



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:56 PM UTC

PDB ID : 1RLB / pdb_00001rlb
Title : RETINOL BINDING PROTEIN COMPLEXED WITH TRANSTHYRETIN
Authors : Monaco, H.L.; Rizzi, M.; Coda, A.
Deposited on : 1995-02-20
Resolution : 3.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

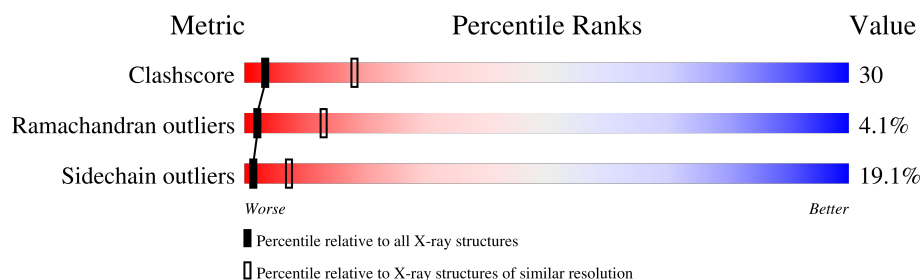
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	43% 35% 17% • •
1	B	127	35% 39% 18% • 6%
1	C	127	33% 36% 24% • •
1	D	127	28% 46% 16% 6% 6%
2	E	174	33% 45% 15% 7%
2	F	174	31% 45% 18% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	REA	E	176	-	-	X	-
3	REA	F	177	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6624 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 TRANSTHYRETIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	27	0	0
			950	604	157	187	2			
1	B	120	Total	C	N	O	S	0	0	0
			930	593	154	181	2			
1	C	123	Total	C	N	O	S	0	0	0
			950	604	157	187	2			
1	D	120	Total	C	N	O	S	0	0	0
			930	593	154	181	2			

- Molecule 2 is a protein called RETINOL BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	174	Total	C	N	O	S	68	0	0
			1411	889	246	266	10			
2	F	174	Total	C	N	O	S	116	0	0
			1411	889	246	266	10			

There are 26 discrepancies between the modelled and reference sequences:

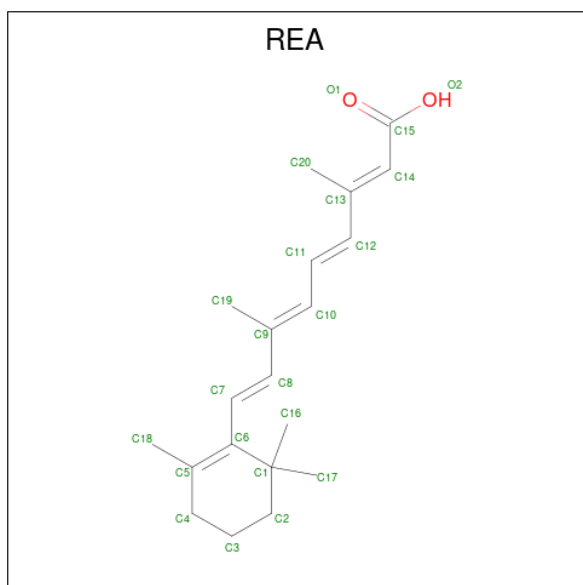
Chain	Residue	Modelled	Actual	Comment	Reference
E	21	ALA	SER	conflict	UNP P02753
E	50	ASN	THR	conflict	UNP P02753
E	52	HIS	GLN	conflict	UNP P02753
E	107	ILE	VAL	conflict	UNP P02753
E	112	GLU	ASP	conflict	UNP P02753
E	114	PHE	TYR	conflict	UNP P02753
E	138	ALA	SER	conflict	UNP P02753
E	142	SER	ASN	conflict	UNP P02753
E	144	PHE	LEU	conflict	UNP P02753
E	145	SER	PRO	conflict	UNP P02753
E	147	GLN	GLU	conflict	UNP P02753
E	148	VAL	ALA	conflict	UNP P02753

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Chain	Residue	Modelled	Actual	Comment	Reference
E	169	PRO	VAL	conflict	UNP P02753
F	21	ALA	SER	conflict	UNP P02753
F	50	ASN	THR	conflict	UNP P02753
F	52	HIS	GLN	conflict	UNP P02753
F	107	ILE	VAL	conflict	UNP P02753
F	112	GLU	ASP	conflict	UNP P02753
F	114	PHE	TYR	conflict	UNP P02753
F	138	ALA	SER	conflict	UNP P02753
F	142	SER	ASN	conflict	UNP P02753
F	144	PHE	LEU	conflict	UNP P02753
F	145	SER	PRO	conflict	UNP P02753
F	147	GLN	GLU	conflict	UNP P02753
F	148	VAL	ALA	conflict	UNP P02753
F	169	PRO	VAL	conflict	UNP P02753

- Molecule 3 is RETINOIC ACID (CCD ID: REA) (formula: C₂₀H₂₈O₂).



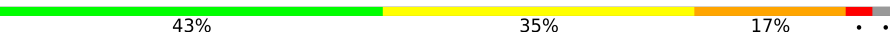
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			21	20	1		
3	F	1	Total	C	O	0	0
			21	20	1		

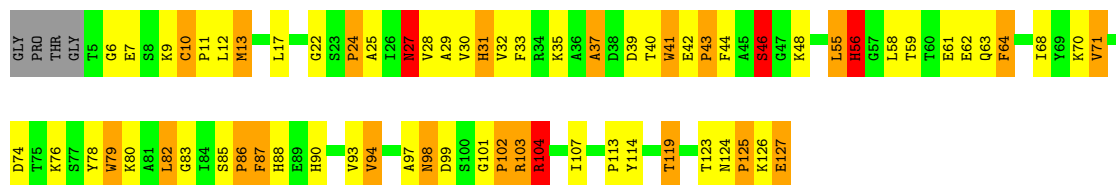
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

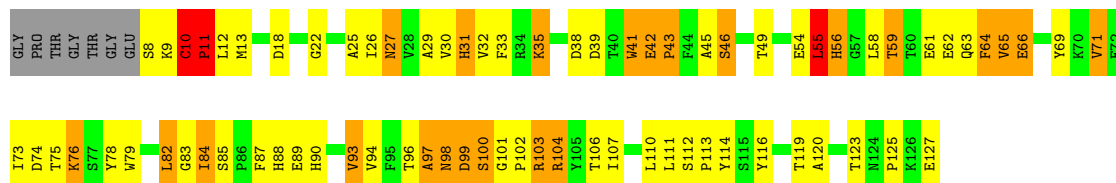
• Molecule 1: TRANSTHYRETIN

Chain A: 

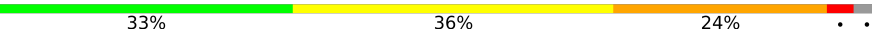


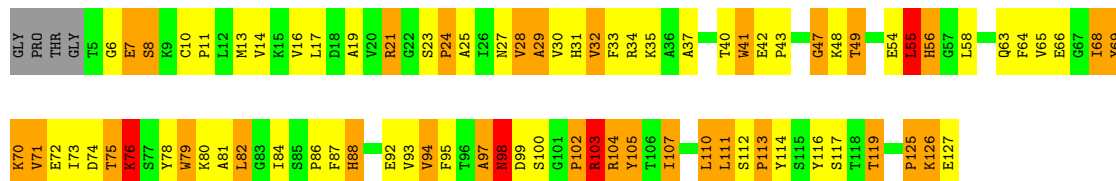
• Molecule 1: TRANSTHYRETIN

Chain B: 

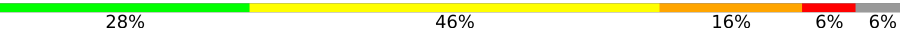


• Molecule 1: TRANSTHYRETIN

Chain C: 



• Molecule 1: TRANSTHYRETIN

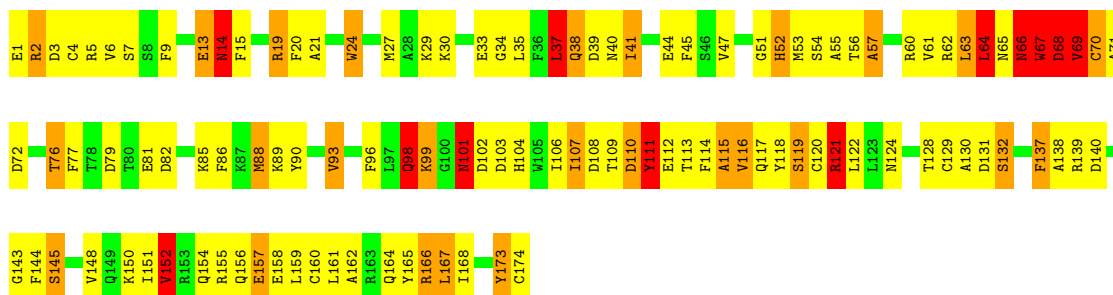
Chain D: 





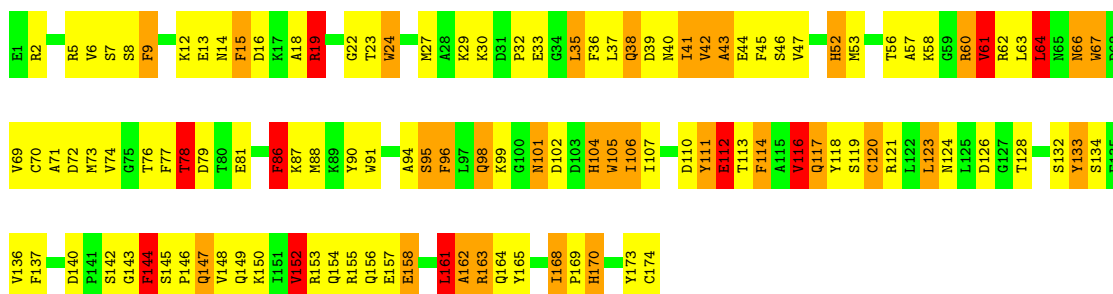
• Molecule 2: RETINOL BINDING PROTEIN

Chain E: 33% 45% 15% 7%



• Molecule 2: RETINOL BINDING PROTEIN

Chain F: 31% 45% 18% 6%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	222.40 Å 163.40 Å 55.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.10	Depositor
% Data completeness (in resolution range)	93.5 (6.00-3.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.215 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6624	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: REA

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	1.43	8/974 (0.8%)	2.06	39/1325 (2.9%)
1	B	1.37	10/954 (1.0%)	2.14	46/1298 (3.5%)
1	C	1.36	5/974 (0.5%)	2.31	53/1325 (4.0%)
1	D	1.20	3/954 (0.3%)	1.73	19/1298 (1.5%)
2	E	1.51	11/1445 (0.8%)	2.60	100/1950 (5.1%)
2	F	1.70	10/1445 (0.7%)	2.66	86/1950 (4.4%)
All	All	1.46	47/6746 (0.7%)	2.32	343/9146 (3.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	E	0	1
All	All	0	2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	162	ALA	C-N	-34.38	0.73	1.34
2	F	163	ARG	N-CA	-24.83	1.19	1.46
2	E	69	VAL	N-CA	18.95	1.70	1.46
1	A	98	ASN	C-O	16.20	1.46	1.23
2	E	99	LYS	N-CA	11.22	1.60	1.45
1	A	98	ASN	CA-C	11.22	1.71	1.52
1	A	31	HIS	CD2-NE2	-7.12	1.30	1.37
2	F	170	HIS	CD2-NE2	-7.09	1.30	1.37
1	C	31	HIS	CD2-NE2	-7.00	1.30	1.37
1	A	90	HIS	CD2-NE2	-6.86	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	161	LEU	CB-CG	-6.70	1.40	1.53
1	B	31	HIS	CD2-NE2	-6.69	1.30	1.37
2	E	104	HIS	CD2-NE2	-6.66	1.30	1.37
1	C	56	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	56	HIS	CD2-NE2	-6.53	1.30	1.37
2	F	104	HIS	CD2-NE2	-6.40	1.30	1.37
2	F	52	HIS	CD2-NE2	-6.37	1.30	1.37
2	E	104	HIS	CG-ND1	-6.17	1.31	1.38
1	A	88	HIS	CD2-NE2	-6.13	1.31	1.37
1	B	41	TRP	CA-C	-6.03	1.45	1.53
2	E	52	HIS	CD2-NE2	-5.97	1.31	1.37
1	B	84	ILE	CA-CB	5.96	1.62	1.54
1	C	49	THR	CA-CB	5.92	1.62	1.53
1	B	8	SER	C-N	5.91	1.41	1.33
2	E	107	ILE	CA-CB	5.76	1.61	1.54
1	A	90	HIS	CG-ND1	-5.73	1.31	1.38
1	C	107	ILE	CA-CB	5.67	1.60	1.53
1	A	79	TRP	NE1-CE2	-5.66	1.31	1.37
1	B	65	VAL	CA-CB	5.58	1.62	1.54
2	F	128	THR	CA-CB	5.56	1.62	1.53
2	F	43	ALA	CA-CB	-5.54	1.45	1.53
1	B	96	THR	C-N	-5.53	1.27	1.33
1	B	56	HIS	CD2-NE2	-5.52	1.31	1.37
1	D	45	ALA	N-CA	5.42	1.52	1.45
1	D	79	TRP	NE1-CE2	-5.37	1.31	1.37
2	E	88	MET	CA-CB	-5.34	1.46	1.53
2	E	120	CYS	CA-CB	-5.34	1.45	1.53
1	B	49	THR	CA-CB	5.33	1.62	1.53
1	B	12	LEU	N-CA	5.33	1.52	1.45
2	E	39	ASP	CA-CB	5.32	1.60	1.53
1	C	19	ALA	C-N	5.30	1.38	1.33
2	F	67	TRP	NE1-CE2	-5.19	1.31	1.37
2	F	105	TRP	CG-CD2	-5.14	1.34	1.43
1	D	41	TRP	NE1-CE2	-5.08	1.31	1.37
2	E	24	TRP	NE1-CE2	-5.04	1.31	1.37
1	B	10	CYS	CA-C	-5.03	1.46	1.52
2	F	43	ALA	CA-C	-5.00	1.46	1.52

All (343) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	162	ALA	O-C-N	32.61	163.29	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	162	ALA	CA-C-N	-32.03	68.66	121.18
2	F	162	ALA	C-N-CA	-32.03	68.66	121.18
2	E	68	ASP	CA-C-N	25.58	168.01	121.97
2	E	68	ASP	C-N-CA	25.58	168.01	121.97
2	E	39	ASP	CA-CB-CG	14.85	127.45	112.60
2	E	68	ASP	CB-CA-C	-13.44	83.67	110.42
2	E	69	VAL	N-CA-CB	12.11	131.21	111.23
2	F	86	PHE	CA-CB-CG	11.56	125.36	113.80
1	C	103	ARG	N-CA-C	11.04	125.88	111.75
2	E	99	LYS	N-CA-C	10.95	126.68	110.48
2	E	110	ASP	N-CA-CB	10.86	126.53	110.35
2	F	140	ASP	CA-CB-CG	10.61	123.21	112.60
2	F	39	ASP	CA-CB-CG	10.51	123.11	112.60
2	F	41	ILE	N-CA-C	9.73	121.73	108.89
2	F	163	ARG	CB-CA-C	-9.69	93.10	110.35
2	F	14	ASN	N-CA-C	9.65	124.64	111.90
2	E	101	ASN	CA-CB-CG	9.62	122.22	112.60
2	F	19	ARG	N-CA-C	-9.57	99.30	112.12
1	C	56	HIS	CB-CG-CD2	-9.43	118.94	131.20
2	E	124	ASN	OD1-CG-ND2	-9.34	113.26	122.60
2	F	96	PHE	CA-CB-CG	9.33	123.13	113.80
1	B	8	SER	CB-CA-C	9.21	127.60	110.10
2	F	14	ASN	CA-CB-CG	-9.20	103.40	112.60
2	E	40	ASN	OD1-CG-ND2	-9.11	113.49	122.60
1	D	67	GLY	O-C-N	9.11	131.46	123.36
1	C	27	ASN	N-CA-C	9.10	123.95	111.39
1	C	105	TYR	N-CA-CB	-9.01	95.74	110.43
2	E	67	TRP	CB-CA-C	-8.79	96.36	110.86
1	B	97	ALA	O-C-N	8.78	132.53	123.13
1	A	55	LEU	O-C-N	-8.73	113.10	122.96
2	E	152	VAL	CA-C-O	-8.67	111.94	120.95
2	F	101	ASN	OD1-CG-ND2	-8.64	113.96	122.60
2	E	71	ALA	N-CA-C	8.60	122.25	108.41
1	A	27	ASN	OD1-CG-ND2	-8.56	114.04	122.60
1	A	103	ARG	N-CA-CB	-8.55	95.79	110.32
1	D	127	GLU	CA-CB-CG	-8.44	97.22	114.10
2	E	38	GLN	OE1-CD-NE2	-8.38	114.22	122.60
2	E	131	ASP	O-C-N	-8.36	113.40	123.27
1	A	126	LYS	O-C-N	8.32	133.09	122.28
2	E	72	ASP	CB-CA-C	-8.32	96.65	110.29
1	A	31	HIS	CB-CG-CD2	-8.28	120.44	131.20
2	F	136	VAL	N-CA-C	-8.08	96.19	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	41	ILE	N-CA-C	8.04	119.35	109.30
2	E	99	LYS	N-CA-CB	-8.03	98.08	110.29
2	F	163	ARG	N-CA-CB	8.00	126.46	111.43
2	E	111	TYR	O-C-N	-7.97	111.99	122.59
2	F	114	PHE	CA-CB-CG	7.96	121.76	113.80
2	F	142	SER	N-CA-C	7.96	120.86	111.71
1	C	42	GLU	N-CA-C	-7.91	100.12	109.93
2	E	67	TRP	N-CA-CB	7.87	121.64	110.07
1	B	35	LYS	N-CA-C	-7.87	98.38	110.10
2	E	117	GLN	OE1-CD-NE2	-7.85	114.75	122.60
1	B	79	TRP	CG-CD2-CE3	7.83	141.73	133.90
1	A	85	SER	CA-C-N	7.83	128.29	119.92
1	A	85	SER	C-N-CA	7.83	128.29	119.92
2	E	77	PHE	N-CA-C	7.80	121.18	109.25
1	C	79	TRP	CG-CD2-CE3	7.75	141.65	133.90
1	A	31	HIS	CA-CB-CG	-7.70	106.11	113.80
1	A	7	GLU	N-CA-C	-7.69	101.32	111.24
2	E	121	ARG	NE-CZ-NH1	7.69	129.19	121.50
1	C	73	ILE	N-CA-CB	-7.67	102.26	111.00
1	C	119	THR	O-C-N	7.63	132.34	123.41
1	D	43	PRO	O-C-N	7.63	132.16	122.85
1	B	88	HIS	CA-CB-CG	-7.59	106.21	113.80
1	A	74	ASP	CA-CB-CG	7.51	120.11	112.60
1	A	56	HIS	CB-CG-CD2	-7.47	121.49	131.20
2	F	64	LEU	O-C-N	-7.45	112.68	122.59
1	B	56	HIS	CB-CG-CD2	-7.42	121.56	131.20
1	C	82	LEU	N-CA-C	-7.42	102.17	113.89
1	D	111	LEU	O-C-N	7.41	132.30	123.33
2	E	140	ASP	CA-CB-CG	7.41	120.01	112.60
2	F	126	ASP	CA-CB-CG	7.40	120.00	112.60
2	E	2	ARG	N-CA-C	-7.40	98.12	109.14
1	B	54	GLU	N-CA-C	7.33	120.85	108.90
1	D	88	HIS	CA-CB-CG	-7.31	106.49	113.80
2	E	165	TYR	CA-C-O	-7.29	112.92	121.16
2	F	23	THR	O-C-N	-7.28	114.42	123.01
2	E	137	PHE	CA-C-O	-7.26	112.59	120.36
2	E	44	GLU	CA-CB-CG	-7.26	99.58	114.10
1	A	98	ASN	N-CA-C	7.24	123.05	113.20
2	E	101	ASN	N-CA-C	-7.24	96.47	108.34
1	C	97	ALA	O-C-N	7.22	132.19	122.59
2	F	101	ASN	CB-CG-ND2	7.15	127.12	116.40
1	C	111	LEU	N-CA-C	7.13	120.35	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	52	HIS	CB-CG-CD2	-7.10	121.97	131.20
2	E	52	HIS	CB-CG-CD2	-7.08	121.99	131.20
2	E	145	SER	CA-C-N	6.99	126.97	119.28
2	E	145	SER	C-N-CA	6.99	126.97	119.28
1	C	80	LYS	N-CA-C	-6.95	103.32	111.03
2	E	88	MET	CA-CB-CG	-6.95	100.21	114.10
1	C	79	TRP	N-CA-C	6.92	119.85	111.82
2	E	72	ASP	N-CA-CB	6.90	121.12	109.87
1	A	98	ASN	CB-CA-C	-6.88	102.69	111.22
2	F	116	VAL	CB-CA-C	-6.88	100.93	111.31
1	B	56	HIS	CB-CG-ND1	6.87	133.01	122.70
2	F	121	ARG	CA-CB-CG	-6.86	100.39	114.10
1	C	102	PRO	CA-N-CD	-6.80	102.48	112.00
1	A	103	ARG	CA-C-O	-6.79	111.27	119.49
1	C	41	TRP	CE2-CD2-CE3	6.79	125.59	118.80
1	C	6	GLY	N-CA-C	-6.79	97.09	113.18
1	A	46	SER	CA-C-O	-6.78	114.01	121.33
2	F	161	LEU	CB-CA-C	-6.75	102.08	112.07
1	A	39	ASP	CA-CB-CG	6.72	119.32	112.60
2	E	33	GLU	N-CA-C	-6.71	99.60	110.20
2	E	121	ARG	NE-CZ-NH2	-6.68	113.19	119.20
1	B	62	GLU	CB-CG-CD	6.67	123.93	112.60
1	C	40	THR	CA-CB-OG1	-6.66	99.61	109.60
2	F	168	ILE	CA-C-N	6.64	128.14	119.84
2	F	168	ILE	C-N-CA	6.64	128.14	119.84
2	F	119	SER	CA-CB-OG	6.62	124.34	111.10
1	C	70	LYS	CA-C-N	-6.61	114.60	122.93
1	C	70	LYS	C-N-CA	-6.61	114.60	122.93
2	E	88	MET	O-C-N	-6.60	115.69	123.22
2	E	158	GLU	CA-CB-CG	-6.59	100.91	114.10
2	F	156	GLN	OE1-CD-NE2	-6.59	116.01	122.60
1	C	71	VAL	CG1-CB-CG2	-6.59	96.30	110.80
2	E	152	VAL	CA-CB-CG2	-6.59	99.20	110.40
1	C	110	LEU	O-C-N	6.58	131.71	123.28
2	F	169	PRO	CA-C-N	-6.55	114.32	122.84
2	F	169	PRO	C-N-CA	-6.55	114.32	122.84
1	B	71	VAL	N-CA-C	-6.53	99.02	108.17
1	A	17	LEU	N-CA-C	6.53	119.35	109.23
1	C	24	PRO	CA-C-O	-6.52	108.73	120.60
2	E	156	GLN	CA-C-O	-6.51	113.59	120.63
2	F	74	VAL	N-CA-C	-6.51	99.75	108.35
1	A	56	HIS	CB-CG-ND1	6.51	132.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	GLU	O-C-N	6.51	133.41	123.00
2	E	20	PHE	N-CA-C	-6.50	105.48	113.41
2	E	122	LEU	O-C-N	-6.49	115.58	123.30
1	C	74	ASP	CA-CB-CG	6.48	119.08	112.60
2	F	162	ALA	N-CA-C	6.45	122.64	113.02
1	C	31	HIS	CB-CG-CD2	-6.45	122.81	131.20
2	F	8	SER	N-CA-C	6.45	119.12	111.71
1	A	41	TRP	CG-CD1-NE1	-6.43	101.84	110.20
2	F	12	LYS	N-CA-C	6.42	119.02	109.59
1	C	56	HIS	CB-CG-ND1	6.40	132.29	122.70
2	F	9	PHE	N-CA-C	6.39	124.42	110.80
1	B	76	LYS	CA-C-O	-6.38	114.08	120.90
2	E	93	VAL	CB-CA-C	-6.37	99.63	111.79
1	B	55	LEU	N-CA-C	-6.34	100.18	110.20
1	B	27	ASN	N-CA-C	6.34	120.30	111.74
2	E	81	GLU	N-CA-C	-6.33	104.82	112.54
1	C	29	ALA	O-C-N	6.33	130.52	122.93
2	F	46	SER	CA-CB-OG	6.32	123.74	111.10
1	A	37	ALA	N-CA-C	6.32	124.26	110.80
2	F	38	GLN	OE1-CD-NE2	-6.31	116.29	122.60
1	B	74	ASP	CA-CB-CG	6.30	118.90	112.60
1	B	55	LEU	O-C-N	-6.28	115.60	123.01
1	A	119	THR	CA-CB-OG1	-6.28	100.18	109.60
2	F	58	LYS	N-CA-C	-6.28	99.93	109.85
2	F	72	ASP	CA-C-O	-6.27	113.65	120.36
2	F	40	ASN	N-CA-C	6.27	120.27	112.24
2	E	82	ASP	N-CA-C	-6.25	102.19	110.07
2	F	163	ARG	N-CA-C	-6.25	103.32	113.19
1	B	35	LYS	O-C-N	6.23	130.68	122.95
1	B	79	TRP	CB-CG-CD1	-6.23	117.55	126.90
2	E	157	GLU	CB-CG-CD	6.22	123.18	112.60
2	F	40	ASN	CA-C-N	6.22	130.25	121.66
2	F	40	ASN	C-N-CA	6.22	130.25	121.66
2	F	124	ASN	N-CA-C	-6.22	100.78	110.17
2	E	72	ASP	CA-CB-CG	6.22	118.82	112.60
2	F	120	CYS	O-C-N	-6.21	115.92	123.19
2	F	162	ALA	CB-CA-C	-6.21	100.00	110.44
2	F	81	GLU	O-C-N	6.17	128.75	122.09
2	F	112	GLU	N-CA-C	-6.15	105.91	113.41
2	E	79	ASP	CA-CB-CG	6.15	118.75	112.60
2	E	88	MET	CA-C-O	-6.14	113.79	120.36
1	C	8	SER	CA-C-O	-6.13	111.75	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	LEU	N-CA-C	-6.12	100.94	110.42
1	D	121	VAL	N-CA-C	-6.10	96.64	109.34
2	F	87	LYS	CA-CB-CG	-6.10	101.90	114.10
1	B	93	VAL	O-C-N	-6.10	116.80	122.71
1	A	55	LEU	N-CA-C	-6.09	101.46	110.48
2	F	76	THR	N-CA-C	-6.09	98.36	108.34
2	E	85	LYS	CB-CG-CD	-6.08	97.31	111.30
2	F	12	LYS	CG-CD-CE	-6.08	97.31	111.30
1	C	84	ILE	CB-CG1-CD1	-6.08	101.03	113.80
1	B	42	GLU	CA-C-O	6.08	125.88	119.80
2	E	116	VAL	O-C-N	-6.06	115.13	122.59
1	A	86	PRO	CA-N-CD	-6.06	103.51	112.00
1	B	8	SER	O-C-N	6.05	132.68	123.00
1	D	10	CYS	N-CA-C	-6.04	96.46	109.81
2	E	19	ARG	N-CA-C	-6.03	105.48	114.64
1	D	101	GLY	O-C-N	-6.03	115.74	121.77
1	B	27	ASN	CB-CG-ND2	5.99	125.39	116.40
1	A	40	THR	CA-CB-OG1	-5.99	100.61	109.60
2	E	14	ASN	CB-CA-C	-5.98	103.07	111.80
1	C	79	TRP	CB-CG-CD1	-5.97	117.94	126.90
1	D	13	MET	CB-CG-SD	-5.97	94.79	112.70
2	F	114	PHE	N-CA-C	5.93	116.93	108.74
2	E	66	ASN	CB-CA-C	-5.92	104.25	111.82
2	F	91	TRP	CG-CD2-CE3	5.89	139.79	133.90
2	F	22	GLY	CA-C-O	-5.84	117.60	122.33
1	A	6	GLY	N-CA-C	-5.84	103.67	112.60
1	C	32	VAL	N-CA-C	-5.84	99.94	108.11
1	B	12	LEU	N-CA-CB	-5.83	101.75	111.20
2	E	34	GLY	CA-C-N	-5.83	114.89	123.05
2	E	34	GLY	C-N-CA	-5.83	114.89	123.05
1	A	35	LYS	N-CA-C	-5.83	101.22	109.96
2	F	71	ALA	N-CA-C	5.81	118.62	109.96
1	A	87	PHE	CA-C-O	5.81	126.69	120.24
2	F	2	ARG	N-CA-C	-5.80	100.24	109.76
1	B	104	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	C	55	LEU	N-CA-C	-5.80	101.09	110.32
1	B	26	ILE	N-CA-C	5.80	117.98	109.63
1	B	59	THR	O-C-N	5.78	128.70	123.26
2	F	42	VAL	CA-C-O	-5.77	114.14	120.43
1	B	64	PHE	CA-CB-CG	5.76	119.56	113.80
2	F	174	CYS	CA-CB-SG	5.76	127.64	114.40
2	F	168	ILE	N-CA-CB	-5.70	103.23	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	70	CYS	N-CA-CB	5.68	119.24	110.21
2	E	3	ASP	N-CA-C	-5.68	98.08	108.02
1	D	112	SER	O-C-N	-5.67	117.85	121.88
2	F	91	TRP	CB-CG-CD1	-5.67	118.39	126.90
1	C	37	ALA	N-CA-C	5.67	117.45	111.28
2	F	170	HIS	CB-CG-CD2	-5.66	123.84	131.20
2	E	5	ARG	N-CA-C	-5.65	100.08	109.46
2	E	66	ASN	O-C-N	-5.62	116.32	122.67
1	D	88	HIS	O-C-N	5.62	129.79	123.27
1	A	41	TRP	CD1-CG-CD2	5.61	115.28	106.30
1	C	23	SER	CA-C-N	5.61	126.85	119.84
1	C	23	SER	C-N-CA	5.61	126.85	119.84
2	E	101	ASN	CA-C-O	5.60	126.18	120.24
2	E	24	TRP	CB-CG-CD1	-5.60	118.50	126.90
2	F	133	TYR	CA-CB-CG	5.60	123.98	113.90
1	B	27	ASN	OD1-CG-ND2	-5.59	117.01	122.60
2	F	33	GLU	N-CA-C	-5.57	99.43	108.52
1	B	8	SER	CA-C-N	5.57	130.46	122.21
1	B	8	SER	C-N-CA	5.57	130.46	122.21
2	F	148	VAL	N-CA-C	-5.57	103.98	111.44
2	F	152	VAL	CA-CB-CG2	-5.56	100.94	110.40
2	F	44	GLU	N-CA-C	-5.55	98.58	108.13
2	E	38	GLN	CB-CG-CD	5.55	122.03	112.60
1	A	102	PRO	CA-N-CD	-5.55	104.23	112.00
2	E	45	PHE	CA-C-O	-5.54	114.39	120.43
1	B	31	HIS	CB-CG-CD2	-5.53	124.02	131.20
2	E	38	GLN	O-C-N	-5.53	115.85	122.15
2	E	56	THR	O-C-N	-5.53	116.01	123.19
2	E	30	LYS	CA-CB-CG	-5.51	103.08	114.10
1	A	119	THR	CA-CB-CG2	5.51	119.87	110.50
1	C	75	THR	CA-C-O	-5.50	115.12	120.89
2	F	164	GLN	O-C-N	-5.49	115.63	122.83
1	C	113	PRO	N-CA-C	5.49	121.32	113.47
1	C	112	SER	CA-C-N	5.49	124.68	118.97
1	C	112	SER	C-N-CA	5.49	124.68	118.97
1	A	62	GLU	CB-CG-CD	5.48	121.91	112.60
1	B	103	ARG	O-C-N	-5.48	115.14	122.43
2	E	101	ASN	OD1-CG-ND2	-5.47	117.13	122.60
2	F	123	LEU	O-C-N	-5.47	114.95	122.23
2	F	57	ALA	CB-CA-C	-5.47	100.26	109.50
2	F	5	ARG	N-CA-C	-5.46	100.79	109.59
2	E	86	PHE	CA-CB-CG	5.46	119.26	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	SER	O-C-N	-5.45	117.58	121.83
2	E	37	LEU	CD1-CG-CD2	-5.45	98.81	110.80
1	C	72	GLU	CA-C-O	5.44	126.11	120.40
2	E	152	VAL	CA-CB-CG1	5.44	119.65	110.40
2	E	76	THR	CA-CB-OG1	-5.44	101.45	109.60
2	F	163	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	B	18	ASP	CA-CB-CG	5.43	118.03	112.60
2	E	132	SER	CA-C-O	-5.43	112.88	120.21
1	C	88	HIS	N-CA-C	5.43	117.37	108.52
2	E	98	GLN	O-C-N	5.42	129.80	122.59
1	B	10	CYS	CB-CA-C	5.41	120.83	110.17
2	F	144	PHE	CA-CB-CG	5.40	119.20	113.80
1	B	64	PHE	CA-C-O	5.39	126.15	120.54
2	F	106	ILE	N-CA-C	-5.38	100.00	108.23
2	F	79	ASP	N-CA-CB	-5.38	103.01	110.38
2	F	153	ARG	N-CA-C	-5.38	105.42	111.28
2	E	131	ASP	CA-C-O	-5.37	114.42	120.32
2	E	3	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	103	ARG	CA-C-N	-5.36	115.40	122.85
1	A	103	ARG	C-N-CA	-5.36	115.40	122.85
1	C	31	HIS	CA-CB-CG	-5.35	108.45	113.80
2	E	24	TRP	CE2-CD2-CG	-5.34	100.79	107.20
1	B	38	ASP	N-CA-C	-5.34	104.11	110.41
1	D	103	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	C	113	PRO	O-C-N	-5.33	116.14	122.17
1	C	119	THR	CA-CB-OG1	-5.33	101.61	109.60
1	B	99	ASP	CB-CA-C	-5.32	100.78	109.56
2	F	36	PHE	CA-CB-CG	-5.32	108.48	113.80
1	C	76	LYS	CA-C-O	-5.31	112.92	120.51
2	E	119	SER	O-C-N	5.31	129.84	123.26
1	B	11	PRO	CB-CA-C	5.31	120.31	111.56
1	B	103	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	E	67	TRP	CB-CG-CD2	-5.29	119.39	126.80
1	C	97	ALA	CA-C-N	5.29	131.64	121.54
1	C	97	ALA	C-N-CA	5.29	131.64	121.54
2	E	40	ASN	N-CA-C	5.28	119.31	112.86
1	C	68	ILE	CA-C-O	5.27	127.05	121.04
1	A	103	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	B	97	ALA	CB-CA-C	-5.25	107.83	114.40
2	F	117	GLN	CA-C-O	-5.25	115.03	120.70
2	F	56	THR	CA-C-O	-5.25	113.64	120.25
2	E	40	ASN	CB-CG-ND2	5.25	124.27	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	167	LEU	N-CA-C	5.24	117.62	110.55
2	E	24	TRP	CG-CD1-NE1	-5.24	103.39	110.20
1	B	85	SER	CA-C-N	5.22	126.37	119.84
1	B	85	SER	C-N-CA	5.22	126.37	119.84
2	E	57	ALA	CA-C-N	5.20	131.49	122.64
2	E	57	ALA	C-N-CA	5.20	131.49	122.64
2	F	152	VAL	CA-CB-CG1	5.20	119.24	110.40
1	A	104	ARG	N-CA-C	5.19	117.40	107.75
2	E	60	ARG	NE-CZ-NH2	5.19	123.87	119.20
2	E	111	TYR	N-CA-CB	-5.19	101.72	110.49
2	E	55	ALA	O-C-N	-5.18	116.45	123.19
2	E	62	ARG	NE-CZ-NH2	5.18	123.87	119.20
1	C	27	ASN	CB-CA-C	-5.18	104.53	111.89
2	E	67	TRP	CA-CB-CG	5.14	123.36	113.60
1	C	54	GLU	CA-C-O	-5.13	114.78	120.38
1	D	111	LEU	CD1-CG-CD2	5.12	122.06	110.80
1	C	116	TYR	N-CA-C	-5.12	100.97	108.79
2	E	21	ALA	CA-C-O	-5.11	113.20	120.51
1	B	41	TRP	CE2-CD2-CE3	5.11	123.91	118.80
1	C	117	SER	CA-CB-OG	5.11	121.31	111.10
1	A	24	PRO	N-CA-C	5.10	118.88	111.03
1	B	8	SER	N-CA-C	5.10	125.27	111.00
1	A	31	HIS	CB-CG-ND1	5.09	130.33	122.70
2	F	61	VAL	CB-CA-C	-5.09	103.55	110.42
1	C	126	LYS	O-C-N	5.09	129.36	122.59
2	F	116	VAL	N-CA-C	-5.08	101.10	108.97
2	E	160	CYS	O-C-N	-5.08	114.94	122.04
1	D	104	ARG	NE-CZ-NH2	5.07	123.77	119.20
2	F	24	TRP	O-C-N	-5.07	116.79	123.28
1	A	126	LYS	CA-C-N	5.07	130.82	121.70
1	A	126	LYS	C-N-CA	5.07	130.82	121.70
1	C	47	GLY	N-CA-C	5.06	117.93	110.80
2	E	24	TRP	CD1-CG-CD2	5.05	114.39	106.30
2	E	130	ALA	CA-C-O	-5.05	115.15	120.55
2	F	91	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	B	12	LEU	N-CA-C	-5.04	101.88	109.85
2	E	70	CYS	CB-CA-C	-5.04	102.49	110.81
1	D	126	LYS	CA-C-N	5.04	130.77	121.70
1	D	126	LYS	C-N-CA	5.04	130.77	121.70
2	E	124	ASN	CB-CG-ND2	5.04	123.96	116.40
2	F	60	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	B	45	ALA	CA-C-O	-5.03	115.89	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	ARG	N-CA-C	5.03	116.84	111.36
1	D	86	PRO	CB-CA-C	-5.03	103.26	111.56
2	F	78	THR	N-CA-C	-5.03	100.84	109.24
2	E	117	GLN	N-CA-C	-5.02	101.92	109.85
2	E	132	SER	N-CA-C	5.02	117.52	108.48
2	E	138	ALA	O-C-N	-5.01	117.37	123.03

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	69	TYR	Sidechain
2	E	68	ASP	Peptide

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	950	0	924	47	0
1	B	930	0	908	47	0
1	C	950	0	924	56	0
1	D	930	0	908	104	5
2	E	1411	0	1334	68	0
2	F	1411	0	1334	58	0
3	E	21	0	27	16	0
3	F	21	0	27	6	0
All	All	6624	0	6386	376	5

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 (376) 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:E:69:VAL:N	2:E:69:VAL:CA	1.70	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLU:HG2	1:B:98:ASN:O	1.14	1.27
1:B:100:SER:O	1:B:102:PRO:HD3	1.41	1.20
1:A:61:GLU:OE2	1:A:103:ARG:HD3	1.40	1.19
1:C:97:ALA:HB3	1:C:98:ASN:ND2	1.58	1.18
2:E:69:VAL:N	2:E:69:VAL:HA	1.61	1.15
1:D:95:PHE:CD2	1:D:97:ALA:HB2	1.83	1.13
1:B:100:SER:C	1:B:102:PRO:HD3	1.76	1.10
2:E:64:LEU:C	2:E:66:ASN:H	1.61	1.02
1:B:66:GLU:CG	1:B:98:ASN:O	2.10	1.00
1:D:66:GLU:HA	1:D:98:ASN:HB3	1.44	0.96
2:E:37:LEU:CD2	3:E:176:REA:H12	1.97	0.94
1:B:100:SER:C	1:B:102:PRO:CD	2.39	0.94
1:D:9:LYS:HA	1:D:104:ARG:NH2	1.84	0.93
1:B:61:GLU:HB3	1:B:103:ARG:HH11	1.34	0.93
3:E:176:REA:C8	3:E:176:REA:H181	1.96	0.92
1:A:61:GLU:OE2	1:A:103:ARG:CD	2.17	0.91
1:C:97:ALA:CB	1:C:98:ASN:ND2	2.32	0.91
2:F:110:ASP:O	2:F:112:GLU:HG2	1.70	0.91
2:F:73:MET:HG3	3:F:177:REA:H10	1.54	0.89
1:D:100:SER:C	1:D:102:PRO:HD3	1.99	0.88
3:E:176:REA:C8	3:E:176:REA:C18	2.44	0.88
1:D:95:PHE:HD2	1:D:97:ALA:HB2	1.27	0.87
1:D:55:LEU:HD13	1:D:58:LEU:HD11	1.58	0.85
2:E:64:LEU:C	2:E:66:ASN:N	2.31	0.85
2:E:67:TRP:O	2:E:68:ASP:HB2	1.74	0.84
1:B:22:GLY:HA3	1:C:114:TYR:CD2	2.13	0.84
2:E:110:ASP:OD1	2:E:110:ASP:O	1.97	0.83
1:D:100:SER:O	1:D:102:PRO:HD3	1.79	0.82
1:D:34:ARG:NH1	1:D:36:ALA:HA	1.95	0.81
1:D:103:ARG:NH1	1:D:103:ARG:HA	1.95	0.81
1:D:95:PHE:CE2	1:D:97:ALA:HB2	2.15	0.81
1:D:30:VAL:HB	1:D:55:LEU:HD12	1.61	0.80
1:B:61:GLU:HB3	1:B:103:ARG:NH1	1.96	0.80
2:E:107:ILE:HD11	2:E:118:TYR:HB3	1.62	0.80
1:D:19:ALA:HB3	1:D:112:SER:OG	1.83	0.79
1:D:95:PHE:CE2	1:D:97:ALA:CB	2.66	0.78
1:B:55:LEU:HD13	1:B:58:LEU:HD11	1.68	0.76
1:D:68:ILE:H	1:D:96:THR:HA	1.50	0.76
1:D:11:PRO:HB3	1:D:103:ARG:HG3	1.68	0.76
3:E:176:REA:C18	3:E:176:REA:H8	2.16	0.75
1:D:100:SER:C	1:D:102:PRO:CD	2.59	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:VAL:HB	1:C:55:LEU:HD12	1.67	0.75
1:C:103:ARG:HA	1:C:103:ARG:NH1	2.01	0.75
1:D:97:ALA:HB1	1:D:105:TYR:CZ	2.22	0.74
1:D:65:VAL:HG23	1:D:66:GLU:N	2.03	0.74
1:C:97:ALA:HB3	1:C:98:ASN:HD21	1.50	0.74
1:D:95:PHE:CD2	1:D:97:ALA:CB	2.70	0.74
2:E:109:THR:HG23	2:E:109:THR:O	1.88	0.73
1:D:68:ILE:O	1:D:68:ILE:HG22	1.87	0.72
1:C:98:ASN:ND2	1:C:98:ASN:H	1.87	0.72
1:C:98:ASN:HB3	1:C:103:ARG:NH2	2.04	0.72
2:F:64:LEU:C	2:F:66:ASN:H	1.97	0.72
1:D:66:GLU:O	1:D:98:ASN:HB2	1.90	0.71
1:D:93:VAL:HG21	1:D:107:ILE:HG21	1.71	0.71
1:D:98:ASN:HA	1:D:103:ARG:NH1	2.07	0.70
1:D:65:VAL:HG23	1:D:66:GLU:H	1.55	0.70
2:E:113:THR:HG21	2:E:148:VAL:HG21	1.72	0.70
1:C:14:VAL:HG21	1:C:71:VAL:HG11	1.72	0.70
1:C:97:ALA:HB3	1:C:98:ASN:HD22	1.54	0.70
1:A:33:PHE:HD2	1:A:41:TRP:HB3	1.57	0.69
1:D:66:GLU:HA	1:D:98:ASN:CB	2.20	0.68
2:E:37:LEU:HD21	3:E:176:REA:H12	1.75	0.68
2:E:37:LEU:HD12	2:E:41:ILE:HG12	1.75	0.68
1:D:34:ARG:HH11	1:D:36:ALA:HA	1.56	0.68
1:A:83:GLY:HA3	2:F:35:LEU:HD22	1.76	0.68
1:C:70:LYS:HD3	1:C:94:VAL:HG13	1.75	0.68
1:D:102:PRO:HA	1:D:125:PRO:HD2	1.75	0.67
1:D:103:ARG:HA	1:D:103:ARG:HH11	1.58	0.67
1:D:79:TRP:HB2	1:D:86:PRO:HG3	1.75	0.67
2:E:114:PHE:CD2	2:E:152:VAL:HG23	2.29	0.67
1:A:27:ASN:ND2	1:A:48:LYS:HD3	2.09	0.66
2:E:37:LEU:HD23	3:E:176:REA:H12	1.77	0.66
1:D:84:ILE:O	1:D:86:PRO:HD3	1.95	0.66
2:F:110:ASP:O	2:F:112:GLU:N	2.24	0.66
1:B:30:VAL:HB	1:B:55:LEU:HD12	1.77	0.66
2:E:113:THR:CG2	2:E:148:VAL:HG21	2.26	0.66
1:A:13:MET:SD	1:A:56:HIS:CE1	2.89	0.65
2:E:98:GLN:NE2	3:E:176:REA:H202	2.10	0.65
2:F:37:LEU:HA	2:F:61:VAL:HG13	1.79	0.65
2:E:29:LYS:HZ2	2:E:166:ARG:HE	1.45	0.65
1:D:65:VAL:C	1:D:66:GLU:HG3	2.22	0.65
1:A:32:VAL:HG21	1:A:58:LEU:HD13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:PHE:CE1	2:F:106:ILE:HG13	2.33	0.64
2:F:16:ASP:HB3	2:F:19:ARG:HB2	1.80	0.64
1:A:113:PRO:HB2	1:A:114:TYR:HD1	1.63	0.63
1:D:21:ARG:NE	1:D:82:LEU:HD21	2.12	0.63
2:E:102:ASP:OD1	2:E:121:ARG:HD3	1.98	0.63
2:F:118:TYR:HE1	2:F:161:LEU:HD21	1.63	0.63
1:B:101:GLY:N	1:B:102:PRO:CD	2.61	0.63
2:F:6:VAL:HA	2:F:9:PHE:CD2	2.34	0.63
1:C:98:ASN:HB3	1:C:103:ARG:CZ	2.29	0.63
2:E:157:GLU:OE1	2:E:162:ALA:HB3	1.99	0.62
2:F:41:ILE:HD12	2:F:168:ILE:HD13	1.80	0.62
1:D:65:VAL:O	1:D:66:GLU:CG	2.47	0.62
1:A:101:GLY:O	1:A:103:ARG:HG3	2.00	0.62
1:C:102:PRO:HA	1:C:125:PRO:HD2	1.81	0.61
2:E:129:CYS:SG	2:E:132:SER:HB3	2.40	0.61
1:A:76:LYS:HD3	1:A:80:LYS:HE2	1.81	0.61
1:C:98:ASN:ND2	1:C:98:ASN:N	2.49	0.61
1:A:87:PHE:CD2	1:B:120:ALA:HB2	2.36	0.60
1:C:21:ARG:HE	1:C:82:LEU:HD21	1.65	0.60
1:C:11:PRO:HB2	1:C:64:PHE:CD2	2.36	0.60
1:D:97:ALA:HB1	1:D:105:TYR:CE1	2.36	0.60
1:A:30:VAL:HB	1:A:55:LEU:HD12	1.82	0.60
1:A:9:LYS:HA	1:A:104:ARG:NH2	2.17	0.60
1:A:10:CYS:SG	1:A:13:MET:HG3	2.42	0.60
1:C:21:ARG:NE	1:C:82:LEU:HD21	2.17	0.60
1:B:104:ARG:HD3	1:B:123:THR:OG1	2.01	0.59
2:E:37:LEU:HD21	3:E:176:REA:C10	2.32	0.59
2:E:27:MET:HE1	2:E:143:GLY:HA2	1.84	0.59
1:D:93:VAL:O	1:D:95:PHE:HD1	1.85	0.59
2:E:88:MET:O	2:E:101:ASN:HA	2.02	0.59
1:D:30:VAL:HB	1:D:55:LEU:CD1	2.32	0.59
1:D:93:VAL:HG11	1:D:107:ILE:HG12	1.83	0.59
1:B:93:VAL:HG21	1:B:107:ILE:HG21	1.85	0.58
2:F:27:MET:HE2	2:F:143:GLY:HA2	1.84	0.58
1:B:100:SER:C	1:B:102:PRO:HD2	2.26	0.58
1:C:93:VAL:HG11	1:C:107:ILE:HG13	1.85	0.58
1:D:30:VAL:HG22	1:D:73:ILE:HG12	1.85	0.58
2:E:103:ASP:O	2:E:119:SER:HB2	2.04	0.58
1:C:55:LEU:HD13	1:C:58:LEU:HD11	1.86	0.58
2:F:37:LEU:CD2	3:F:177:REA:H12	2.34	0.58
1:D:9:LYS:HA	1:D:104:ARG:HH22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:VAL:CB	1:D:55:LEU:HD12	2.31	0.57
1:D:101:GLY:N	1:D:102:PRO:CD	2.67	0.57
2:E:29:LYS:NZ	2:E:166:ARG:HE	2.01	0.57
2:E:107:ILE:HG22	2:E:155:ARG:NH2	2.19	0.57
2:F:110:ASP:C	2:F:112:GLU:H	2.11	0.57
1:D:35:LYS:HB3	1:D:68:ILE:CG2	2.34	0.57
1:D:97:ALA:CB	1:D:105:TYR:CZ	2.87	0.57
2:F:88:MET:HE3	2:F:90:TYR:HB3	1.86	0.57
1:D:17:LEU:HB2	1:D:110:LEU:HD12	1.86	0.57
1:D:95:PHE:HE2	1:D:97:ALA:CB	2.16	0.56
1:C:33:PHE:HB3	1:C:41:TRP:CE3	2.40	0.56
1:D:65:VAL:O	1:D:66:GLU:HG3	2.06	0.56
2:F:147:GLN:O	2:F:150:LYS:HB3	2.05	0.56
1:B:33:PHE:HD2	1:B:41:TRP:HB3	1.70	0.56
1:B:73:ILE:O	1:B:90:HIS:HB2	2.06	0.56
2:E:70:CYS:SG	2:E:173:TYR:O	2.63	0.56
1:A:113:PRO:HB2	1:A:114:TYR:CD1	2.41	0.55
1:D:97:ALA:HA	1:D:105:TYR:OH	2.06	0.55
2:F:37:LEU:HD21	3:F:177:REA:H12	1.87	0.55
1:D:67:GLY:HA3	1:D:96:THR:HG23	1.88	0.55
1:C:103:ARG:HA	1:C:103:ARG:CZ	2.36	0.55
3:F:177:REA:H171	3:F:177:REA:C8	2.35	0.55
1:A:12:LEU:HD21	1:A:32:VAL:HG11	1.87	0.55
1:C:41:TRP:HH2	1:C:68:ILE:HG22	1.71	0.55
2:F:64:LEU:C	2:F:66:ASN:N	2.65	0.55
1:C:41:TRP:CH2	1:C:68:ILE:HG22	2.42	0.55
2:E:148:VAL:HA	2:E:151:ILE:HD12	1.88	0.55
1:C:125:PRO:O	1:C:126:LYS:HG3	2.07	0.54
2:E:67:TRP:O	2:E:68:ASP:CB	2.53	0.54
1:A:113:PRO:HG2	1:D:20:VAL:O	2.08	0.54
3:E:176:REA:H8	3:E:176:REA:H182	1.86	0.54
1:B:32:VAL:HG22	1:B:71:VAL:HG22	1.89	0.54
2:F:60:ARG:HG3	2:F:173:TYR:CD2	2.42	0.54
1:B:33:PHE:HB3	1:B:41:TRP:HE3	1.72	0.53
1:D:11:PRO:HB2	1:D:64:PHE:CD2	2.43	0.53
1:B:83:GLY:HA3	2:E:35:LEU:HD22	1.91	0.53
1:B:76:LYS:HE3	1:B:89:GLU:OE2	2.08	0.53
1:D:35:LYS:HB3	1:D:68:ILE:HG22	1.90	0.53
1:C:25:ALA:HA	1:C:78:TYR:OH	2.09	0.53
1:D:11:PRO:HB2	1:D:64:PHE:HD2	1.73	0.53
1:D:97:ALA:O	1:D:98:ASN:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:H	1:A:125:PRO:HD3	1.73	0.52
2:E:114:PHE:CE2	2:E:152:VAL:HG23	2.44	0.52
2:F:94:ALA:HB1	2:F:96:PHE:CD1	2.45	0.52
1:D:103:ARG:HA	1:D:103:ARG:CZ	2.40	0.52
1:C:11:PRO:HB2	1:C:64:PHE:HD2	1.75	0.52
2:F:47:VAL:HA	2:F:52:HIS:O	2.10	0.52
1:A:70:LYS:HB2	1:A:94:VAL:HG12	1.91	0.52
1:D:16:VAL:HG23	1:D:49:THR:HG21	1.92	0.52
2:F:155:ARG:HA	2:F:158:GLU:HG3	1.92	0.52
1:A:11:PRO:HB2	1:A:64:PHE:CD2	2.44	0.52
1:B:35:LYS:NZ	1:B:39:ASP:HA	2.25	0.52
1:C:103:ARG:O	1:C:105:TYR:HD1	1.93	0.52
1:D:47:GLY:HA3	1:D:55:LEU:HD21	1.92	0.52
1:B:11:PRO:HB2	1:B:59:THR:HG23	1.92	0.51
1:B:55:LEU:HD22	1:B:58:LEU:HG	1.93	0.51
1:C:8:SER:HB3	1:C:104:ARG:HH12	1.74	0.51
2:F:105:TRP:CE3	2:F:118:TYR:HD2	2.29	0.51
1:D:12:LEU:HD12	1:D:13:MET:H	1.75	0.51
2:E:29:LYS:HB3	2:E:168:ILE:HD11	1.92	0.51
2:E:57:ALA:CB	3:E:176:REA:H41	2.41	0.51
2:F:29:LYS:HA	2:F:134:SER:O	2.11	0.50
1:B:64:PHE:HD1	1:B:69:TYR:CZ	2.30	0.50
1:D:98:ASN:HA	1:D:103:ARG:CZ	2.42	0.50
1:D:98:ASN:HA	1:D:103:ARG:HH12	1.73	0.50
3:F:177:REA:C8	3:F:177:REA:C17	2.90	0.50
1:A:41:TRP:CH2	1:A:68:ILE:HG22	2.46	0.50
2:E:13:GLU:HG2	2:E:14:ASN:HB2	1.94	0.50
2:E:114:PHE:HD2	2:E:152:VAL:CG2	2.25	0.50
1:B:33:PHE:CD2	1:B:41:TRP:HB3	2.46	0.50
1:C:28:VAL:O	1:C:48:LYS:HA	2.12	0.50
2:F:161:LEU:O	2:F:165:TYR:CE1	2.64	0.50
1:C:16:VAL:CG1	1:C:111:LEU:HD12	2.41	0.50
1:D:84:ILE:HG13	2:F:67:TRP:HB3	1.93	0.50
1:B:75:THR:HG22	1:B:111:LEU:HD21	1.94	0.50
2:E:109:THR:O	2:E:109:THR:CG2	2.58	0.50
2:E:4:CYS:O	2:E:128:THR:HA	2.11	0.49
2:F:15:PHE:HE1	2:F:106:ILE:HG21	1.76	0.49
2:F:77:PHE:HE2	2:F:104:HIS:CD2	2.31	0.49
2:F:161:LEU:O	2:F:165:TYR:HE1	1.95	0.49
1:A:28:VAL:O	1:A:48:LYS:HA	2.12	0.49
2:E:15:PHE:CE1	2:E:106:ILE:HG13	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ALA:HB1	1:B:31:HIS:HE1	1.77	0.49
1:D:23:SER:OG	1:D:24:PRO:HD2	2.11	0.49
1:D:32:VAL:N	1:D:45:ALA:O	2.41	0.49
1:D:65:VAL:C	1:D:66:GLU:CG	2.85	0.49
2:F:168:ILE:HG22	2:F:170:HIS:NE2	2.27	0.49
1:B:87:PHE:HB2	1:B:114:TYR:CD2	2.47	0.49
2:F:116:VAL:HG22	2:F:152:VAL:CG2	2.43	0.49
1:A:32:VAL:HG22	1:A:71:VAL:HG22	1.94	0.49
1:A:102:PRO:HA	1:A:125:PRO:CD	2.43	0.49
1:A:103:ARG:N	1:A:125:PRO:HD3	2.28	0.49
1:D:65:VAL:CG2	1:D:66:GLU:H	2.23	0.49
2:F:168:ILE:HG22	2:F:170:HIS:CD2	2.48	0.49
1:B:84:ILE:CG2	2:E:96:PHE:HB2	2.43	0.49
1:C:64:PHE:HD1	1:C:69:TYR:CZ	2.30	0.49
1:D:64:PHE:HB3	1:D:98:ASN:HD21	1.78	0.49
1:D:32:VAL:HG22	1:D:71:VAL:CG2	2.43	0.48
1:A:25:ALA:HA	1:A:78:TYR:OH	2.13	0.48
1:A:44:PHE:HE2	1:A:59:THR:HB	1.77	0.48
2:F:78:THR:O	2:F:86:PHE:HB3	2.14	0.48
1:A:29:ALA:HB1	1:A:31:HIS:HE1	1.78	0.48
1:B:104:ARG:HB3	1:B:123:THR:O	2.13	0.48
1:C:13:MET:C	1:C:13:MET:SD	2.97	0.48
2:E:6:VAL:HA	2:E:9:PHE:CD2	2.48	0.48
2:E:37:LEU:HD21	3:E:176:REA:H10	1.95	0.48
2:E:98:GLN:NE2	3:E:176:REA:C20	2.77	0.48
2:E:107:ILE:HG22	2:E:155:ARG:CZ	2.43	0.48
1:D:28:VAL:O	1:D:48:LYS:HA	2.14	0.48
2:E:110:ASP:O	2:E:110:ASP:CG	2.57	0.48
1:B:97:ALA:O	1:B:99:ASP:N	2.47	0.48
1:C:32:VAL:HG22	1:C:71:VAL:HG22	1.96	0.48
1:D:80:LYS:C	1:D:82:LEU:H	2.22	0.48
1:A:55:LEU:HD22	1:A:58:LEU:HG	1.96	0.47
1:D:73:ILE:O	1:D:90:HIS:HB2	2.14	0.47
2:E:57:ALA:HB2	3:E:176:REA:H41	1.94	0.47
1:B:83:GLY:HA3	2:E:35:LEU:CD2	2.44	0.47
2:E:6:VAL:HG21	2:E:129:CYS:HB2	1.96	0.47
2:F:6:VAL:HG12	2:F:6:VAL:O	2.12	0.47
2:F:53:MET:O	2:F:77:PHE:HD1	1.98	0.47
2:F:157:GLU:OE1	2:F:162:ALA:HB3	2.14	0.47
1:A:99:ASP:C	2:E:89:LYS:HZ3	2.23	0.47
1:D:64:PHE:CD1	1:D:98:ASN:ND2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ALA:HA	1:B:78:TYR:OH	2.15	0.47
1:D:65:VAL:CG2	1:D:66:GLU:N	2.71	0.47
2:E:38:GLN:OE1	2:E:61:VAL:HA	2.15	0.47
1:B:110:LEU:O	1:B:116:TYR:HA	2.15	0.46
2:E:107:ILE:HG13	2:E:159:LEU:HD11	1.98	0.46
2:F:77:PHE:CE2	2:F:104:HIS:CD2	3.03	0.46
2:F:117:GLN:O	2:F:134:SER:HA	2.15	0.46
1:A:55:LEU:HD13	1:A:58:LEU:HD11	1.96	0.46
1:A:114:TYR:OH	2:F:95:SER:HB2	2.15	0.46
1:C:71:VAL:O	1:C:92:GLU:HA	2.16	0.46
1:C:95:PHE:CE2	1:C:105:TYR:CD2	3.03	0.46
1:C:98:ASN:O	1:C:99:ASP:C	2.58	0.46
2:F:30:LYS:O	2:F:133:TYR:HA	2.15	0.46
1:B:101:GLY:N	1:B:102:PRO:HD2	2.30	0.46
2:E:29:LYS:NZ	2:E:166:ARG:NE	2.64	0.46
2:E:150:LYS:HE3	2:E:150:LYS:HB3	1.91	0.46
1:D:28:VAL:HG11	1:D:73:ILE:HG23	1.98	0.46
1:D:32:VAL:HA	1:D:70:LYS:O	2.16	0.46
1:A:9:LYS:HA	1:A:104:ARG:CZ	2.46	0.46
2:E:37:LEU:CD2	3:E:176:REA:C12	2.83	0.46
2:E:108:ASP:O	2:E:115:ALA:HA	2.16	0.46
1:A:41:TRP:HH2	1:A:68:ILE:HG22	1.81	0.46
1:C:64:PHE:HA	1:C:69:TYR:OH	2.15	0.46
2:E:47:VAL:HA	2:E:52:HIS:O	2.15	0.46
2:F:107:ILE:HD11	2:F:118:TYR:HB2	1.97	0.46
1:A:93:VAL:HG21	1:A:107:ILE:HG21	1.98	0.46
1:B:31:HIS:CD2	1:B:46:SER:OG	2.69	0.46
1:B:75:THR:O	1:B:78:TYR:HB3	2.16	0.46
1:A:11:PRO:HB2	1:A:64:PHE:HD2	1.79	0.45
1:A:124:ASN:HD21	1:A:127:GLU:HA	1.81	0.45
1:A:79:TRP:O	1:A:80:LYS:C	2.58	0.45
1:D:66:GLU:O	1:D:98:ASN:CB	2.62	0.45
1:D:103:ARG:O	1:D:105:TYR:HD1	1.98	0.45
1:C:64:PHE:CD1	1:C:69:TYR:CZ	3.05	0.45
2:E:37:LEU:HD21	3:E:176:REA:C12	2.46	0.45
1:C:35:LYS:N	1:C:41:TRP:CZ3	2.85	0.45
2:E:114:PHE:CD2	2:E:152:VAL:CG2	2.97	0.45
2:F:114:PHE:HB2	2:F:144:PHE:HE2	1.81	0.45
2:F:146:PRO:HA	2:F:149:GLN:HB3	1.98	0.45
1:B:35:LYS:HZ2	1:B:39:ASP:HA	1.82	0.45
2:E:19:ARG:O	2:E:111:TYR:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:VAL:HB	1:D:25:ALA:HB3	1.98	0.45
2:E:37:LEU:HA	2:E:61:VAL:CG1	2.47	0.45
1:C:13:MET:SD	1:C:14:VAL:N	2.90	0.45
1:A:79:TRP:HA	1:A:79:TRP:CE3	2.52	0.45
1:C:64:PHE:HD1	1:C:69:TYR:OH	2.00	0.44
1:A:33:PHE:CD2	1:A:41:TRP:HB3	2.45	0.44
1:D:10:CYS:SG	1:D:56:HIS:CD2	3.11	0.44
1:A:80:LYS:C	1:A:82:LEU:H	2.25	0.44
1:C:17:LEU:HB2	1:C:110:LEU:HD12	2.00	0.44
1:D:95:PHE:CE2	1:D:97:ALA:HB3	2.52	0.44
2:E:6:VAL:CG2	2:E:129:CYS:HB2	2.48	0.44
2:E:24:TRP:HB3	2:E:137:PHE:HB3	2.00	0.44
1:B:41:TRP:O	1:B:43:PRO:HD3	2.18	0.44
1:C:113:PRO:C	1:C:114:TYR:HD1	2.26	0.44
1:C:29:ALA:HA	1:C:47:GLY:O	2.17	0.44
1:C:70:LYS:HD2	1:C:92:GLU:CD	2.42	0.43
1:D:125:PRO:HG2	1:D:127:GLU:OXT	2.18	0.43
1:C:79:TRP:HE1	1:C:111:LEU:HD22	1.83	0.43
1:C:98:ASN:HA	1:C:103:ARG:HH12	1.82	0.43
2:F:116:VAL:HG22	2:F:152:VAL:HG22	2.00	0.43
1:B:13:MET:O	1:B:106:THR:HA	2.18	0.43
1:A:93:VAL:HG21	1:A:107:ILE:CG2	2.49	0.43
1:D:75:THR:O	1:D:78:TYR:N	2.51	0.43
2:F:24:TRP:HB3	2:F:137:PHE:HB3	2.01	0.43
1:D:64:PHE:CB	1:D:98:ASN:HD21	2.31	0.43
1:D:72:GLU:HA	1:D:91:ALA:O	2.19	0.43
3:E:176:REA:H192	3:E:176:REA:H7	1.33	0.43
1:D:35:LYS:HA	1:D:41:TRP:HA	2.01	0.43
1:D:93:VAL:HG11	1:D:107:ILE:CG1	2.49	0.43
1:D:107:ILE:N	1:D:107:ILE:HD12	2.34	0.43
1:C:75:THR:O	1:C:76:LYS:C	2.61	0.43
1:D:32:VAL:HG22	1:D:71:VAL:HG23	2.01	0.43
1:B:64:PHE:CD1	1:B:69:TYR:CZ	3.07	0.43
1:D:64:PHE:CE1	1:D:69:TYR:CE2	3.06	0.43
2:E:27:MET:CE	2:E:143:GLY:HA2	2.48	0.43
1:B:84:ILE:HG23	2:E:96:PHE:HD2	1.84	0.43
1:C:10:CYS:HA	1:C:11:PRO:HD2	1.79	0.43
1:C:33:PHE:CD2	1:C:41:TRP:HB3	2.54	0.43
1:D:35:LYS:HB3	1:D:68:ILE:HG21	2.01	0.43
2:F:19:ARG:HB3	2:F:111:TYR:CD1	2.54	0.43
2:F:43:ALA:HB1	2:F:45:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:LYS:HZ2	2:E:166:ARG:NE	2.12	0.42
1:C:87:PHE:HD2	1:C:88:HIS:CE1	2.37	0.42
1:D:34:ARG:HB2	1:D:44:PHE:HB2	2.00	0.42
1:D:101:GLY:N	1:D:102:PRO:HD2	2.34	0.42
2:E:90:TYR:O	2:E:99:LYS:HA	2.19	0.42
2:F:27:MET:CE	2:F:143:GLY:HA2	2.48	0.42
1:A:102:PRO:HA	1:A:125:PRO:HD2	2.01	0.42
1:D:65:VAL:O	1:D:66:GLU:HG2	2.18	0.42
1:D:124:ASN:HA	1:D:125:PRO:HD2	1.78	0.42
2:F:15:PHE:CZ	2:F:106:ILE:HG13	2.55	0.42
1:A:102:PRO:HA	1:A:125:PRO:HD3	2.02	0.42
1:B:114:TYR:N	1:B:114:TYR:CD1	2.87	0.42
1:D:66:GLU:CA	1:D:98:ASN:CB	2.95	0.42
1:A:31:HIS:CD2	1:A:46:SER:OG	2.72	0.42
1:A:33:PHE:HB3	1:A:41:TRP:HE3	1.84	0.42
2:E:107:ILE:HD11	2:E:118:TYR:CB	2.43	0.42
1:B:33:PHE:HB3	1:B:41:TRP:CE3	2.53	0.42
1:D:60:THR:OG1	1:D:63:GLN:HB2	2.18	0.42
1:D:89:GLU:O	1:D:90:HIS:HB3	2.19	0.42
2:F:168:ILE:O	2:F:170:HIS:HD2	2.03	0.42
1:C:93:VAL:HG21	1:C:107:ILE:CG2	2.49	0.42
1:D:25:ALA:HA	1:D:78:TYR:OH	2.20	0.42
2:F:6:VAL:HG21	2:F:120:CYS:SG	2.60	0.42
1:D:79:TRP:CH2	1:D:113:PRO:HD3	2.54	0.41
2:F:15:PHE:CE1	2:F:106:ILE:HG21	2.54	0.41
2:F:62:ARG:HH11	2:F:66:ASN:ND2	2.18	0.41
1:B:65:VAL:O	1:B:69:TYR:HE1	2.03	0.41
1:D:98:ASN:OD1	1:D:103:ARG:NH2	2.53	0.41
2:E:6:VAL:HA	2:E:9:PHE:CE2	2.55	0.41
2:E:63:LEU:HA	2:E:63:LEU:HD12	1.67	0.41
2:F:90:TYR:O	2:F:99:LYS:HA	2.20	0.41
1:A:41:TRP:O	1:A:43:PRO:HD3	2.21	0.41
1:D:8:SER:N	1:D:9:LYS:HD2	2.35	0.41
1:D:70:LYS:HG3	1:D:71:VAL:N	2.35	0.41
1:D:101:GLY:HA2	1:D:103:ARG:NH2	2.35	0.41
2:F:37:LEU:HD21	3:F:177:REA:C12	2.50	0.41
1:D:13:MET:SD	1:D:56:HIS:CE1	3.14	0.41
1:B:10:CYS:HA	1:B:11:PRO:HD2	1.80	0.41
2:F:157:GLU:OE1	2:F:162:ALA:CB	2.69	0.41
1:C:34:ARG:HE	1:C:65:VAL:HG23	1.86	0.40
1:C:97:ALA:HB1	1:C:98:ASN:ND2	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:112:GLU:HG2	2:F:112:GLU:H	1.70	0.40
2:F:144:PHE:CD1	2:F:144:PHE:N	2.89	0.40
1:C:76:LYS:HE3	1:C:76:LYS:HB2	1.92	0.40
1:C:98:ASN:CB	1:C:103:ARG:NH2	2.82	0.40
1:D:114:TYR:N	1:D:114:TYR:CD1	2.90	0.40
1:D:64:PHE:C	1:D:98:ASN:HD21	2.30	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:GLU:CD	1:D:66:GLU:OE1[3_655]	0.16	2.04
1:D:66:GLU:OE1	1:D:66:GLU:OE1[3_655]	1.18	1.02
1:D:66:GLU:CD	1:D:66:GLU:CD[3_655]	1.41	0.79
1:D:66:GLU:OE1	1:D:66:GLU:OE2[3_655]	1.43	0.77
1:D:66:GLU:CG	1:D:66:GLU:OE1[3_655]	1.51	0.69

5.3 Torsion angles

5.3.1 Protein backbone

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	121/127 (95%)	100 (83%)	17 (14%)	4 (3%)	3	17
1	B	118/127 (93%)	97 (82%)	16 (14%)	5 (4%)	2	13
1	C	121/127 (95%)	93 (77%)	23 (19%)	5 (4%)	2	13
1	D	118/127 (93%)	89 (75%)	21 (18%)	8 (7%)	1	5
2	E	172/174 (99%)	145 (84%)	20 (12%)	7 (4%)	2	13
2	F	172/174 (99%)	143 (83%)	24 (14%)	5 (3%)	3	19
All	All	822/856 (96%)	667 (81%)	121 (15%)	34 (4%)	2	13

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ALA
1	A	125	PRO
1	B	98	ASN
1	B	125	PRO
1	C	98	ASN
1	D	98	ASN
1	D	99	ASP
1	D	125	PRO
2	E	51	GLY
2	E	65	ASN
2	F	111	TYR
1	B	66	GLU
1	B	82	LEU
1	C	76	LYS
1	D	68	ILE
2	E	64	LEU
2	E	111	TYR
2	E	173	TYR
1	C	7	GLU
1	C	81	ALA
1	C	125	PRO
1	D	10	CYS
1	D	50	SER
2	E	115	ALA
2	F	15	PHE
2	F	18	ALA
2	F	98	GLN
1	D	66	GLU
1	D	90	HIS
2	E	69	VAL
2	F	32	PRO
1	A	97	ALA
1	B	11	PRO
1	A	22	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	103/105 (98%)	84 (82%)	19 (18%)	1	8
1	B	101/105 (96%)	86 (85%)	15 (15%)	3	13
1	C	103/105 (98%)	85 (82%)	18 (18%)	2	9
1	D	101/105 (96%)	77 (76%)	24 (24%)	1	3
2	E	150/150 (100%)	122 (81%)	28 (19%)	1	7
2	F	150/150 (100%)	119 (79%)	31 (21%)	1	5
All	All	708/720 (98%)	573 (81%)	135 (19%)	1	7

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	CYS
1	A	13	MET
1	A	24	PRO
1	A	27	ASN
1	A	42	GLU
1	A	43	PRO
1	A	46	SER
1	A	56	HIS
1	A	63	GLN
1	A	64	PHE
1	A	71	VAL
1	A	82	LEU
1	A	86	PRO
1	A	94	VAL
1	A	98	ASN
1	A	104	ARG
1	A	119	THR
1	A	123	THR
1	A	127	GLU
1	B	9	LYS
1	B	10	CYS
1	B	27	ASN
1	B	42	GLU
1	B	43	PRO
1	B	46	SER
1	B	55	LEU
1	B	56	HIS
1	B	63	GLN
1	B	82	LEU
1	B	94	VAL

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Mol	Chain	Res	Type
1	B	100	SER
1	B	113	PRO
1	B	119	THR
1	B	127	GLU
1	C	7	GLU
1	C	21	ARG
1	C	24	PRO
1	C	28	VAL
1	C	43	PRO
1	C	49	THR
1	C	55	LEU
1	C	56	HIS
1	C	63	GLN
1	C	66	GLU
1	C	86	PRO
1	C	94	VAL
1	C	98	ASN
1	C	100	SER
1	C	103	ARG
1	C	104	ARG
1	C	119	THR
1	C	127	GLU
1	D	10	CYS
1	D	12	LEU
1	D	13	MET
1	D	16	VAL
1	D	27	ASN
1	D	31	HIS
1	D	40	THR
1	D	46	SER
1	D	48	LYS
1	D	52	SER
1	D	54	GLU
1	D	55	LEU
1	D	56	HIS
1	D	63	GLN
1	D	64	PHE
1	D	68	ILE
1	D	71	VAL
1	D	82	LEU
1	D	94	VAL
1	D	98	ASN

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Mol	Chain	Res	Type
1	D	103	ARG
1	D	113	PRO
1	D	119	THR
1	D	127	GLU
2	E	2	ARG
2	E	7	SER
2	E	13	GLU
2	E	14	ASN
2	E	37	LEU
2	E	53	MET
2	E	54	SER
2	E	63	LEU
2	E	64	LEU
2	E	66	ASN
2	E	67	TRP
2	E	69	VAL
2	E	76	THR
2	E	93	VAL
2	E	98	GLN
2	E	101	ASN
2	E	112	GLU
2	E	116	VAL
2	E	121	ARG
2	E	139	ARG
2	E	144	PHE
2	E	145	SER
2	E	152	VAL
2	E	154	GLN
2	E	164	GLN
2	E	166	ARG
2	E	167	LEU
2	E	174	CYS
2	F	7	SER
2	F	13	GLU
2	F	19	ARG
2	F	35	LEU
2	F	38	GLN
2	F	42	VAL
2	F	61	VAL
2	F	63	LEU
2	F	64	LEU
2	F	66	ASN

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Mol	Chain	Res	Type
2	F	69	VAL
2	F	70	CYS
2	F	78	THR
2	F	86	PHE
2	F	95	SER
2	F	98	GLN
2	F	101	ASN
2	F	102	ASP
2	F	112	GLU
2	F	113	THR
2	F	116	VAL
2	F	123	LEU
2	F	132	SER
2	F	144	PHE
2	F	145	SER
2	F	147	GLN
2	F	152	VAL
2	F	154	GLN
2	F	158	GLU
2	F	161	LEU
2	F	163	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	31	HIS
1	A	98	ASN
1	B	31	HIS
1	B	90	HIS
1	C	98	ASN
1	D	56	HIS
1	D	98	ASN
2	E	40	ASN
2	E	98	GLN
2	E	104	HIS
2	E	117	GLN
2	E	124	ASN
2	E	156	GLN
2	F	66	ASN
2	F	98	GLN
2	F	104	HIS

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Mol	Chain	Res	Type
2	F	124	ASN
2	F	156	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	REA	E	176	-	21,21,22	1.51	2 (9%)	27,28,30	6.09	20 (74%)
3	REA	F	177	-	21,21,22	1.75	5 (23%)	27,28,30	8.60	20 (74%)

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	REA	E	176	-	-	6/14/31/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	REA	F	177	-	-	9/14/31/32	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	177	REA	O1-C15	5.54	1.38	1.22
3	E	176	REA	O1-C15	4.96	1.37	1.22
3	F	177	REA	C11-C12	2.35	1.40	1.34
3	F	177	REA	C8-C7	2.22	1.39	1.33
3	F	177	REA	C11-C10	2.20	1.50	1.43
3	F	177	REA	C10-C9	2.09	1.40	1.35
3	E	176	REA	C20-C13	2.05	1.55	1.50

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	177	REA	C18-C5-C6	-27.45	94.54	124.48
3	F	177	REA	C16-C1-C6	15.66	134.79	110.24
3	E	176	REA	C7-C8-C9	-13.19	106.73	126.23
3	F	177	REA	O1-C15-C14	-12.28	107.18	123.68
3	F	177	REA	C1-C6-C5	-10.94	107.69	122.64
3	E	176	REA	O1-C15-C14	-10.44	109.66	123.68
3	E	176	REA	C19-C9-C10	10.16	139.28	122.82
3	E	176	REA	C20-C13-C14	-10.13	106.41	122.82
3	F	177	REA	C7-C8-C9	-9.82	111.70	126.23
3	F	177	REA	C17-C1-C6	-9.71	95.02	110.24
3	F	177	REA	C11-C10-C9	-9.32	114.20	127.28
3	E	176	REA	C19-C9-C8	-9.20	104.03	118.09
3	F	177	REA	C20-C13-C14	-9.16	107.98	122.82
3	E	176	REA	C11-C10-C9	-8.94	114.74	127.28
3	F	177	REA	C12-C13-C14	-8.60	105.49	119.01
3	E	176	REA	C8-C7-C6	-7.81	106.15	127.00
3	F	177	REA	C19-C9-C8	-7.33	106.89	118.09
3	E	176	REA	C1-C6-C7	6.74	133.94	115.65
3	F	177	REA	C20-C13-C12	-6.47	108.20	118.09
3	F	177	REA	C19-C9-C10	5.99	132.53	122.82
3	E	176	REA	C8-C9-C10	-5.76	109.94	119.01
3	E	176	REA	C7-C6-C5	-5.70	108.43	121.56
3	E	176	REA	C1-C6-C5	-5.63	114.94	122.64
3	F	177	REA	C18-C5-C4	-5.40	102.08	113.60
3	E	176	REA	C10-C11-C12	-5.09	108.45	123.20
3	F	177	REA	C16-C1-C2	-5.06	89.53	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	176	REA	C11-C12-C13	-4.56	113.85	126.36
3	F	177	REA	C8-C9-C10	-4.45	112.01	119.01
3	E	176	REA	C18-C5-C6	-4.42	119.67	124.48
3	F	177	REA	C1-C6-C7	4.06	126.66	115.65
3	F	177	REA	C7-C6-C5	-3.94	112.49	121.56
3	E	176	REA	C2-C1-C6	3.93	116.15	110.44
3	F	177	REA	C11-C12-C13	-3.93	115.58	126.36
3	F	177	REA	C2-C1-C6	3.86	116.05	110.44
3	E	176	REA	C12-C13-C14	-3.86	112.94	119.01
3	E	176	REA	C16-C1-C6	-3.66	104.50	110.24
3	F	177	REA	C8-C7-C6	-3.62	117.33	127.00
3	E	176	REA	C18-C5-C4	-3.26	106.64	113.60
3	E	176	REA	C20-C13-C12	-3.01	113.48	118.09
3	E	176	REA	C17-C1-C6	2.80	114.63	110.24

There are no chirality outliers.

All (15) torsion outliers are listed below:

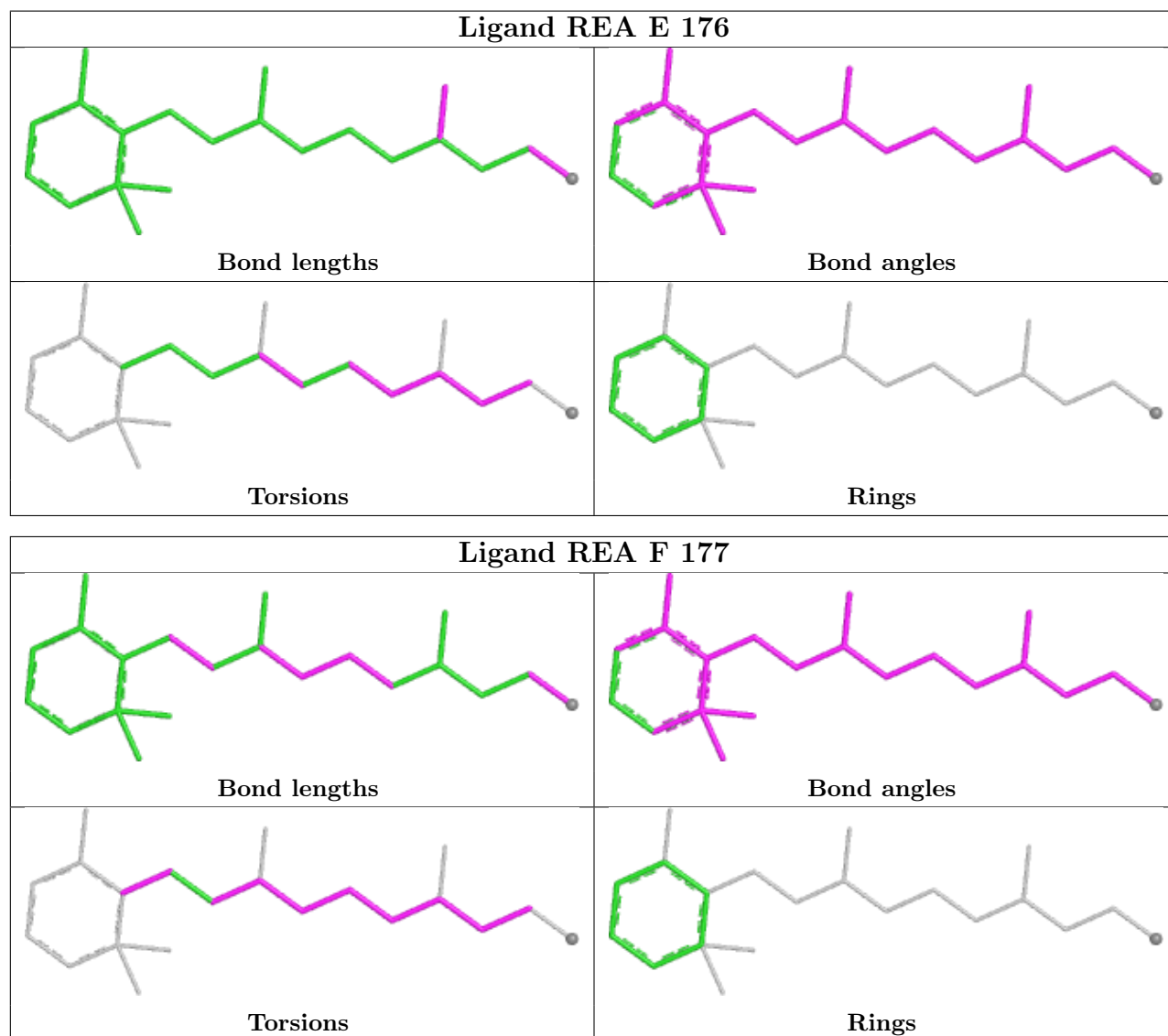
Mol	Chain	Res	Type	Atoms
3	E	176	REA	C11-C10-C9-C19
3	E	176	REA	C20-C13-C14-C15
3	E	176	REA	C13-C14-C15-O1
3	F	177	REA	C11-C10-C9-C19
3	F	177	REA	C20-C13-C14-C15
3	F	177	REA	C13-C14-C15-O1
3	E	176	REA	C11-C12-C13-C20
3	F	177	REA	C7-C8-C9-C19
3	F	177	REA	C11-C12-C13-C20
3	E	176	REA	C10-C11-C12-C13
3	F	177	REA	C1-C6-C7-C8
3	F	177	REA	C10-C11-C12-C13
3	F	177	REA	C9-C10-C11-C12
3	F	177	REA	C7-C8-C9-C10
3	E	176	REA	C12-C13-C14-C15

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	176	REA	16	0
3	F	177	REA	6	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	162:ALA	C	163:ARG	N	0.73

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.