ILE	2.4
1	U	449	THR	2.4
3	E	685	GLU	2.4
1	A	242	VAL	2.4
1	A	260	SER	2.4
2	D	263	LYS	2.4
2	X	464	SER	2.4
1	U	261	PRO	2.4
1	A	263	ASP	2.3
1	A	437	PHE	2.3
1	A	332	VAL	2.3
1	A	262	ASN	2.3
2	X	308	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	U	382	GLY	2.3
1	A	439	PHE	2.3
1	U	447	ILE	2.3
1	U	265	VAL	2.3
1	A	330	LEU	2.3
1	U	291	GLU	2.2
1	U	246	THR	2.2
2	D	461	THR	2.2
1	U	330	LEU	2.2
2	D	463	MET	2.2
1	U	322	ASP	2.2
1	U	241	ALA	2.1
2	D	268	THR	2.1
1	A	241	ALA	2.1
1	A	247	GLU	2.1
1	A	246	THR	2.1
1	A	442	ILE	2.1
2	X	244	LYS	2.1
2	D	405	PRO	2.1
2	X	266	HIS	2.1
1	U	229	ASP	2.0
2	D	252	MET	2.0
1	U	431	LYS	2.0
1	A	351	THR	2.0
2	X	241	THR	2.0
3	V	640	GLY	2.0
1	U	408	TYR	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,

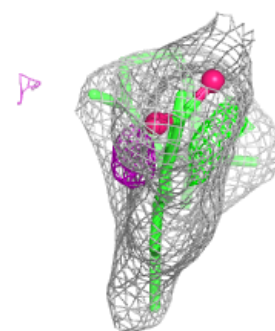
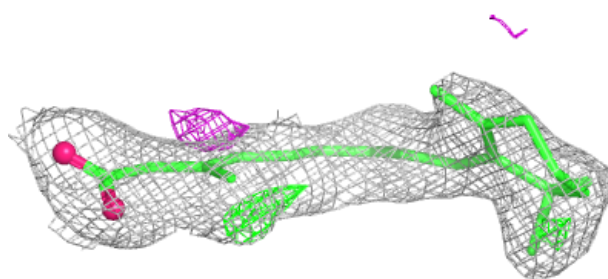
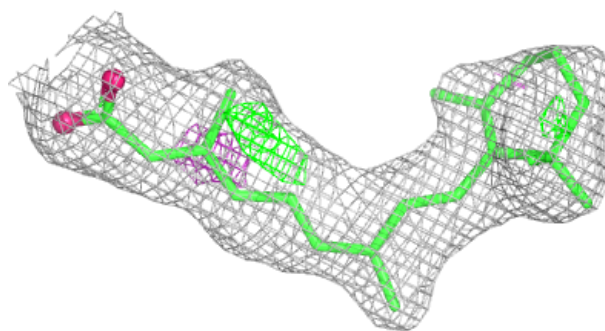
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	9CR	A	501	22/22	0.85	0.16	44,61,71,72	0
4	9CR	U	502	22/22	0.88	0.13	41,49,63,64	0
5	BRL	D	503	25/25	0.93	0.08	41,45,47,49	0
5	BRL	X	504	25/25	0.94	0.07	37,40,48,48	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.

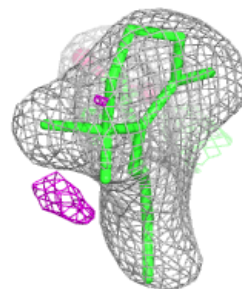
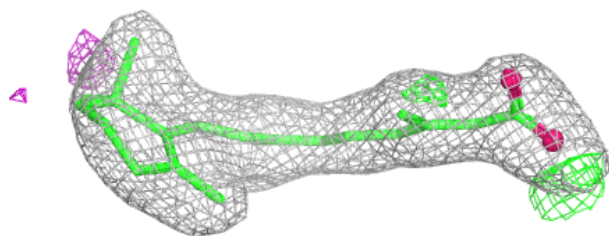
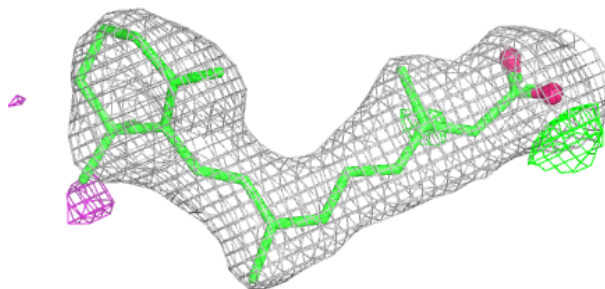
Electron density around 9CR A 501:

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

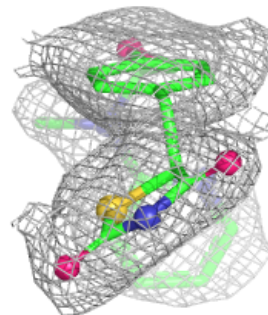
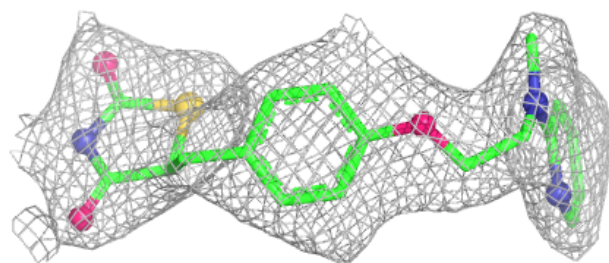
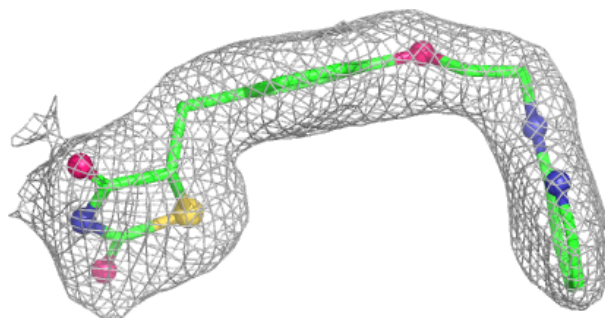


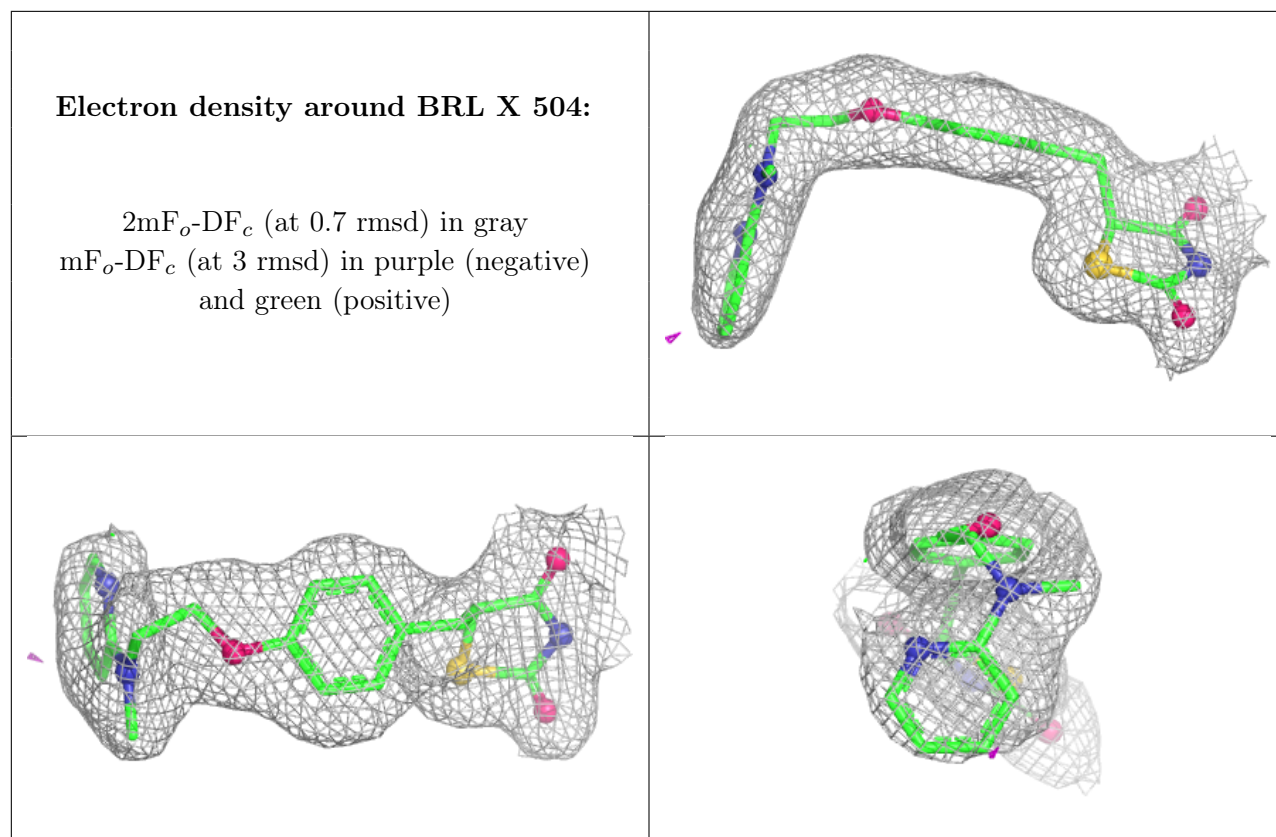
Electron density around 9CR U 502:

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

**Electron density around BRL D 503:**

$2mF_o-DF_c$ (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.