



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:00 PM GMT

PDB ID : 1RLB
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

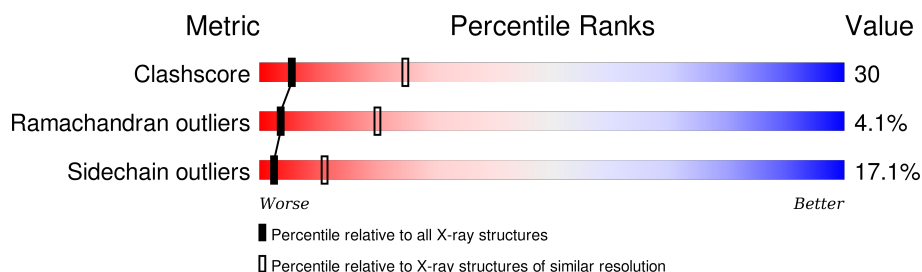
1 Overall quality at a glance

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	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	
1	B	127	
1	C	127	
1	D	127	
2	E	174	
2	F	174	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	REA	E	176	-	-	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:

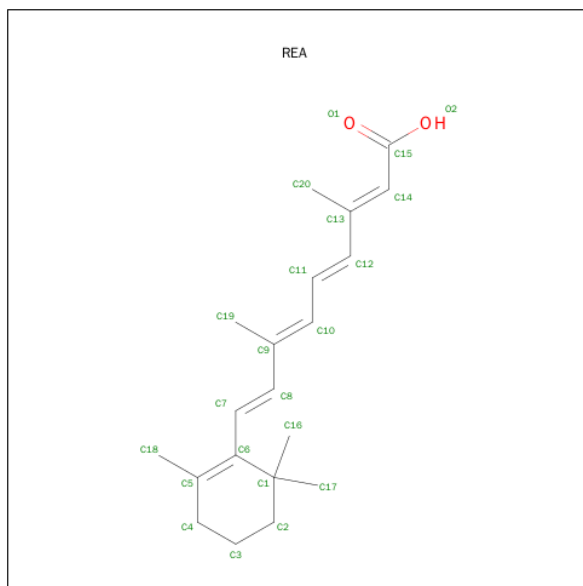
Chain	Residue	Modelled	Actual	Comment	Reference
E	21	ALA	SER	CONFLICT	UNP P02753
E	50	ASN	THR	CONFLICT	UNP P02753
E	52	HIS	GLN	CONFLICT	UNP P02753
E	107	ILE	VAL	CONFLICT	UNP P02753
E	112	GLU	ASP	CONFLICT	UNP P02753
E	114	PHE	TYR	CONFLICT	UNP P02753
E	138	ALA	SER	CONFLICT	UNP P02753
E	142	SER	ASN	CONFLICT	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 (three-letter code: REA) (formula: C₂₀H₂₈O₂).



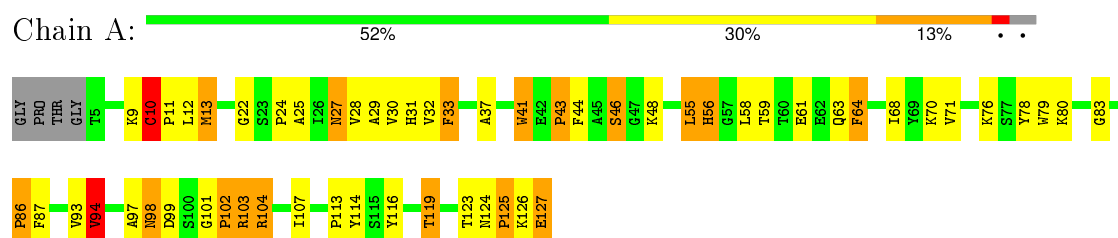
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			21	20	1		
3	F	1	Total	C	O	0	0
			21	20	1		

3 Residue-property plots

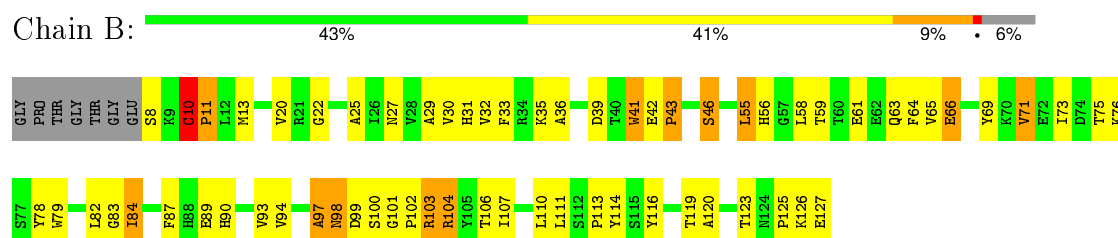
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

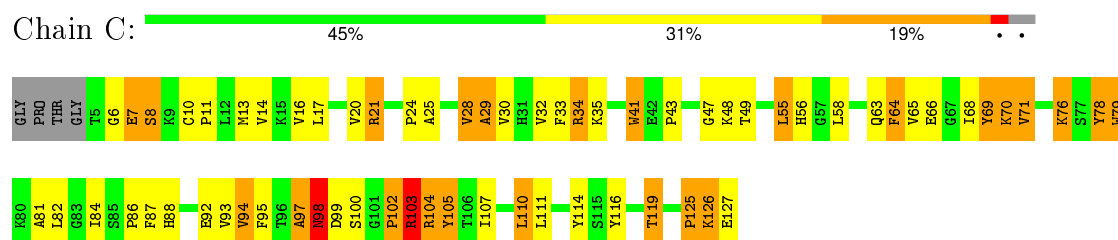
• Molecule 1: TRANSTHYRETIN



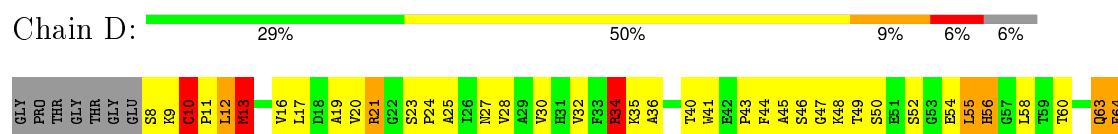
• Molecule 1: TRANSTHYRETIN

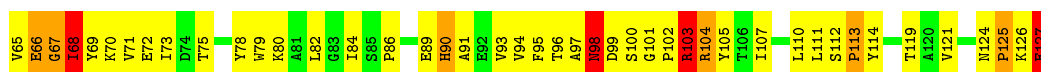


• Molecule 1: TRANSTHYRETIN

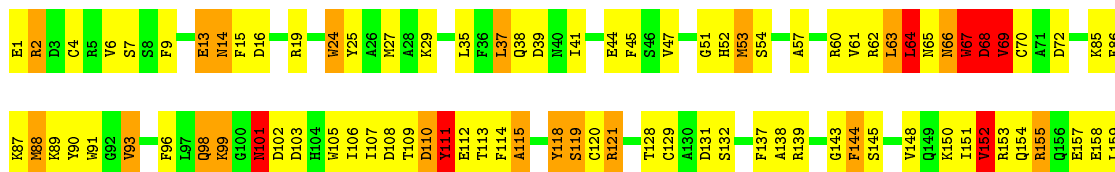


• Molecule 1: TRANSTHYRETIN

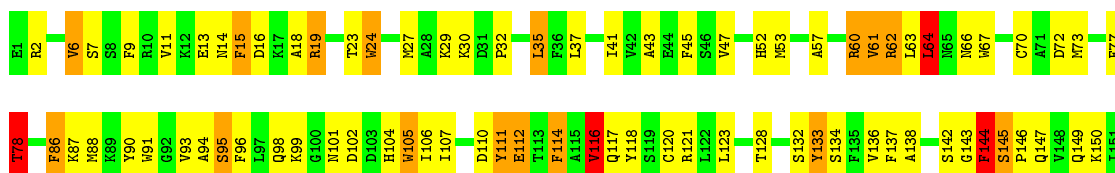




• Molecule 2: RETINOL BINDING PROTEIN



• Molecule 2: RETINOL BINDING PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 [i](#)

5.1 Standard geometry [i](#)

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	1.11	2/974 (0.2%)	1.74	16/1325 (1.2%)
1	B	1.07	0/954	1.82	23/1298 (1.8%)
1	C	1.06	0/974	1.93	28/1325 (2.1%)
1	D	1.04	0/954	1.52	13/1298 (1.0%)
2	E	1.21	5/1445 (0.3%)	2.22	59/1950 (3.0%)
2	F	1.30	3/1445 (0.2%)	2.11	45/1950 (2.3%)
All	All	1.15	10/6746 (0.1%)	1.94	184/9146 (2.0%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	162	ALA	C-N	-26.18	0.73	1.34
2	F	163	ARG	N-CA	-13.27	1.19	1.46
1	A	98	ASN	C-O	12.00	1.46	1.23
2	E	69	VAL	N-CA	11.84	1.70	1.46
2	E	99	LYS	N-CA	7.11	1.60	1.46
1	A	98	ASN	CA-C	6.93	1.71	1.52
2	E	119	SER	CA-CB	-5.79	1.44	1.52
2	F	105	TRP	CG-CD2	-5.38	1.34	1.43
2	E	24	TRP	CG-CD2	-5.19	1.34	1.43
2	E	24	TRP	CD1-NE1	-5.02	1.29	1.38

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	162	ALA	O-C-N	25.37	163.29	122.70
2	F	162	ALA	C-N-CA	-21.22	68.66	121.70
2	E	68	ASP	C-N-CA	18.52	168.01	121.70
2	F	162	ALA	CA-C-N	-17.98	77.66	117.20
2	E	121	ARG	NE-CZ-NH1	17.79	129.19	120.30
2	E	121	ARG	NE-CZ-NH2	-14.22	113.19	120.30
2	E	68	ASP	CB-CA-C	-13.36	83.67	110.40
1	A	41	TRP	CD1-CG-CD2	11.22	115.28	106.30
2	E	24	TRP	CD1-CG-CD2	10.11	114.39	106.30
1	B	8	SER	CB-CA-C	9.21	127.60	110.10
1	C	71	VAL	CG1-CB-CG2	-9.12	96.30	110.90
1	C	78	TYR	CB-CG-CD1	-8.99	115.61	121.00
2	E	69	VAL	N-CA-CB	8.96	131.21	111.50
2	E	110	ASP	N-CA-CB	8.85	126.53	110.60
1	B	79	TRP	CD1-CG-CD2	8.82	113.36	106.30
2	F	163	ARG	N-CA-CB	8.81	126.46	110.60
2	E	105	TRP	CD1-CG-CD2	8.79	113.33	106.30
1	B	79	TRP	CG-CD2-CE3	8.70	141.73	133.90
2	F	163	ARG	CB-CA-C	-8.65	93.10	110.40
1	C	79	TRP	CG-CD2-CE3	8.61	141.65	133.90
1	C	41	TRP	CD1-CG-CD2	8.59	113.17	106.30
2	E	91	TRP	CD1-CG-CD2	8.57	113.16	106.30
2	F	91	TRP	CD1-CG-CD2	8.33	112.96	106.30
1	B	41	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	A	41	TRP	CG-CD1-NE1	-8.26	101.84	110.10
1	C	105	TYR	N-CA-CB	-8.25	95.74	110.60
1	B	104	ARG	NE-CZ-NH2	8.25	124.42	120.30
1	A	103	ARG	N-CA-CB	-8.23	95.79	110.60
2	E	24	TRP	CE2-CD2-CG	-8.14	100.79	107.30
1	C	79	TRP	CD1-CG-CD2	7.93	112.65	106.30
2	E	2	ARG	NE-CZ-NH2	-7.92	116.34	120.30
2	F	121	ARG	NE-CZ-NH2	-7.87	116.36	120.30
2	E	152	VAL	CA-CB-CG2	-7.80	99.20	110.90
2	E	88	MET	CA-CB-CG	-7.70	100.21	113.30
2	F	91	TRP	CE2-CD2-CG	-7.70	101.14	107.30
2	F	163	ARG	NE-CZ-NH2	7.58	124.09	120.30
2	F	174	CYS	CA-CB-SG	7.58	127.64	114.00
2	E	91	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	C	79	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	D	103	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	B	79	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	D	127	GLU	CA-CB-CG	-7.36	97.22	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	A	103	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	B	79	TRP	CB-CG-CD1	-7.27	117.55	127.00
2	F	24	TRP	CD1-CG-CD2	7.20	112.06	106.30
2	E	118	TYR	CB-CG-CD2	-7.17	116.70	121.00
2	E	105	TRP	CE2-CD2-CG	-7.17	101.56	107.30
2	E	60	ARG	NE-CZ-NH2	7.14	123.87	120.30
2	E	62	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	A	41	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	C	116	TYR	CB-CG-CD2	-7.11	116.74	121.00
2	E	67	TRP	CB-CA-C	-7.02	96.36	110.40
1	C	103	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	126	LYS	CA-C-N	-7.00	101.80	117.20
1	C	79	TRP	CB-CG-CD1	-6.97	117.94	127.00
2	E	99	LYS	N-CA-CB	-6.96	98.08	110.60
2	F	78	THR	CA-CB-CG2	-6.95	102.67	112.40
1	D	104	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	C	41	TRP	CE2-CD2-CG	-6.91	101.78	107.30
2	E	72	ASP	CB-CA-C	-6.87	96.65	110.40
2	F	60	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	C	8	SER	CA-C-N	6.84	132.24	117.20
1	B	41	TRP	CE2-CD2-CG	-6.74	101.91	107.30
2	F	162	ALA	CB-CA-C	-6.73	100.00	110.10
2	E	131	ASP	CA-C-N	6.73	132.00	117.20
2	E	24	TRP	CG-CD1-NE1	-6.71	103.39	110.10
1	D	34	ARG	NE-CZ-NH2	6.70	123.65	120.30
2	E	1	GLU	O-C-N	6.70	133.41	122.70
2	E	111	TYR	O-C-N	-6.69	111.99	122.70
2	F	6	VAL	CG1-CB-CG2	-6.66	100.24	110.90
2	E	166	ARG	NE-CZ-NH1	6.65	123.63	120.30
2	F	152	VAL	CA-CB-CG2	-6.64	100.94	110.90
2	F	91	TRP	CB-CG-CD1	-6.62	118.39	127.00
2	F	57	ALA	CB-CA-C	-6.56	100.26	110.10
1	D	21	ARG	NE-CZ-NH2	6.55	123.57	120.30
2	F	91	TRP	CG-CD2-CE3	6.55	139.79	133.90
2	E	24	TRP	CB-CG-CD1	-6.54	118.50	127.00
2	E	155	ARG	NE-CZ-NH2	6.53	123.56	120.30
2	E	165	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	A	126	LYS	O-C-N	6.50	133.09	122.70
2	F	24	TRP	CE2-CD2-CG	-6.48	102.12	107.30
1	C	102	PRO	CA-N-CD	-6.44	102.48	111.50
2	F	105	TRP	CD1-CG-CD2	6.41	111.43	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	GLY	N-CA-C	-6.40	97.09	113.10
2	E	39	ASP	CA-CB-CG	6.39	127.45	113.40
2	E	44	GLU	CA-CB-CG	-6.28	99.58	113.40
2	F	64	LEU	O-C-N	-6.26	112.68	122.70
1	B	8	SER	O-C-N	6.24	132.68	122.70
2	E	93	VAL	CB-CA-C	-6.20	99.63	111.40
1	C	34	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	B	97	ALA	O-C-N	6.14	132.53	122.70
2	E	67	TRP	N-CA-CB	6.13	121.64	110.60
2	E	153	ARG	NE-CZ-NH2	6.11	123.35	120.30
2	F	62	ARG	NE-CZ-NH2	6.07	123.33	120.30
2	E	105	TRP	CG-CD1-NE1	-6.06	104.04	110.10
1	C	119	THR	O-C-N	6.03	132.34	122.70
2	E	88	MET	CA-C-N	6.01	130.42	117.20
2	E	160	CYS	CA-CB-SG	-6.01	103.19	114.00
1	A	55	LEU	O-C-N	-6.00	113.10	122.70
2	E	144	PHE	CB-CG-CD2	-6.00	116.60	120.80
1	D	111	LEU	O-C-N	6.00	132.30	122.70
1	B	126	LYS	CA-C-N	-5.98	104.04	117.20
2	F	2	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	C	97	ALA	O-C-N	5.93	132.19	122.70
1	A	116	TYR	CB-CG-CD2	-5.93	117.44	121.00
2	E	25	TYR	CB-CG-CD1	-5.93	117.44	121.00
2	F	121	ARG	CA-CB-CG	-5.92	100.39	113.40
1	D	43	PRO	O-C-N	5.91	132.16	122.70
2	E	111	TYR	CA-C-N	5.89	130.16	117.20
2	F	144	PHE	CB-CG-CD2	-5.88	116.68	120.80
1	D	13	MET	CB-CG-SD	-5.87	94.79	112.40
1	C	126	LYS	CA-C-N	-5.87	104.29	117.20
2	E	72	ASP	N-CA-CB	5.85	121.12	110.60
2	F	145	SER	N-CA-CB	-5.84	101.74	110.50
2	E	152	VAL	CA-CB-CG1	5.83	119.65	110.90
1	C	79	TRP	CG-CD1-NE1	-5.82	104.28	110.10
2	E	131	ASP	O-C-N	-5.81	113.40	122.70
2	E	99	LYS	N-CA-C	5.81	126.68	111.00
1	B	8	SER	CA-C-N	-5.77	104.51	117.20
2	E	1	GLU	CA-C-N	-5.77	104.51	117.20
1	A	94	VAL	CA-CB-CG1	-5.75	102.28	110.90
1	C	41	TRP	CE2-CD2-CE3	5.75	125.59	118.70
1	B	79	TRP	CG-CD1-NE1	-5.73	104.37	110.10
1	A	86	PRO	CA-N-CD	-5.71	103.51	111.50
2	E	158	GLU	CA-CB-CG	-5.68	100.91	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	TYR	CG-CD2-CE2	-5.64	116.79	121.30
1	C	110	LEU	O-C-N	5.63	131.71	122.70
1	C	29	ALA	CA-C-N	-5.61	104.86	117.20
2	E	16	ASP	CB-CG-OD1	5.60	123.34	118.30
2	E	45	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	C	20	VAL	CG1-CB-CG2	-5.57	101.99	110.90
2	F	133	TYR	CA-CB-CG	5.57	123.98	113.40
2	F	152	VAL	CA-CB-CG1	5.56	119.24	110.90
2	E	91	TRP	CG-CD1-NE1	-5.55	104.55	110.10
2	F	105	TRP	CE2-CD2-CG	-5.55	102.86	107.30
2	E	67	TRP	CB-CG-CD2	-5.54	119.39	126.60
1	C	103	ARG	N-CA-C	5.51	125.88	111.00
2	F	116	VAL	CB-CA-C	-5.51	100.93	111.40
2	F	121	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	71	VAL	CA-CB-CG2	-5.50	102.66	110.90
2	E	85	LYS	CB-CG-CD	-5.50	97.31	111.60
2	F	136	VAL	N-CA-C	-5.48	96.19	111.00
1	D	67	GLY	O-C-N	5.48	131.46	122.70
2	F	138	ALA	CB-CA-C	-5.45	101.92	110.10
1	A	33	PHE	CB-CG-CD2	-5.45	116.99	120.80
1	A	10	CYS	CA-CB-SG	5.44	123.79	114.00
1	C	119	THR	CA-C-N	-5.41	105.30	117.20
2	F	91	TRP	CG-CD1-NE1	-5.40	104.70	110.10
2	F	128	THR	CA-CB-CG2	-5.39	104.86	112.40
1	D	10	CYS	N-CA-C	-5.38	96.46	111.00
2	E	101	ASN	N-CA-C	-5.38	96.47	111.00
1	B	84	ILE	CG1-CB-CG2	-5.38	99.56	111.40
1	A	119	THR	CA-CB-CG2	5.33	119.87	112.40
2	E	24	TRP	CG-CD2-CE3	5.33	138.69	133.90
1	D	121	VAL	N-CA-C	-5.32	96.64	111.00
2	F	23	THR	CA-C-N	5.32	128.90	117.20
1	B	8	SER	N-CA-C	5.29	125.27	111.00
2	F	11	VAL	CG1-CB-CG2	5.28	119.34	110.90
2	F	87	LYS	CA-CB-CG	-5.23	101.90	113.40
1	B	10	CYS	CB-CA-C	5.21	120.83	110.40
1	B	20	VAL	CG1-CB-CG2	-5.20	102.58	110.90
2	F	142	SER	N-CA-CB	-5.20	102.70	110.50
1	A	102	PRO	CA-N-CD	-5.19	104.23	111.50
1	B	36	ALA	CB-CA-C	5.18	117.87	110.10
2	F	23	THR	O-C-N	-5.18	114.42	122.70
2	F	57	ALA	N-CA-CB	5.16	117.32	110.10
1	D	10	CYS	CA-CB-SG	5.12	123.21	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	133	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	A	41	TRP	CD1-NE1-CE2	5.10	113.59	109.00
1	B	41	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	B	71	VAL	CA-CB-CG1	5.08	118.53	110.90
2	E	67	TRP	CA-CB-CG	5.08	123.36	113.70
2	E	120	CYS	CA-CB-SG	-5.08	104.85	114.00
2	E	53	MET	CA-CB-CG	5.07	121.92	113.30
2	E	119	SER	CA-C-N	-5.06	106.07	117.20
2	E	91	TRP	CG-CD2-CE3	5.06	138.45	133.90
2	E	138	ALA	CB-CA-C	-5.06	102.51	110.10
1	B	71	VAL	CG1-CB-CG2	-5.05	102.81	110.90
2	F	14	ASN	N-CA-C	5.05	124.64	111.00
1	C	103	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	F	93	VAL	CA-CB-CG1	-5.02	103.38	110.90
1	D	126	LYS	CA-C-N	-5.01	106.17	117.20
1	C	84	ILE	CG1-CB-CG2	-5.01	100.39	111.40

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	53	0
1	D	930	0	908	103	5
2	E	1411	0	1334	69	0
2	F	1411	0	1334	58	0
3	E	21	0	27	16	0
3	F	21	0	27	7	0
All	All	6624	0	6386	372	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 (372) 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:CA	2:E:69:VAL:N	1.70	1.51
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	1.05
1:B:66:GLU:CG	1:B:98:ASN:O	2.10	1.00
2:E:64:LEU:C	2:E:66:ASN:H	1.61	0.97
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: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:H181	3:E:176:REA:C8	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
1:B:100:SER:C	1:B:102:PRO:CD	2.39	0.90
2:F:73:MET:HG3	3:F:177:REA:H10	1.54	0.89
3:E:176:REA:C18	3:E:176:REA:C8	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: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
1:D:100:SER:C	1:D:102:PRO:HD3	1.99	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:HA	1:D:103:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:103:ARG:NH1	1:C:103:ARG:HA	2.01	0.75
1:C:30:VAL:HB	1:C:55:LEU:HD12	1.67	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:68:ILE:O	1:D:68:ILE:HG22	1.87	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:C:98:ASN:H	1:C:98:ASN:ND2	1.87	0.72
1:C:98:ASN:HB3	1:C:103:ARG:NH2	2.04	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:100:SER:C	1:D:102:PRO:CD	2.59	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:97:ALA:HB3	1:C:98:ASN:HD22	1.54	0.70
1:C:14:VAL:HG21	1:C:71:VAL:HG11	1.72	0.70
1:A:33:PHE:HD2	1:A:41:TRP:HB3	1.57	0.69
2:E:29:LYS:HZ2	2:E:166:ARG:HE	1.41	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
2:F:64:LEU:C	2:F:66:ASN:H	1.97	0.67
1:D:103:ARG:HA	1:D:103:ARG:HH11	1.58	0.67
2:E:27:MET:HE1	2:E:143:GLY:HA2	1.77	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
2:E:37:LEU:HD23	3:E:176:REA:H12	1.77	0.66
1:A:27:ASN:ND2	1:A:48:LYS:HD3	2.09	0.66
2:F:110:ASP:O	2:F:112:GLU:N	2.24	0.66
1:D:84:ILE:O	1:D:86:PRO:HD3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:98:GLN:NE2	3:E:176:REA:H202	2.10	0.65
1:A:13:MET:SD	1:A:56:HIS:CE1	2.89	0.65
2:F:37:LEU:HA	2:F:61:VAL:HG13	1.79	0.65
1:A:32:VAL:HG21	1:A:58:LEU:HD13	1.78	0.64
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
2:F:118:TYR:HE1	2:F:161:LEU:HD21	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
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:N	1:C:98:ASN:ND2	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:D:97:ALA:HB1	1:D:105:TYR:CE1	2.36	0.60
1:C:11:PRO:HB2	1:C:64:PHE:CD2	2.36	0.60
1:A:30:VAL:HB	1:A:55:LEU:HD12	1.82	0.60
1:D:65:VAL:C	1:D:66:GLU:HG3	2.22	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
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:93:VAL:HG11	1:D:107:ILE:HG12	1.83	0.59
1:D:30:VAL:HB	1:D:55:LEU:CD1	2.32	0.59
1:B:35:LYS:HZ3	1:B:39:ASP:HA	1.68	0.59
1:B:93:VAL:HG21	1:B:107:ILE:HG21	1.85	0.58
1:D:30:VAL:HG22	1:D:73:ILE:HG12	1.85	0.58
1:C:93:VAL:HG11	1:C:107:ILE:HG13	1.85	0.58
2:E:103:ASP:O	2:E:119:SER:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:D:97:ALA:CB	1:D:105:TYR:CZ	2.87	0.57
1:D:35:LYS:HB3	1:D:68:ILE:CG2	2.34	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:B:100:SER:C	1:B:102:PRO:HD2	2.26	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:D:97:ALA:HA	1:D:105:TYR:OH	2.06	0.55
1:A:113:PRO:HB2	1:A:114:TYR:CD1	2.41	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:CZ	1:C:103:ARG:HA	2.36	0.55
3:F:177:REA:C8	3:F:177:REA:H171	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:E:64:LEU:C	2:E:66:ASN:N	2.31	0.55
2:E:148:VAL:HA	2:E:151:ILE:HD12	1.88	0.55
1:C:41:TRP:CH2	1:C:68:ILE:HG22	2.42	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
3:E:176:REA:H182	3:E:176:REA:H8	1.86	0.54
1:A:113:PRO:HG2	1:D:20:VAL:O	2.08	0.54
2:F:60:ARG:HG3	2:F:173:TYR:CD2	2.42	0.54
1:B:32:VAL:HG22	1:B:71:VAL:HG22	1.89	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:D:11:PRO:HB2	1:D:64:PHE:HD2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ALA:HA	1:C:78:TYR:OH	2.09	0.53
1:D:97:ALA:O	1:D:98:ASN:HB2	2.08	0.52
1:A:103:ARG:H	1:A:125:PRO:HD3	1.73	0.52
2:F:110:ASP:C	2:F:112:GLU:H	2.11	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
2:F:155:ARG:HA	2:F:158:GLU:HG3	1.92	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
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:A:11:PRO:HB2	1:A:64:PHE:CD2	2.44	0.52
1:B:11:PRO:HB2	1:B:59:THR:HG23	1.92	0.51
1:B:35:LYS:NZ	1:B:39:ASP:HA	2.25	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
2:E:29:LYS:HB3	2:E:168:ILE:HD11	1.92	0.51
1:D:12:LEU:HD12	1:D:13:MET:H	1.75	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:D:98:ASN:HA	1:D:103:ARG:HH12	1.73	0.50
1:D:98:ASN:HA	1:D:103:ARG:CZ	2.42	0.50
3:F:177:REA:C17	3:F:177:REA:C8	2.90	0.50
1:B:64:PHE:HD1	1:B:69:TYR:CZ	2.30	0.50
1:A:41:TRP:CH2	1:A:68:ILE:HG22	2.46	0.50
2:E:114:PHE:HD2	2:E:152:VAL:CG2	2.25	0.50
2:E:13:GLU:HG2	2:E:14:ASN:HB2	1.94	0.50
2:F:161:LEU:O	2:F:165:TYR:CE1	2.64	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
1:D:84:ILE:HG13	2:F:67:TRP:HB3	1.93	0.50
1:C:16:VAL:CG1	1:C:111:LEU:HD12	2.41	0.50
2:E:109:THR:CG2	2:E:109:THR:O	2.58	0.50
2:F:64:LEU:C	2:F:66:ASN:N	2.65	0.50
1:B:75:THR:HG22	1:B:111:LEU:HD21	1.94	0.50
2:F:15:PHE:HE1	2:F:106:ILE:HG21	1.76	0.49
2:E:4:CYS:O	2:E:128:THR:HA	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:168:ILE:HG22	2:F:170:HIS:NE2	2.27	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:B:29:ALA:HB1	1:B:31:HIS:HE1	1.77	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: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
1:A:32:VAL:HG22	1:A:71:VAL:HG22	1.94	0.49
2:F:168:ILE:HG22	2:F:170:HIS:CD2	2.48	0.49
1:D:64:PHE:HB3	1:D:98:ASN:HD21	1.78	0.49
1:C:64:PHE:HD1	1:C:69:TYR:CZ	2.30	0.49
1:B:84:ILE:CG2	2:E:96:PHE:HB2	2.43	0.49
1:D:32:VAL:HG22	1:D:71:VAL:CG2	2.43	0.48
2:F:78:THR:O	2:F:86:PHE:HB3	2.14	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:E:98:GLN:NE2	3:E:176:REA:C20	2.77	0.48
2:E:37:LEU:HD21	3:E:176:REA:H10	1.95	0.48
2:E:107:ILE:HG22	2:E:155:ARG:CZ	2.43	0.48
2:E:6:VAL:HA	2:E:9:PHE:CD2	2.48	0.48
1:B:104:ARG:HB3	1:B:123:THR:O	2.13	0.48
1:A:29:ALA:HB1	1:A:31:HIS:HE1	1.78	0.48
1:D:28:VAL:O	1:D:48:LYS:HA	2.14	0.48
2:F:6:VAL:O	2:F:6:VAL:HG12	2.12	0.48
1:C:32:VAL:HG22	1:C:71:VAL:HG22	1.96	0.48
1:B:97:ALA:O	1:B:99:ASP:N	2.47	0.48
1:A:55:LEU:HD22	1:A:58:LEU:HG	1.96	0.47
2:E:57:ALA:HB2	3:E:176:REA:H41	1.94	0.47
1:D:73:ILE:O	1:D:90:HIS:HB2	2.14	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: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:D:64:PHE:CD1	1:D:98:ASN:ND2	2.82	0.47
1:D:65:VAL:CG2	1:D:66:GLU:N	2.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:38:GLN:OE1	2:E:61:VAL:HA	2.15	0.47
1:B:25:ALA:HA	1:B:78:TYR:OH	2.15	0.47
2:E:29:LYS:HZ2	2:E:166:ARG:NE	2.08	0.46
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:117:GLN:O	2:F:134:SER:HA	2.15	0.46
2:F:77:PHE:CE2	2:F:104:HIS:CD2	3.03	0.46
1:C:95:PHE:CE2	1:C:105:TYR:CD2	3.03	0.46
1:C:71:VAL:O	1:C:92:GLU:HA	2.16	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
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
2:E:37:LEU:CD2	3:E:176:REA:C12	2.83	0.46
1:A:9:LYS:HA	1:A:104:ARG:CZ	2.46	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
2:F:107:ILE:HD11	2:F:118:TYR:HB2	1.97	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
1:B:75:THR:O	1:B:78:TYR:HB3	2.16	0.46
1:B:31:HIS:CD2	1:B:46:SER:OG	2.69	0.46
1:A:93:VAL:HG21	1:A:107:ILE:HG21	1.98	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:D:103:ARG:O	1:D:105:TYR:HD1	1.98	0.45
1:D:65:VAL:C	1:D:66:GLU:CG	2.85	0.45
1:D:66:GLU:O	1:D:98:ASN:CB	2.62	0.45
2:E:37:LEU:HD21	3:E:176:REA:C12	2.46	0.45
1:C:64:PHE:CD1	1:C:69:TYR:CZ	3.05	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:146:PRO:HA	2:F:149:GLN:HB3	1.98	0.45
2:F:114:PHE:HB2	2:F:144:PHE:HE2	1.81	0.45
2:E:19:ARG:O	2:E:111:TYR:HB3	2.16	0.45
2:E:37:LEU:HA	2:E:61:VAL:CG1	2.47	0.45
1:D:16:VAL:HB	1:D:25:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:ASP:HB3	2:E:89:LYS:HZ1	1.82	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: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:F:27:MET:HE1	2:F:143:GLY:HA2	1.99	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
2:F:88:MET:HE3	3:F:177:REA:H183	2.00	0.44
1:B:41:TRP:O	1:B:43:PRO:HD3	2.18	0.44
1:C:29:ALA:HA	1:C:47:GLY:O	2.17	0.44
1:D:125:PRO:HG2	1:D:127:GLU:OXT	2.18	0.43
1:C:98:ASN:HA	1:C:103:ARG:HH12	1.82	0.43
1:C:79:TRP:HE1	1:C:111:LEU:HD22	1.83	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:C:13:MET:SD	1:C:13:MET:C	2.97	0.43
1:D:75:THR:O	1:D:78:TYR:N	2.51	0.43
1:A:93:VAL:HG21	1:A:107:ILE:CG2	2.49	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
3:E:176:REA:H192	3:E:176:REA:H7	1.33	0.43
2:E:110:ASP:CG	2:E:110:ASP:O	2.57	0.43
1:D:72:GLU:HA	1:D:91:ALA:O	2.19	0.43
1:D:93:VAL:HG11	1:D:107:ILE:CG1	2.49	0.43
1:D:35:LYS:HA	1:D:41:TRP:HA	2.01	0.43
1:D:107:ILE:N	1:D:107:ILE:HD12	2.34	0.43
1:D:80:LYS:C	1:D:82:LEU:H	2.22	0.43
1:D:32:VAL:HG22	1:D:71:VAL:HG23	2.01	0.43
2:F:27:MET:CE	2:F:143:GLY:HA2	2.48	0.43
1:D:64:PHE:CE1	1:D:69:TYR:CE2	3.06	0.43
1:B:64:PHE:CD1	1:B:69:TYR:CZ	3.07	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
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:B:84:ILE:HG23	2:E:96:PHE:HD2	1.84	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)
1:D:101:GLY:N	1:D:102:PRO:HD2	2.34	0.42
1:D:34:ARG:HB2	1:D:44:PHE:HB2	2.00	0.42
1:C:87:PHE:HD2	1:C:88:HIS:CE1	2.37	0.42
2:E:90:TYR:O	2:E:99:LYS:HA	2.19	0.42
1:A:102:PRO:HA	1:A:125:PRO:HD2	2.01	0.42
1:D:124:ASN:HA	1:D:125:PRO:HD2	1.78	0.42
1:D:65:VAL:O	1:D:66:GLU:HG2	2.18	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:D:66:GLU:CA	1:D:98:ASN:CB	2.95	0.42
1:B:114:TYR:N	1:B:114:TYR:CD1	2.87	0.42
2:E:107:ILE:HD11	2:E:118:TYR:CB	2.43	0.42
1:A:33:PHE:HB3	1:A:41:TRP:HE3	1.84	0.42
1:A:31:HIS:CD2	1:A:46:SER:OG	2.72	0.42
1:A:99:ASP:C	2:E:89:LYS:HZ3	2.23	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: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:C:98:ASN:O	1:C:99:ASP:C	2.58	0.42
2:F:6:VAL:HG21	2:F:120:CYS:SG	2.60	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:62:ARG:HH11	2:F:66:ASN:ND2	2.18	0.41
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
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
1:B:65:VAL:O	1:B:69:TYR:HE1	2.03	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:101:GLY:HA2	1:D:103:ARG:NH2	2.35	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
2:F:37:LEU:HD21	3:F:177:REA:C12	2.50	0.41
2:E:27:MET:CE	2:E:143:GLY:HA2	2.48	0.41
1:D:13:MET:SD	1:D:56:HIS:CE1	3.14	0.41
1:A:79:TRP:O	1:A:80:LYS:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ALA:HB1	1:C:98:ASN:ND2	2.30	0.40
2:F:112:GLU:H	2:F:112:GLU:HG2	1.70	0.40
1:C:34:ARG:HE	1:C:65:VAL:HG23	1.86	0.40
2:F:144:PHE:CD1	2:F:144:PHE:N	2.89	0.40
1:C:98:ASN:CB	1:C:103:ARG:NH2	2.82	0.40
1:C:76:LYS:HB2	1:C:76:LYS:HE3	1.92	0.40
1:D:114:TYR:CD1	1:D:114:TYR:N	2.90	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%)	5	26
1	B	118/127 (93%)	97 (82%)	16 (14%)	5 (4%)	3	19
1	C	121/127 (95%)	93 (77%)	23 (19%)	5 (4%)	3	20
1	D	118/127 (93%)	89 (75%)	21 (18%)	8 (7%)	1	8
2	E	172/174 (99%)	145 (84%)	20 (12%)	7 (4%)	3	20
2	F	172/174 (99%)	143 (83%)	24 (14%)	5 (3%)	6	29
All	All	822/856 (96%)	667 (81%)	121 (15%)	34 (4%)	3	20

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%)	87 (84%)	16 (16%)	3	14
1	B	101/105 (96%)	89 (88%)	12 (12%)	6	25
1	C	103/105 (98%)	83 (81%)	20 (19%)	2	7
1	D	101/105 (96%)	81 (80%)	20 (20%)	1	7
2	E	150/150 (100%)	123 (82%)	27 (18%)	2	10
2	F	150/150 (100%)	124 (83%)	26 (17%)	2	11
All	All	708/720 (98%)	587 (83%)	121 (17%)	2	11

All (121) 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	43	PRO
1	A	46	SER
1	A	56	HIS
1	A	63	GLN
1	A	64	PHE
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	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	94	VAL
1	B	113	PRO
1	B	119	THR
1	B	127	GLU

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Mol	Chain	Res	Type
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	64	PHE
1	C	66	GLU
1	C	70	LYS
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	27	ASN
1	D	34	ARG
1	D	40	THR
1	D	46	SER
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	94	VAL
1	D	98	ASN
1	D	103	ARG
1	D	113	PRO
1	D	119	THR
1	D	127	GLU
2	E	2	ARG
2	E	7	SER

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Mol	Chain	Res	Type
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	86	PHE
2	E	87	LYS
2	E	93	VAL
2	E	98	GLN
2	E	101	ASN
2	E	112	GLU
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	61	VAL
2	F	63	LEU
2	F	64	LEU
2	F	70	CYS
2	F	72	ASP
2	F	78	THR
2	F	86	PHE
2	F	95	SER
2	F	101	ASN
2	F	102	ASP
2	F	112	GLU
2	F	114	PHE
2	F	116	VAL

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Mol	Chain	Res	Type
2	F	123	LEU
2	F	132	SER
2	F	144	PHE
2	F	145	SER
2	F	152	VAL
2	F	154	GLN
2	F	158	GLU
2	F	161	LEU
2	F	164	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	31	HIS
1	B	27	ASN
1	B	31	HIS
1	B	90	HIS
1	C	27	ASN
1	C	31	HIS
1	C	98	ASN
1	D	56	HIS
1	D	98	ASN
2	E	40	ASN
2	E	98	GLN
2	E	124	ASN
2	E	156	GLN
2	F	66	ASN
2	F	101	ASN
2	F	104	HIS
2	F	117	GLN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	1.60	3 (14%)	27,28,30	6.09	21 (77%)
3	REA	F	177	-	21,21,22	1.85	5 (23%)	27,28,30	8.97	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	-	-	1/14/31/32	0/1/1/1
3	REA	F	177	-	-	1/14/31/32	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	177	REA	C11-C10	2.01	1.50	1.43
3	F	177	REA	C8-C7	2.28	1.39	1.33
3	F	177	REA	C11-C12	2.42	1.40	1.34
3	E	176	REA	C14-C13	2.43	1.39	1.35
3	E	176	REA	C10-C9	2.45	1.39	1.35
3	F	177	REA	C10-C9	3.69	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	176	REA	O1-C15	4.83	1.37	1.22
3	F	177	REA	O1-C15	5.41	1.38	1.22

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	177	REA	C18-C5-C6	-30.62	94.54	124.61
3	E	176	REA	C7-C8-C9	-12.79	106.73	126.22
3	F	177	REA	O1-C15-C14	-12.79	107.18	123.65
3	E	176	REA	C20-C13-C14	-11.16	106.41	122.90
3	E	176	REA	O1-C15-C14	-10.87	109.66	123.65
3	F	177	REA	C1-C6-C5	-10.19	107.69	122.66
3	F	177	REA	C20-C13-C14	-10.10	107.98	122.90
3	F	177	REA	C17-C1-C6	-9.75	95.02	110.30
3	F	177	REA	C7-C8-C9	-9.52	111.70	126.22
3	F	177	REA	C11-C10-C9	-9.00	114.20	127.20
3	E	176	REA	C11-C10-C9	-8.62	114.74	127.20
3	E	176	REA	C19-C9-C8	-8.45	104.03	118.10
3	F	177	REA	C12-C13-C14	-8.38	105.49	118.98
3	E	176	REA	C8-C7-C6	-7.05	106.15	127.32
3	F	177	REA	C19-C9-C8	-6.73	106.89	118.10
3	F	177	REA	C18-C5-C4	-5.98	102.08	113.43
3	F	177	REA	C20-C13-C12	-5.94	108.20	118.10
3	E	176	REA	C7-C6-C5	-5.65	108.43	121.37
3	E	176	REA	C8-C9-C10	-5.61	109.94	118.98
3	F	177	REA	C16-C1-C2	-5.38	89.53	108.79
3	E	176	REA	C1-C6-C5	-5.26	114.94	122.66
3	E	176	REA	C18-C5-C6	-5.03	119.67	124.61
3	E	176	REA	C10-C11-C12	-4.82	108.45	123.13
3	F	177	REA	C8-C9-C10	-4.33	112.01	118.98
3	E	176	REA	C11-C12-C13	-4.23	113.85	126.32
3	F	177	REA	C7-C6-C5	-3.88	112.49	121.37
3	E	176	REA	C12-C13-C14	-3.75	112.94	118.98
3	E	176	REA	C16-C1-C6	-3.70	104.50	110.30
3	F	177	REA	C11-C12-C13	-3.65	115.58	126.32
3	E	176	REA	C18-C5-C4	-3.58	106.64	113.43
3	F	177	REA	C8-C7-C6	-3.33	117.33	127.32
3	E	176	REA	C20-C13-C12	-2.77	113.48	118.10
3	E	176	REA	C16-C1-C2	-2.08	101.32	108.79
3	E	176	REA	C17-C1-C6	2.76	114.63	110.30
3	F	177	REA	C2-C1-C6	3.59	116.05	110.36
3	E	176	REA	C2-C1-C6	3.66	116.15	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	177	REA	C1-C6-C7	3.87	126.66	115.82
3	E	176	REA	C1-C6-C7	6.47	133.94	115.82
3	F	177	REA	C19-C9-C10	6.52	132.53	122.90
3	E	176	REA	C19-C9-C10	11.09	139.28	122.90
3	F	177	REA	C16-C1-C6	15.62	134.79	110.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	176	REA	O1-C15-C14-C13
3	F	177	REA	O1-C15-C14-C13

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	176	REA	16	0
3	F	177	REA	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.