



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:31 AM UTC

PDB ID : 2Q5E / pdb_00002q5e
Title : Crystal structure of human carboxy-terminal domain RNA polymerase II polypeptide A small phosphatase 2
Authors : Bonanno, J.B.; Dickey, M.; Bain, K.T.; Lau, C.; Romero, R.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-05-31
Resolution : 2.51 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

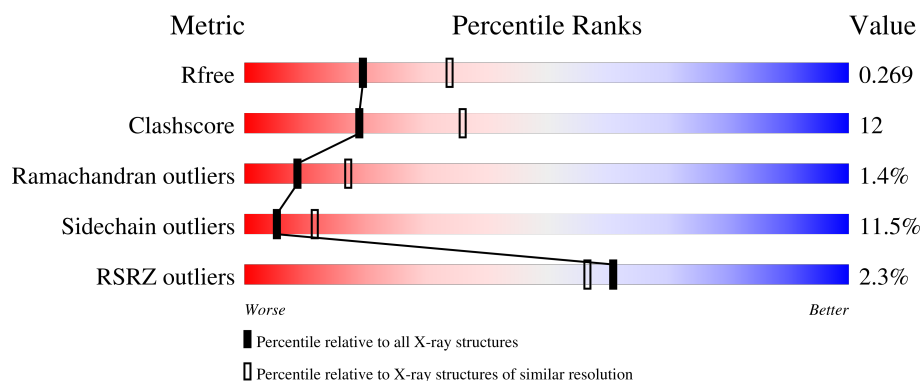
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	187	2% 68% 22% 6% • •
1	B	187	66% 24% 5% 5%
1	C	187	3% 68% 20% 6% • 5%
1	D	187	3% 67% 21% • • 6%
1	E	187	2% 60% 30% 5% •

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Mol	Chain	Length	Quality of chain
1	F	187	2% 56% 34% 5% 5%
1	G	187	5% 62% 28% 5%
1	H	187	% 66% 26% • • •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11566 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 Carboxy-terminal domain RNA polymerase II polypeptide A small phosphatase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1454	930	241	276	7			
1	B	178	Total	C	N	O	S	0	0	0
			1433	919	236	271	7			
1	C	178	Total	C	N	O	S	0	0	0
			1433	919	236	271	7			
1	D	175	Total	C	N	O	S	0	0	0
			1405	902	229	267	7			
1	E	179	Total	C	N	O	S	0	0	0
			1436	918	236	274	8			
1	F	178	Total	C	N	O	S	0	0	0
			1428	916	233	271	8			
1	G	179	Total	C	N	O	S	0	0	0
			1439	922	237	272	8			
1	H	179	Total	C	N	O	S	0	0	0
			1439	922	237	272	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	SER	-	cloning artifact	UNP O14595
A	86	LEU	-	cloning artifact	UNP O14595
B	85	SER	-	cloning artifact	UNP O14595
B	86	LEU	-	cloning artifact	UNP O14595
C	85	SER	-	cloning artifact	UNP O14595
C	86	LEU	-	cloning artifact	UNP O14595
D	85	SER	-	cloning artifact	UNP O14595
D	86	LEU	-	cloning artifact	UNP O14595
E	85	SER	-	cloning artifact	UNP O14595
E	86	LEU	-	cloning artifact	UNP O14595
F	85	SER	-	cloning artifact	UNP O14595
F	86	LEU	-	cloning artifact	UNP O14595

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Chain	Residue	Modelled	Actual	Comment	Reference
G	85	SER	-	cloning artifact	UNP O14595
G	86	LEU	-	cloning artifact	UNP O14595
H	85	SER	-	cloning artifact	UNP O14595
H	86	LEU	-	cloning artifact	UNP O14595

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	12	Total O 12 12	0	0
3	C	11	Total O 11 11	0	0
3	D	11	Total O 11 11	0	0
3	E	11	Total O 11 11	0	0
3	F	7	Total O 7 7	0	0
3	G	11	Total O 11 11	0	0

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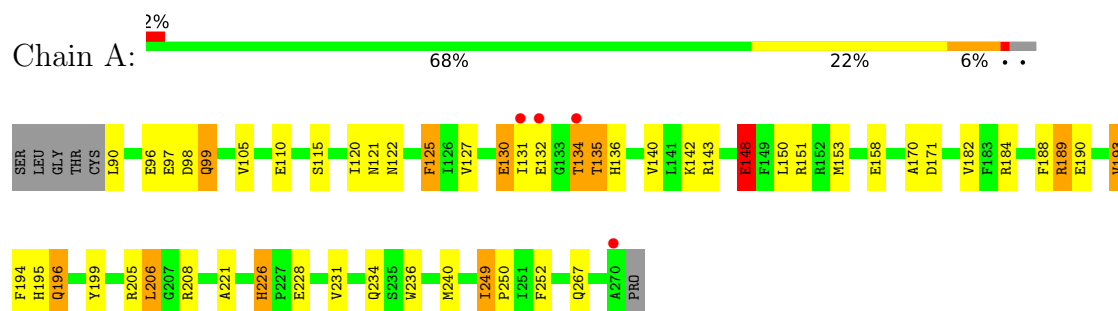
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	17	Total	O	0	0
			17	17		

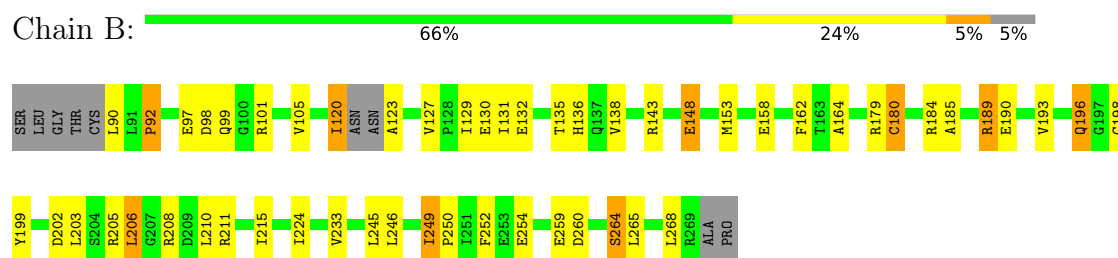
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

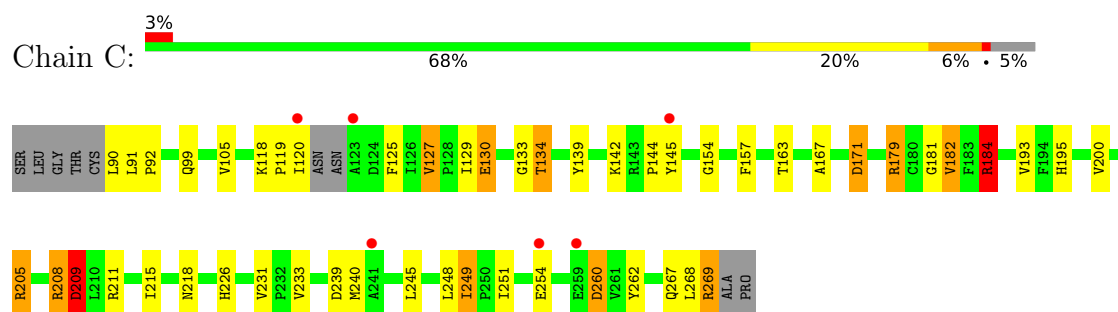
- Molecule 1: Carboxy-terminal domain RNA polymerase II polypeptide A small phosphatase 2



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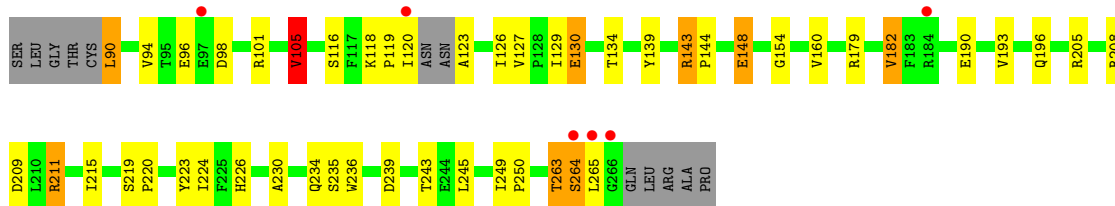


- Molecule 1: Carboxy-terminal domain RNA polymerase II polypeptide A small phosphatase 2

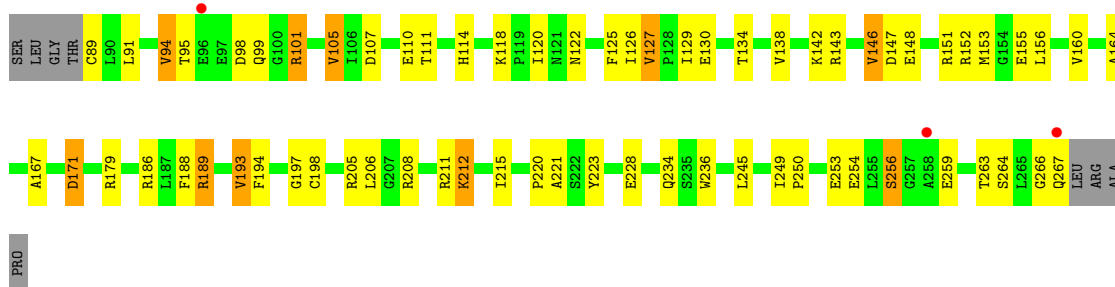


- Molecule 1: Carboxy-terminal domain RNA polymerase II polypeptide A small phosphatase 2

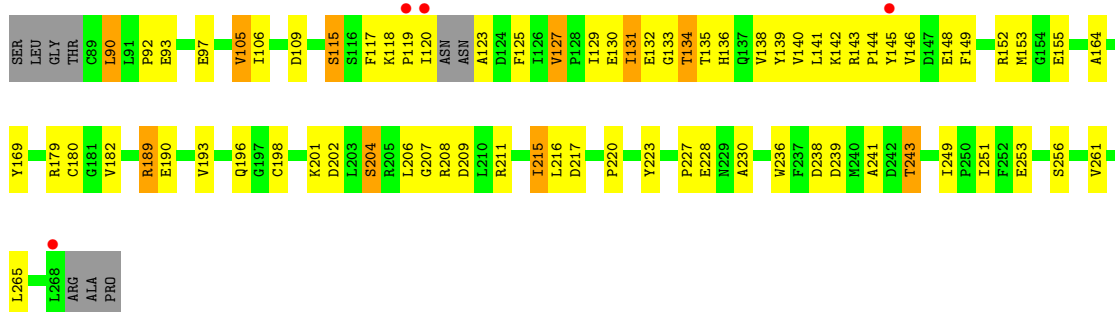




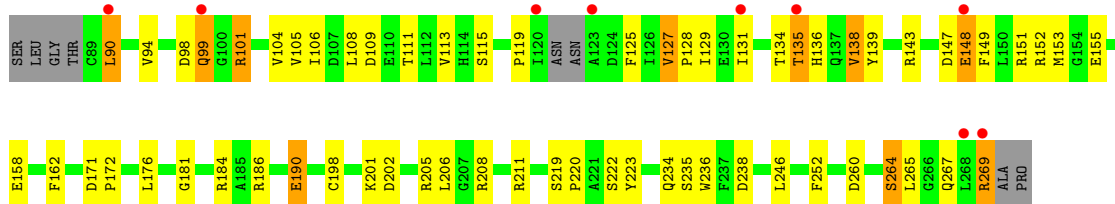
- Molecule 1: Carboxy-terminal domain RNA polymerase II polypeptide A small phosphatase 2



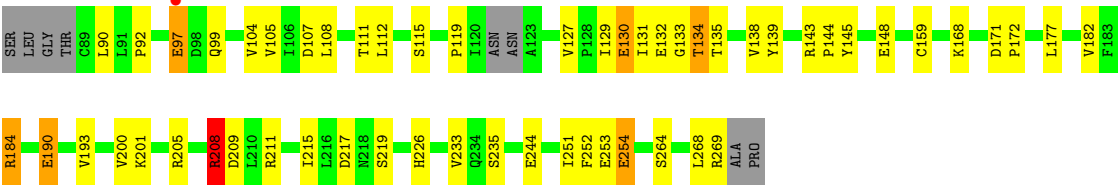
- Molecule 1: Carboxy-terminal domain RNA polymerase II polypeptide A small phosphatase 2



- Molecule 1: Carboxy-terminal domain RNA polymerase II polypeptide A small phosphatase 2



- Molecule 1: Carboxy-terminal domain RNA polymerase II polypeptide A small phosphatase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.64Å 117.64Å 170.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.51 20.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-2.51) 96.1 (20.00-2.51)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.278 0.211 , 0.269	Depositor DCC
R_{free} test set	3635 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11566	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.38	2/1485 (0.1%)	1.36	9/2018 (0.4%)
1	B	1.32	4/1463 (0.3%)	1.30	6/1986 (0.3%)
1	C	1.31	3/1463 (0.2%)	1.36	10/1986 (0.5%)
1	D	1.26	2/1435 (0.1%)	1.25	7/1949 (0.4%)
1	E	1.24	3/1467 (0.2%)	1.25	1/1994 (0.1%)
1	F	1.25	1/1458 (0.1%)	1.22	2/1980 (0.1%)
1	G	1.16	3/1469 (0.2%)	1.25	5/1994 (0.3%)
1	H	1.37	1/1469 (0.1%)	1.37	6/1994 (0.3%)
All	All	1.29	19/11709 (0.2%)	1.30	46/15901 (0.3%)

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	D	0	1
1	E	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	ILE	CA-CB	-10.51	1.48	1.54
1	E	221	ALA	CA-CB	-7.28	1.41	1.53
1	D	160	VAL	C-O	-6.94	1.16	1.24
1	G	198	CYS	CB-SG	-6.79	1.58	1.81
1	A	249	ILE	C-O	-6.65	1.19	1.24
1	E	127	VAL	CA-CB	6.49	1.62	1.54
1	G	138	VAL	CA-CB	6.16	1.61	1.54
1	B	233	VAL	N-CA	-5.96	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	230	ALA	CA-CB	-5.92	1.44	1.53
1	C	195	HIS	N-CA	-5.87	1.39	1.46
1	B	135	THR	CA-CB	5.77	1.61	1.53
1	F	134	THR	CA-CB	5.67	1.62	1.53
1	C	171	ASP	N-CA	-5.54	1.42	1.46
1	A	221	ALA	CA-CB	-5.52	1.44	1.53
1	H	104	VAL	CA-CB	5.37	1.60	1.54
1	C	157	PHE	CA-C	-5.31	1.46	1.52
1	G	104	VAL	CA-CB	-5.16	1.47	1.54
1	B	198	CYS	CB-SG	-5.10	1.64	1.81
1	E	198	CYS	CB-SG	-5.04	1.64	1.81

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	ILE	CA-C-N	-8.81	110.57	119.56
1	B	249	ILE	C-N-CA	-8.81	110.57	119.56
1	C	205	ARG	N-CA-C	-8.22	100.90	113.89
1	A	182	VAL	N-CA-C	7.85	119.57	110.62
1	H	99	GLN	N-CA-C	7.08	123.06	111.37
1	D	226	HIS	CA-C-N	-6.99	112.49	120.04
1	D	226	HIS	C-N-CA	-6.99	112.49	120.04
1	A	231	VAL	CB-CA-C	-6.82	104.60	111.08
1	G	151	ARG	N-CA-C	-6.48	103.50	111.40
1	B	268	LEU	N-CA-C	-6.42	103.34	112.13
1	B	259	GLU	N-CA-C	-6.24	106.20	113.88
1	D	129	ILE	CB-CA-C	6.14	118.70	110.42
1	D	126	ILE	N-CA-C	-6.10	98.69	107.78
1	C	249	ILE	N-CA-CB	5.98	114.52	110.52
1	C	91	LEU	CA-C-N	5.97	125.94	120.21
1	C	91	LEU	C-N-CA	5.97	125.94	120.21
1	C	208	ARG	N-CA-C	-5.92	100.06	109.23
1	A	226	HIS	CA-C-N	-5.89	113.61	119.56
1	A	226	HIS	C-N-CA	-5.89	113.61	119.56
1	A	135	THR	N-CA-C	5.86	118.36	107.99
1	D	143	ARG	N-CA-C	-5.85	101.70	110.24
1	H	208	ARG	CG-CD-NE	-5.79	99.27	112.00
1	D	179	ARG	N-CA-C	5.78	119.59	112.54
1	H	219	SER	CB-CA-C	-5.78	104.45	110.17
1	C	209	ASP	CB-CA-C	5.75	119.21	109.84
1	B	210	LEU	N-CA-C	-5.70	106.33	113.28
1	H	105	VAL	N-CA-CB	-5.66	104.59	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	181	GLY	N-CA-C	5.62	121.68	113.48
1	C	231	VAL	CA-C-N	5.55	125.56	119.90
1	C	231	VAL	C-N-CA	5.55	125.56	119.90
1	C	184	ARG	N-CA-C	-5.52	106.54	113.28
1	E	266	GLY	N-CA-C	-5.52	105.81	112.49
1	G	109	ASP	N-CA-C	5.46	118.39	110.42
1	A	122	ASN	N-CA-CB	-5.45	101.91	110.46
1	G	101	ARG	N-CA-C	5.39	118.03	109.24
1	G	113	VAL	N-CA-C	5.29	114.99	108.53
1	H	226	HIS	CA-C-N	-5.26	114.40	119.87
1	H	226	HIS	C-N-CA	-5.26	114.40	119.87
1	A	148	GLU	CA-CB-CG	5.23	124.56	114.10
1	B	180	CYS	N-CA-C	5.22	119.34	112.92
1	A	121	ASN	CA-C-N	5.21	131.74	122.06
1	A	121	ASN	C-N-CA	5.21	131.74	122.06
1	C	134	THR	N-CA-C	5.19	117.36	108.90
1	F	105	VAL	N-CA-CB	-5.14	104.98	111.46
1	D	105	VAL	N-CA-C	-5.13	100.17	107.77
1	F	207	GLY	N-CA-C	-5.12	108.00	115.63

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	263	THR	Peptide
1	E	89	CYS	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	1454	0	1431	36	0
1	B	1433	0	1413	31	0
1	C	1433	0	1413	31	1
1	D	1405	0	1381	24	0
1	E	1436	0	1407	36	0
1	F	1428	0	1405	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1439	0	1418	41	0
1	H	1439	0	1418	30	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	11	0	0	3	0
3	B	12	0	0	0	0
3	C	11	0	0	3	0
3	D	11	0	0	0	0
3	E	11	0	0	0	0
3	F	7	0	0	0	0
3	G	11	0	0	3	0
3	H	17	0	0	4	0
All	All	11566	0	11286	269	1

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 12.

All (269) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:ASP:O	1:E:101:ARG:HG3	1.59	1.02
1:G:147:ASP:HA	3:G:282:HOH:O	1.57	1.02
1:F:227:PRO:HD2	1:F:228:GLU:OE2	1.63	0.96
1:A:131:ILE:N	1:A:134:THR:O	1.98	0.95
1:H:264:SER:O	1:H:268:LEU:HD13	1.72	0.90
1:F:164:ALA:O	1:F:189:ARG:HD3	1.70	0.90
1:B:98:ASP:HA	1:B:101:ARG:HD2	1.57	0.86
1:E:164:ALA:O	1:E:189:ARG:HD3	1.79	0.82
1:G:152:ARG:NH1	1:G:155:GLU:OE1	2.14	0.80
1:C:92:PRO:O	1:C:208:ARG:NH2	2.14	0.80
1:F:143:ARG:CZ	1:F:236:TRP:HB2	2.15	0.77
1:E:98:ASP:HA	1:E:101:ARG:HD2	1.67	0.76
1:H:168:LYS:HD2	3:H:281:HOH:O	1.85	0.76
1:F:145:TYR:CE1	1:F:243:THR:HG22	2.21	0.75
1:D:148:GLU:N	1:D:148:GLU:OE2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ASP:OD2	1:D:211:ARG:NH1	2.21	0.73
1:E:171:ASP:OD1	1:E:186:ARG:NH1	2.21	0.73
1:A:98:ASP:OD2	3:A:279:HOH:O	2.07	0.73
1:E:143:ARG:O	1:E:146:VAL:HG12	1.89	0.73
1:E:107:ASP:O	1:E:111:THR:HB	1.88	0.72
1:C:144:PRO:O	1:C:145:TYR:HB2	1.90	0.72
1:A:130:GLU:HB2	1:A:135:THR:HG22	1.71	0.72
1:B:90:LEU:HB2	1:B:205:ARG:O	1.89	0.71
1:F:92:PRO:O	1:F:208:ARG:NH2	2.19	0.70
1:A:90:LEU:HB2	1:A:205:ARG:O	1.90	0.70
1:A:131:ILE:HG13	1:A:136:HIS:CD2	2.27	0.69
1:B:158:GLU:OE2	1:B:208:ARG:NH1	2.29	0.66
1:F:190:GLU:CD	1:F:190:GLU:H	2.04	0.66
1:F:209:ASP:OD2	1:F:211:ARG:NH1	2.28	0.66
1:E:253:GLU:O	1:E:256:SER:OG	2.14	0.66
1:G:190:GLU:OE2	3:G:274:HOH:O	2.14	0.65
1:A:130:GLU:OE1	1:A:135:THR:HG23	1.96	0.65
1:C:181:GLY:O	1:E:205:ARG:NH1	2.30	0.63
1:A:148:GLU:OE2	1:A:148:GLU:N	2.25	0.63
1:H:171:ASP:HB2	1:H:172:PRO:HD3	1.82	0.62
1:E:250:PRO:HA	1:E:253:GLU:HB2	1.82	0.61
1:H:131:ILE:O	1:H:132:GLU:C	2.42	0.61
1:A:130:GLU:HB2	1:A:135:THR:CG2	2.29	0.61
1:H:269:ARG:HG3	1:H:269:ARG:HH11	1.66	0.60
1:C:269:ARG:HH11	1:C:269:ARG:CG	2.15	0.60
1:C:226:HIS:HD2	3:C:272:HOH:O	1.83	0.60
1:H:168:LYS:CD	3:H:281:HOH:O	2.45	0.59
1:A:189:ARG:HD2	1:A:199:TYR:CZ	2.38	0.59
1:F:220:PRO:HA	1:F:223:TYR:CZ	2.38	0.59
1:B:131:ILE:HG13	1:B:136:HIS:CD2	2.37	0.58
1:C:90:LEU:HB2	1:C:205:ARG:O	2.03	0.58
1:C:125:PHE:CZ	1:C:142:LYS:HD3	2.39	0.58
1:E:152:ARG:NH1	1:E:155:GLU:OE1	2.35	0.58
1:H:209:ASP:OD2	1:H:211:ARG:NH1	2.36	0.58
1:E:101:ARG:NH2	1:E:155:GLU:O	2.37	0.58
1:D:263:THR:O	1:D:265:LEU:N	2.37	0.57
1:H:129:ILE:HD12	1:H:138:VAL:HG21	1.86	0.57
1:F:115:SER:HB3	1:F:140:VAL:HG22	1.85	0.57
1:B:202:ASP:HB3	1:B:205:ARG:HD2	1.87	0.57
1:D:143:ARG:HG3	1:D:236:TRP:CG	2.39	0.57
1:A:131:ILE:HG13	1:A:136:HIS:HD2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:ARG:HD2	1:F:155:GLU:OE1	2.05	0.57
1:F:118:LYS:O	1:F:120:ILE:HG23	2.06	0.56
1:G:101:ARG:NH1	1:G:184:ARG:NH2	2.53	0.56
1:G:115:SER:HB3	1:G:138:VAL:CG1	2.35	0.56
1:B:131:ILE:HG13	1:B:136:HIS:HD2	1.69	0.56
1:H:111:THR:HG23	1:H:233:VAL:HG11	1.87	0.56
1:C:184:ARG:O	1:E:193:VAL:HG23	2.06	0.56
1:F:201:LYS:NZ	1:F:217:ASP:OD2	2.33	0.56
1:G:264:SER:O	1:G:267:GLN:HG2	2.06	0.56
1:D:190:GLU:H	1:D:190:GLU:CD	2.13	0.56
1:G:220:PRO:HA	1:G:223:TYR:CZ	2.41	0.56
1:C:144:PRO:O	1:C:145:TYR:CB	2.54	0.55
1:F:180:CYS:HB2	1:F:182:VAL:HG23	1.89	0.55
1:C:154:GLY:HA3	1:C:182:VAL:HG22	1.87	0.55
1:G:171:ASP:OD1	1:G:186:ARG:NH1	2.38	0.55
1:E:94:VAL:HG22	1:E:95:THR:H	1.72	0.55
1:C:260:ASP:OD1	1:C:262:TYR:N	2.39	0.55
1:E:98:ASP:OD1	1:E:101:ARG:NH1	2.36	0.55
1:F:117:PHE:O	1:F:119:PRO:HD3	2.07	0.55
1:B:211:ARG:HG2	1:B:260:ASP:OD2	2.07	0.54
1:D:209:ASP:OD1	1:D:211:ARG:HB2	2.06	0.54
1:G:211:ARG:HG2	1:G:260:ASP:OD2	2.08	0.54
1:B:90:LEU:CB	1:B:205:ARG:O	2.54	0.54
1:F:143:ARG:NE	1:F:236:TRP:HB2	2.23	0.54
1:A:115:SER:OG	1:A:140:VAL:HG22	2.08	0.54
1:A:188:PHE:O	1:A:189:ARG:C	2.51	0.54
1:F:90:LEU:HD23	1:F:206:LEU:HD12	1.90	0.53
1:D:143:ARG:HG3	1:D:236:TRP:CD2	2.44	0.53
1:F:202:ASP:OD1	1:F:204:SER:OG	2.23	0.53
1:F:143:ARG:HG3	1:F:236:TRP:CG	2.44	0.53
1:H:201:LYS:NZ	1:H:217:ASP:OD2	2.38	0.53
1:A:130:GLU:HA	1:A:134:THR:O	2.09	0.53
1:B:105:VAL:HG13	1:B:162:PHE:CB	2.38	0.53
1:H:129:ILE:HD12	1:H:138:VAL:CG2	2.38	0.53
1:C:125:PHE:HZ	1:C:142:LYS:HD3	1.74	0.52
1:E:212:LYS:HZ3	1:E:259:GLU:HG2	1.74	0.52
1:A:96:GLU:O	1:A:99:GLN:HB2	2.08	0.52
1:E:194:PHE:CZ	1:E:197:GLY:N	2.73	0.52
1:G:131:ILE:HD12	1:G:136:HIS:CD2	2.44	0.52
1:G:101:ARG:HH12	1:G:184:ARG:NH2	2.08	0.52
1:G:147:ASP:CA	3:G:282:HOH:O	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:143:ARG:CZ	1:G:236:TRP:HB2	2.40	0.52
1:G:101:ARG:NH1	1:G:184:ARG:HH21	2.07	0.52
1:G:158:GLU:OE2	1:G:208:ARG:NH1	2.38	0.51
1:D:90:LEU:HB2	1:D:205:ARG:O	2.09	0.51
1:E:143:ARG:HD3	1:E:245:LEU:HG	1.91	0.51
1:G:131:ILE:HD12	1:G:136:HIS:HD2	1.76	0.51
1:B:264:SER:O	1:B:265:LEU:C	2.52	0.51
1:B:105:VAL:HG13	1:B:162:PHE:HB3	1.93	0.51
1:B:164:ALA:O	1:B:189:ARG:HD3	2.10	0.51
1:D:143:ARG:HD3	1:D:245:LEU:HG	1.92	0.51
1:H:269:ARG:HH11	1:H:269:ARG:CG	2.23	0.51
1:G:158:GLU:OE1	1:G:208:ARG:NH1	2.44	0.51
1:H:205:ARG:NE	3:H:279:HOH:O	2.41	0.50
1:G:153:MET:HE1	1:G:252:PHE:CD2	2.47	0.50
1:G:265:LEU:HB3	1:G:269:ARG:HH12	1.76	0.50
1:D:105:VAL:HG12	1:D:215:ILE:HG13	1.93	0.50
1:E:125:PHE:CZ	1:E:142:LYS:HD3	2.47	0.50
1:C:184:ARG:HD2	1:E:193:VAL:HA	1.93	0.50
1:F:120:ILE:CD1	1:F:141:LEU:HD11	2.41	0.50
1:B:189:ARG:HD2	1:B:199:TYR:CZ	2.46	0.50
1:G:148:GLU:OE2	1:G:148:GLU:N	2.41	0.50
1:A:131:ILE:O	1:A:134:THR:N	2.39	0.49
1:D:98:ASP:HA	1:D:101:ARG:HD2	1.95	0.49
1:E:143:ARG:CZ	1:E:236:TRP:HB2	2.43	0.49
1:A:125:PHE:CE2	1:A:142:LYS:HD2	2.48	0.49
1:A:193:VAL:HG23	1:A:194:PHE:N	2.28	0.49
1:G:158:GLU:CD	1:G:208:ARG:NH1	2.71	0.49
1:G:158:GLU:HG3	1:G:184:ARG:HG3	1.93	0.49
1:C:118:LYS:HB3	3:C:282:HOH:O	2.13	0.49
1:B:92:PRO:O	1:B:208:ARG:NH2	2.46	0.48
1:C:218:ASN:HA	1:C:233:VAL:O	2.13	0.48
1:H:190:GLU:CD	1:H:190:GLU:H	2.20	0.48
1:A:125:PHE:CZ	1:A:142:LYS:HD2	2.48	0.48
1:A:234:GLN:NE2	1:C:119:PRO:O	2.47	0.48
1:F:119:PRO:HA	1:F:139:TYR:CZ	2.48	0.48
1:A:110:GLU:OE2	3:A:275:HOH:O	2.20	0.48
1:F:143:ARG:HG3	1:F:236:TRP:CD2	2.49	0.48
1:G:202:ASP:HB3	1:G:205:ARG:HD2	1.94	0.48
1:A:148:GLU:H	1:A:148:GLU:CD	2.19	0.48
1:C:119:PRO:HA	1:C:139:TYR:CZ	2.49	0.48
1:E:129:ILE:HD12	1:E:138:VAL:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:GLY:HA3	1:C:182:VAL:CG2	2.44	0.47
1:F:123:ALA:HA	1:F:141:LEU:HD21	1.95	0.47
1:E:125:PHE:HZ	1:E:142:LYS:HD3	1.78	0.47
1:C:267:GLN:O	1:C:268:LEU:C	2.58	0.47
1:C:209:ASP:OD1	1:C:211:ARG:HB2	2.13	0.47
1:D:219:SER:HA	1:D:220:PRO:HD2	1.80	0.47
1:F:106:ILE:HG23	1:F:216:LEU:HD23	1.96	0.47
1:F:109:ASP:OD1	1:F:169:TYR:OH	2.32	0.47
1:A:105:VAL:HG21	1:A:206:LEU:HD21	1.96	0.47
1:C:269:ARG:HH11	1:C:269:ARG:HG2	1.80	0.47
1:F:120:ILE:HD11	1:F:141:LEU:HD11	1.97	0.47
1:A:226:HIS:HD2	3:A:274:HOH:O	1.98	0.46
1:G:115:SER:HB3	1:G:138:VAL:HG12	1.97	0.46
1:H:251:ILE:O	1:H:254:GLU:HB3	2.14	0.46
1:A:131:ILE:O	1:A:132:GLU:C	2.59	0.46
1:C:127:VAL:HG23	1:C:129:ILE:HD11	1.98	0.46
1:F:239:ASP:OD1	1:F:241:ALA:HB3	2.15	0.46
1:F:127:VAL:HG23	1:F:138:VAL:HB	1.97	0.46
1:H:112:LEU:O	1:H:143:ARG:HB3	2.15	0.46
1:E:110:GLU:OE2	1:E:114:HIS:ND1	2.43	0.46
1:E:153:MET:HB3	1:E:153:MET:HE3	1.81	0.45
1:H:119:PRO:HA	1:H:139:TYR:CE1	2.50	0.45
1:F:131:ILE:C	1:F:133:GLY:N	2.72	0.45
1:H:159:CYS:HB2	1:H:182:VAL:HG12	1.99	0.45
1:D:249:ILE:N	1:D:250:PRO:HD2	2.31	0.45
1:G:162:PHE:CD2	1:G:201:LYS:HG2	2.52	0.45
1:B:158:GLU:CD	1:B:208:ARG:NH1	2.75	0.45
1:C:130:GLU:O	1:C:130:GLU:HG3	2.17	0.45
1:E:105:VAL:HG22	1:E:160:VAL:HB	1.98	0.45
1:G:147:ASP:HB2	1:G:148:GLU:OE2	2.16	0.45
1:B:143:ARG:HD3	1:B:245:LEU:HG	1.98	0.45
1:B:203:LEU:O	1:B:206:LEU:HB2	2.16	0.45
1:F:115:SER:HA	1:F:139:TYR:O	2.17	0.45
1:B:164:ALA:O	1:B:189:ARG:HB2	2.16	0.45
1:D:120:ILE:HG13	1:D:123:ALA:HB2	1.99	0.45
1:F:227:PRO:CD	1:F:228:GLU:OE2	2.51	0.45
1:A:249:ILE:N	1:A:250:PRO:HD2	2.32	0.45
1:E:220:PRO:HA	1:E:223:TYR:CZ	2.51	0.45
1:C:254:GLU:HB3	1:C:268:LEU:HD11	1.99	0.44
1:C:118:LYS:O	1:C:120:ILE:HG23	2.16	0.44
1:E:167:ALA:HB2	1:E:188:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:TYR:HE1	1:F:243:THR:HG22	1.73	0.44
1:F:211:ARG:O	1:F:261:VAL:HG22	2.17	0.44
1:C:269:ARG:CG	1:C:269:ARG:NH1	2.81	0.44
1:B:249:ILE:O	1:B:250:PRO:C	2.59	0.44
1:B:127:VAL:CG2	1:B:138:VAL:HB	2.47	0.44
1:B:224:ILE:HG12	1:H:134:THR:HB	2.00	0.44
1:B:153:MET:HE1	1:B:252:PHE:CD2	2.52	0.44
1:B:196:GLN:HE22	1:D:190:GLU:HB2	1.82	0.44
1:E:249:ILE:N	1:E:250:PRO:HD2	2.33	0.44
1:H:97:GLU:H	1:H:97:GLU:HG3	1.58	0.44
1:A:90:LEU:HD22	1:A:205:ARG:HB3	1.99	0.44
1:G:119:PRO:HA	1:G:139:TYR:CZ	2.53	0.44
1:G:171:ASP:O	1:G:172:PRO:C	2.61	0.44
1:A:228:GLU:CD	1:A:228:GLU:H	2.26	0.43
1:B:158:GLU:HG3	1:B:184:ARG:HG3	1.99	0.43
1:D:119:PRO:HB3	1:D:139:TYR:CZ	2.53	0.43
1:D:143:ARG:HG2	1:D:144:PRO:HD2	2.00	0.43
1:G:98:ASP:O	1:G:101:ARG:HB2	2.18	0.43
1:A:143:ARG:CZ	1:A:236:TRP:HB2	2.48	0.43
1:H:144:PRO:O	1:H:145:TYR:HB2	2.18	0.43
1:G:149:PHE:O	1:G:153:MET:HG2	2.18	0.43
1:A:150:LEU:HD23	1:A:150:LEU:HA	1.85	0.43
1:G:148:GLU:H	1:G:148:GLU:CD	2.25	0.43
1:E:126:ILE:HA	1:E:138:VAL:O	2.17	0.43
1:H:130:GLU:OE1	1:H:133:GLY:CA	2.66	0.43
1:D:143:ARG:CZ	1:D:236:TRP:HB2	2.49	0.43
1:E:98:ASP:CA	1:E:101:ARG:HD2	2.44	0.43
1:F:215:ILE:HG23	1:F:230:ALA:HA	2.01	0.43
1:G:98:ASP:O	1:G:99:GLN:C	2.62	0.43
1:H:131:ILE:HD13	1:H:168:LYS:NZ	2.33	0.43
1:A:195:HIS:O	1:A:196:GLN:C	2.61	0.43
1:F:190:GLU:CD	1:F:190:GLU:N	2.75	0.43
1:H:130:GLU:OE1	1:H:133:GLY:HA2	2.19	0.42
1:B:246:LEU:HA	1:B:246:LEU:HD12	1.77	0.42
1:C:248:LEU:HA	1:C:251:ILE:HD12	1.99	0.42
1:F:131:ILE:HG13	1:F:136:HIS:HD2	1.84	0.42
1:F:149:PHE:HA	1:F:249:ILE:HD11	2.01	0.42
1:C:260:ASP:OD1	1:C:260:ASP:C	2.62	0.42
1:D:105:VAL:HG12	1:D:105:VAL:O	2.18	0.42
1:F:139:TYR:CD1	1:F:139:TYR:N	2.87	0.42
1:F:131:ILE:O	1:F:132:GLU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:PRO:O	1:H:208:ARG:NH2	2.37	0.42
1:B:101:ARG:NH1	1:B:184:ARG:HH21	2.17	0.42
1:D:94:VAL:O	1:D:94:VAL:HG13	2.19	0.42
1:F:220:PRO:HA	1:F:223:TYR:CE2	2.55	0.42
1:G:98:ASP:HA	1:G:101:ARG:HD2	2.01	0.42
1:G:119:PRO:HA	1:G:139:TYR:CE1	2.55	0.42
1:A:130:GLU:HA	1:A:135:THR:HA	2.01	0.42
1:B:148:GLU:CD	1:B:148:GLU:H	2.28	0.42
1:F:143:ARG:HG2	1:F:144:PRO:HD2	2.02	0.42
1:F:149:PHE:CE2	1:F:153:MET:HG3	2.55	0.42
1:G:129:ILE:O	1:G:135:THR:HA	2.20	0.41
1:B:105:VAL:HG13	1:B:162:PHE:HB2	2.01	0.41
1:C:167:ALA:O	1:C:171:ASP:HB2	2.20	0.41
1:C:226:HIS:CD2	3:C:272:HOH:O	2.65	0.41
1:H:252:PHE:O	1:H:253:GLU:C	2.59	0.41
1:E:147:ASP:O	1:E:151:ARG:HB2	2.20	0.41
1:H:184:ARG:O	1:H:184:ARG:HG2	2.20	0.41
1:A:170:ALA:HB3	1:A:188:PHE:CE2	2.56	0.41
1:B:105:VAL:CG1	1:B:162:PHE:HB3	2.49	0.41
1:D:220:PRO:HA	1:D:223:TYR:CZ	2.56	0.41
1:E:91:LEU:HD21	1:E:160:VAL:HG11	2.03	0.41
1:G:219:SER:O	1:G:222:SER:HB2	2.20	0.41
1:H:107:ASP:OD1	1:H:108:LEU:N	2.50	0.41
1:B:120:ILE:HG13	1:B:123:ALA:HB2	2.01	0.41
1:H:205:ARG:HD3	3:H:279:HOH:O	2.21	0.41
1:B:127:VAL:HG23	1:B:138:VAL:HB	2.03	0.41
1:E:94:VAL:HG22	1:E:95:THR:N	2.36	0.41
1:F:145:TYR:O	1:F:146:VAL:C	2.64	0.41
1:A:151:ARG:HH11	1:A:151:ARG:HD2	1.73	0.41
1:A:158:GLU:HG3	1:A:184:ARG:HG3	2.01	0.41
1:C:245:LEU:O	1:C:249:ILE:HG13	2.21	0.41
1:D:119:PRO:HA	1:D:139:TYR:CD1	2.55	0.41
1:G:264:SER:O	1:G:267:GLN:N	2.53	0.41
1:D:130:GLU:O	1:D:130:GLU:HG3	2.20	0.41
1:F:131:ILE:O	1:F:133:GLY:N	2.54	0.41
1:G:190:GLU:H	1:G:190:GLU:HG3	1.31	0.41
1:A:153:MET:HE1	1:A:252:PHE:CD2	2.56	0.41
1:D:154:GLY:HA3	1:D:182:VAL:HG22	2.02	0.41
1:G:127:VAL:HA	1:G:128:PRO:HD3	1.68	0.40
1:G:171:ASP:CB	1:G:172:PRO:CD	2.98	0.40
1:A:189:ARG:HD2	1:A:199:TYR:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:PRO:HA	1:F:139:TYR:CE2	2.56	0.40
1:E:264:SER:HA	1:E:267:GLN:HG2	2.04	0.40
1:F:131:ILE:HG13	1:F:136:HIS:CD2	2.57	0.40
1:E:152:ARG:HG2	1:E:249:ILE:CG2	2.52	0.40
1:E:156:LEU:HD13	1:E:256:SER:HB3	2.04	0.40
1:F:143:ARG:NH2	1:F:236:TRP:HB2	2.37	0.40
1:G:153:MET:HE3	1:G:153:MET:HB3	1.93	0.40
1:H:115:SER:HB3	1:H:138:VAL:CG1	2.52	0.40

All (1) 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:C:179:ARG:NH2	1:H:145:TYR:OH[4_455]	2.16	0.04

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	179/187 (96%)	166 (93%)	12 (7%)	1 (1%)	21	38
1	B	174/187 (93%)	161 (92%)	11 (6%)	2 (1%)	11	22
1	C	174/187 (93%)	158 (91%)	13 (8%)	3 (2%)	7	13
1	D	171/187 (91%)	156 (91%)	12 (7%)	3 (2%)	6	12
1	E	177/187 (95%)	157 (89%)	18 (10%)	2 (1%)	11	22
1	F	174/187 (93%)	158 (91%)	14 (8%)	2 (1%)	11	22
1	G	175/187 (94%)	159 (91%)	11 (6%)	5 (3%)	3	5
1	H	175/187 (94%)	169 (97%)	5 (3%)	1 (1%)	21	38
All	All	1399/1496 (94%)	1284 (92%)	96 (7%)	19 (1%)	9	17

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	264	SER
1	E	99	GLN
1	G	99	GLN
1	B	185	ALA
1	A	196	GLN
1	C	239	ASP
1	D	196	GLN
1	D	239	ASP
1	G	90	LEU
1	C	240	MET
1	E	94	VAL
1	F	238	ASP
1	G	238	ASP
1	H	190	GLU
1	B	92	PRO
1	G	108	LEU
1	G	264	SER
1	C	133	GLY
1	F	251	ILE

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	163/168 (97%)	147 (90%)	16 (10%)	7	16
1	B	161/168 (96%)	144 (89%)	17 (11%)	6	14
1	C	161/168 (96%)	146 (91%)	15 (9%)	8	18
1	D	158/168 (94%)	140 (89%)	18 (11%)	5	12
1	E	162/168 (96%)	138 (85%)	24 (15%)	3	6
1	F	161/168 (96%)	136 (84%)	25 (16%)	2	5
1	G	162/168 (96%)	145 (90%)	17 (10%)	6	14
1	H	162/168 (96%)	146 (90%)	16 (10%)	7	16
All	All	1290/1344 (96%)	1142 (88%)	148 (12%)	5	11

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

Mol	Chain	Res	Type
1	A	97	GLU
1	A	99	GLN
1	A	120	ILE
1	A	125	PHE
1	A	127	VAL
1	A	130	GLU
1	A	134	THR
1	A	148	GLU
1	A	171	ASP
1	A	189	ARG
1	A	190	GLU
1	A	193	VAL
1	A	206	LEU
1	A	208	ARG
1	A	240	MET
1	A	267	GLN
1	B	97	GLU
1	B	99	GLN
1	B	120	ILE
1	B	129	ILE
1	B	130	GLU
1	B	132	GLU
1	B	148	GLU
1	B	179	ARG
1	B	180	CYS
1	B	189	ARG
1	B	190	GLU
1	B	193	VAL
1	B	196	GLN
1	B	206	LEU
1	B	215	ILE
1	B	254	GLU
1	B	264	SER
1	C	99	GLN
1	C	105	VAL
1	C	127	VAL
1	C	130	GLU
1	C	134	THR
1	C	163	THR
1	C	179	ARG
1	C	182	VAL
1	C	184	ARG

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Mol	Chain	Res	Type
1	C	193	VAL
1	C	200	VAL
1	C	209	ASP
1	C	215	ILE
1	C	260	ASP
1	C	269	ARG
1	D	90	LEU
1	D	96	GLU
1	D	105	VAL
1	D	116	SER
1	D	118	LYS
1	D	127	VAL
1	D	130	GLU
1	D	134	THR
1	D	148	GLU
1	D	182	VAL
1	D	193	VAL
1	D	208	ARG
1	D	211	ARG
1	D	224	ILE
1	D	234	GLN
1	D	235	SER
1	D	243	THR
1	D	264	SER
1	E	101	ARG
1	E	105	VAL
1	E	118	LYS
1	E	120	ILE
1	E	122	ASN
1	E	127	VAL
1	E	130	GLU
1	E	134	THR
1	E	146	VAL
1	E	148	GLU
1	E	171	ASP
1	E	179	ARG
1	E	189	ARG
1	E	193	VAL
1	E	206	LEU
1	E	208	ARG
1	E	211	ARG
1	E	212	LYS

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Mol	Chain	Res	Type
1	E	215	ILE
1	E	228	GLU
1	E	234	GLN
1	E	254	GLU
1	E	256	SER
1	E	263	THR
1	F	90	LEU
1	F	93	GLU
1	F	97	GLU
1	F	105	VAL
1	F	115	SER
1	F	125	PHE
1	F	127	VAL
1	F	129	ILE
1	F	130	GLU
1	F	131	ILE
1	F	134	THR
1	F	135	THR
1	F	142	LYS
1	F	148	GLU
1	F	179	ARG
1	F	189	ARG
1	F	193	VAL
1	F	196	GLN
1	F	198	CYS
1	F	204	SER
1	F	215	ILE
1	F	243	THR
1	F	253	GLU
1	F	256	SER
1	F	265	LEU
1	G	90	LEU
1	G	94	VAL
1	G	105	VAL
1	G	106	ILE
1	G	111	THR
1	G	125	PHE
1	G	127	VAL
1	G	134	THR
1	G	135	THR
1	G	148	GLU
1	G	176	LEU

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Mol	Chain	Res	Type
1	G	190	GLU
1	G	206	LEU
1	G	234	GLN
1	G	235	SER
1	G	246	LEU
1	G	269	ARG
1	H	90	LEU
1	H	97	GLU
1	H	127	VAL
1	H	130	GLU
1	H	134	THR
1	H	135	THR
1	H	148	GLU
1	H	177	LEU
1	H	184	ARG
1	H	193	VAL
1	H	200	VAL
1	H	208	ARG
1	H	215	ILE
1	H	235	SER
1	H	244	GLU
1	H	254	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
1	A	137	GLN
1	A	226	HIS
1	A	234	GLN
1	B	136	HIS
1	B	226	HIS
1	C	99	GLN
1	C	226	HIS
1	C	229	ASN
1	D	99	GLN
1	D	247	ASN
1	E	122	ASN
1	E	226	HIS
1	E	247	ASN
1	F	137	GLN
1	F	196	GLN

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Mol	Chain	Res	Type
1	G	136	HIS
1	G	226	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	181/187 (96%)	-0.29	4 (2%) 62 58	24, 34, 63, 81	0
1	B	178/187 (95%)	-0.18	0 100 100	26, 39, 65, 74	0
1	C	178/187 (95%)	-0.01	6 (3%) 48 43	27, 42, 63, 81	0
1	D	175/187 (93%)	-0.02	6 (3%) 48 43	27, 42, 60, 82	0
1	E	179/187 (95%)	0.11	3 (1%) 69 65	30, 45, 73, 84	0
1	F	178/187 (95%)	0.13	4 (2%) 62 58	27, 47, 67, 81	0
1	G	179/187 (95%)	0.36	9 (5%) 34 30	29, 54, 78, 89	0
1	H	179/187 (95%)	-0.18	1 (0%) 85 83	22, 38, 56, 74	0
All	All	1427/1496 (95%)	-0.01	33 (2%) 61 57	22, 42, 70, 89	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	265	LEU	3.8
1	D	266	GLY	3.6
1	G	123	ALA	3.4
1	A	270	ALA	3.2
1	C	259	GLU	3.0
1	G	99	GLN	2.9
1	D	264	SER	2.8
1	E	267	GLN	2.8
1	F	145	TYR	2.8
1	G	268	LEU	2.8
1	D	97	GLU	2.7
1	D	184	ARG	2.7
1	G	135	THR	2.7
1	G	131	ILE	2.7
1	A	134	THR	2.6
1	G	120	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	148	GLU	2.6
1	C	123	ALA	2.6
1	F	119	PRO	2.5
1	H	97	GLU	2.5
1	F	120	ILE	2.5
1	D	120	ILE	2.4
1	E	258	ALA	2.4
1	G	90	LEU	2.3
1	C	145	TYR	2.3
1	A	131	ILE	2.3
1	A	132	GLU	2.2
1	C	120	ILE	2.2
1	G	269	ARG	2.2
1	E	96	GLU	2.1
1	F	268	LEU	2.0
1	C	241	ALA	2.0
1	C	254	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	F	1	1/1	0.62	0.13	59,59,59,59	0
2	MG	C	1	1/1	0.66	0.16	60,60,60,60	0
2	MG	G	1	1/1	0.76	0.11	50,50,50,50	0
2	MG	D	1	1/1	0.79	0.13	58,58,58,58	0
2	MG	A	1	1/1	0.80	0.09	38,38,38,38	0
2	MG	H	1	1/1	0.81	0.11	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	E	1	1/1	0.84	0.09	47,47,47,47	0
2	MG	B	1	1/1	0.92	0.05	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.