



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:15 AM UTC

PDB ID : 3BN9 / pdb_00003bn9
Title : Crystal Structure of MT-SP1 in complex with Fab Inhibitor E2
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Deposited on : 2007-12-13
Resolution : 2.17 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

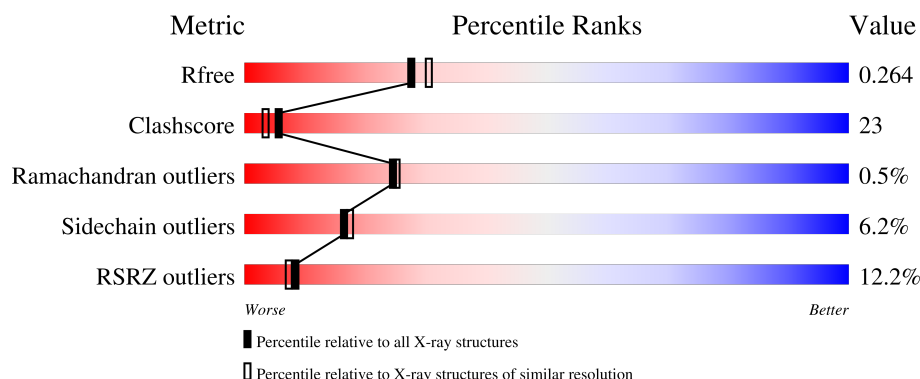
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	241	73% 22% .
1	B	241	78% 20% .
2	C	214	27% 60% 34% . ..
2	E	214	13% 57% 35% 6% ..
3	D	257	16% 51% 27% . 18%

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Mol	Chain	Length	Quality of chain
3	F	257	

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
4	EDO	A	2	-	-	X	-
4	EDO	B	6	-	-	X	-
4	EDO	B	7	-	-	X	-
4	EDO	C	216	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11103 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 Membrane-type serine protease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	241	Total	C	N	O	S	2	3	0
			1882	1188	331	352	11			
1	A	241	Total	C	N	O	S	2	4	0
			1891	1194	334	352	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	122	SER	CYS	engineered mutation	UNP Q9Y5Y6
A	122	SER	CYS	engineered mutation	UNP Q9Y5Y6

- Molecule 2 is a protein called E2 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	210	Total	C	N	O	S	0	0	0
			1593	996	266	326	5			
2	E	211	Total	C	N	O	S	0	1	0
			1609	1007	269	328	5			

- Molecule 3 is a protein called E2 Fab Heavy Chain.

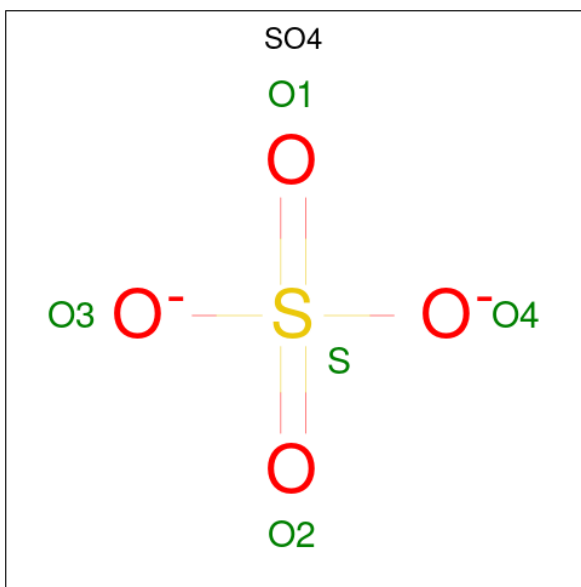
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	1	0
			1575	998	267	302	8			
3	F	224	Total	C	N	O	S	0	1	0
			1667	1050	285	325	7			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

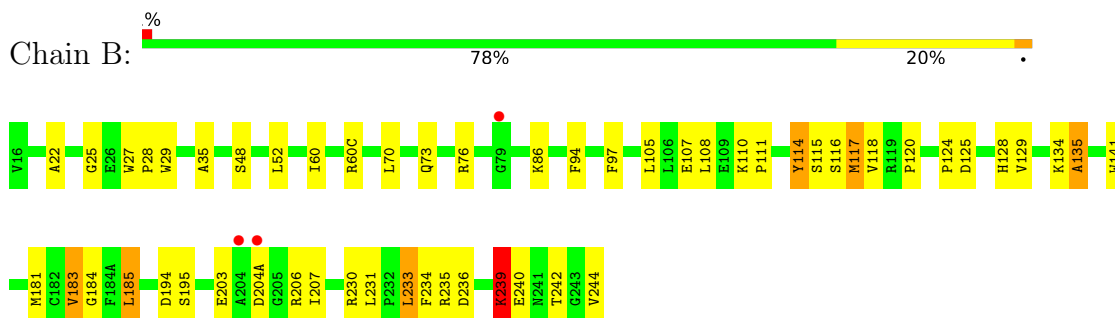
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	199	Total	O	0	0
			199	199		
6	C	118	Total	O	0	0
			118	118		
6	D	105	Total	O	0	0
			105	105		
6	A	175	Total	O	0	0
			175	175		
6	E	124	Total	O	0	0
			124	124		
6	F	103	Total	O	0	0
			103	103		

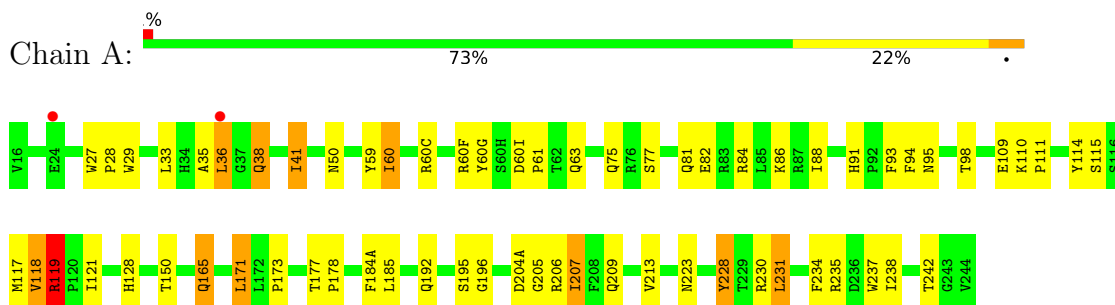
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

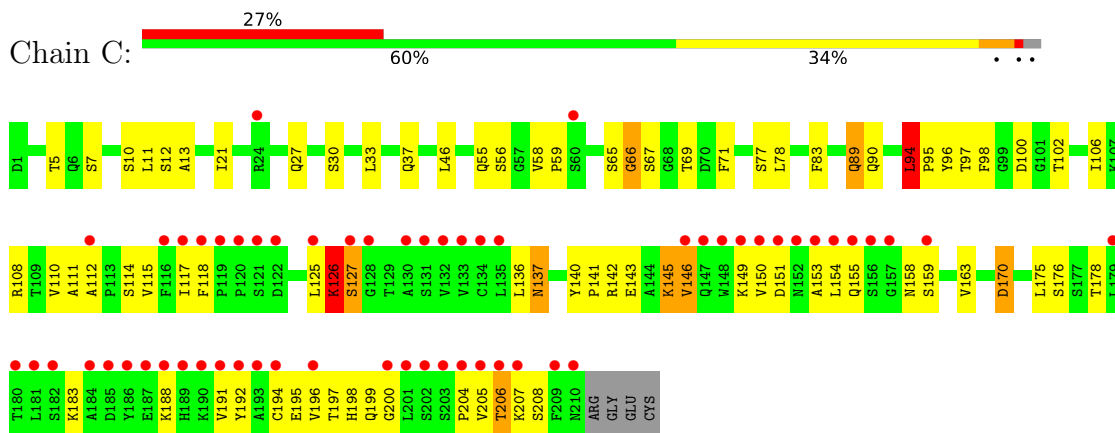
- Molecule 1: Membrane-type serine protease 1



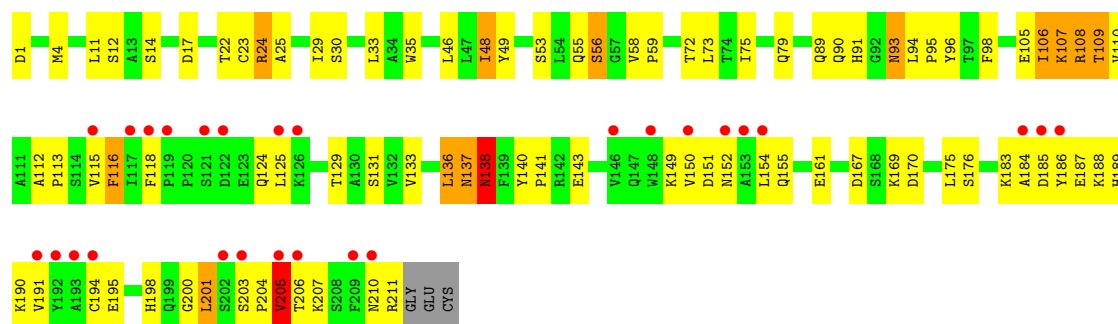
- Molecule 1: Membrane-type serine protease 1



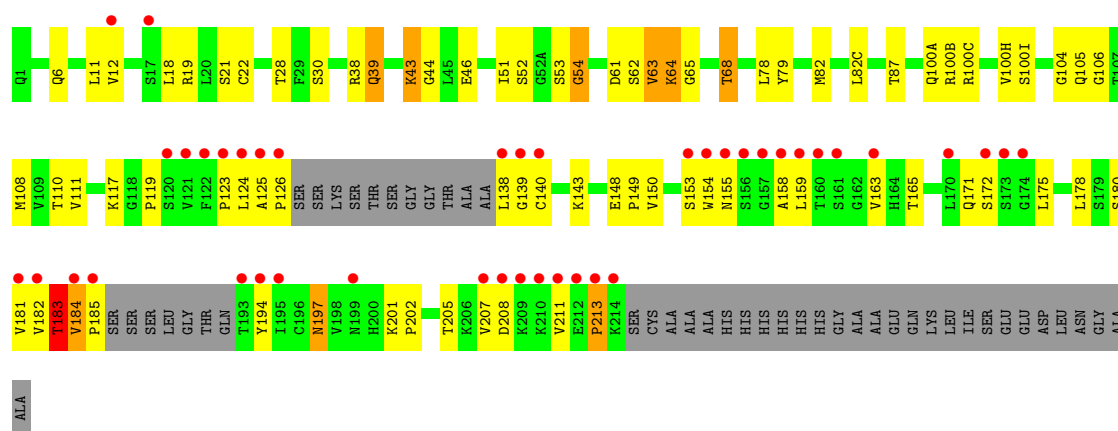
- Molecule 2: E2 Fab Light Chain



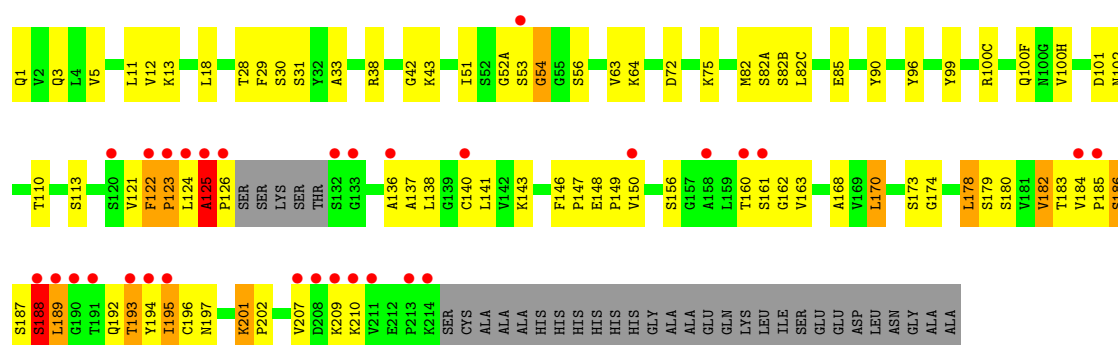
- Molecule 2: E2 Fab Light Chain



• Molecule 3: E2 Fab Heavy Chain



• Molecule 3: E2 Fab Heavy Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.62Å 163.28Å 201.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.64 – 2.17 85.64 – 2.17	Depositor EDS
% Data completeness (in resolution range)	87.4 (85.64-2.17) 87.4 (85.64-2.17)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.18Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.267 0.225 , 0.264	Depositor DCC
R_{free} test set	5781 reflections (6.83%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtrriage
Anisotropy	0.731	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11103	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4561e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO

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	1.32	17/1946 (0.9%)	1.04	11/2647 (0.4%)
1	B	1.25	16/1934 (0.8%)	0.95	0/2630
2	C	1.21	9/1627 (0.6%)	1.03	4/2212 (0.2%)
2	E	1.26	10/1644 (0.6%)	1.09	12/2235 (0.5%)
3	D	0.92	6/1618 (0.4%)	0.96	5/2207 (0.2%)
3	F	1.16	9/1708 (0.5%)	1.11	14/2326 (0.6%)
All	All	1.20	67/10477 (0.6%)	1.03	46/14257 (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
2	C	0	2
3	D	0	4
3	F	0	2
All	All	0	8

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	43	LYS	C-N	-10.53	1.20	1.33
1	A	60	ILE	C-O	-10.19	1.12	1.24
1	B	184	GLY	C-O	-9.68	1.17	1.23
3	F	42	GLY	C-N	-8.27	1.22	1.33
1	B	115	SER	C-O	-7.50	1.16	1.24
1	A	115	SER	C-O	-7.44	1.15	1.23
2	C	89	GLN	C-O	-6.84	1.16	1.23
1	B	22	ALA	C-N	-6.76	1.24	1.33
3	D	39	GLN	C-N	-6.75	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	231	LEU	C-O	-6.75	1.18	1.24
1	B	135	ALA	CA-CB	-6.47	1.45	1.53
3	D	30	SER	C-O	-6.42	1.15	1.24
2	E	205	VAL	CA-CB	-6.39	1.46	1.53
1	A	231	LEU	C-O	-6.38	1.18	1.24
1	A	118	VAL	C-O	-6.35	1.17	1.24
3	F	180	SER	C-N	6.21	1.41	1.33
1	A	60	ILE	C-N	6.17	1.48	1.34
2	C	37	GLN	C-O	-6.14	1.17	1.24
3	F	43	LYS	C-N	-6.10	1.25	1.33
1	A	242	THR	CA-CB	-6.09	1.45	1.54
3	F	30	SER	C-O	-5.99	1.16	1.24
2	C	77	SER	C-O	-5.94	1.18	1.23
1	A	82	GLU	C-O	-5.91	1.16	1.24
2	E	107	LYS	C-O	-5.87	1.17	1.24
1	B	107	GLU	C-O	-5.87	1.16	1.24
2	C	90	GLN	C-O	-5.84	1.16	1.24
2	E	75	ILE	C-O	-5.74	1.17	1.24
1	B	183	VAL	C-O	-5.73	1.18	1.24
1	A	117	MET	C-O	-5.70	1.16	1.23
2	C	10	SER	C-O	-5.65	1.17	1.23
3	D	53	SER	C-O	-5.60	1.16	1.24
2	E	90	GLN	C-O	-5.58	1.17	1.24
1	B	239	LYS	C-O	-5.57	1.17	1.24
1	A	59	TYR	CE1-CZ	-5.55	1.25	1.38
1	A	228	TYR	C-O	-5.52	1.17	1.23
2	C	66	GLY	C-O	-5.51	1.18	1.23
2	E	93	ASN	C-O	-5.49	1.17	1.23
1	B	194	ASP	C-O	-5.47	1.16	1.24
1	B	114	TYR	C-O	-5.40	1.17	1.23
3	F	29	PHE	C-O	-5.36	1.18	1.24
3	F	125	ALA	CA-CB	-5.36	1.43	1.52
2	E	167	ASP	C-O	-5.35	1.17	1.23
3	F	182	VAL	CA-CB	-5.26	1.50	1.55
1	B	35	ALA	CA-CB	-5.24	1.45	1.53
2	E	48	ILE	C-O	-5.24	1.18	1.24
2	E	79	GLN	C-O	-5.21	1.17	1.24
3	D	46	GLU	C-O	-5.21	1.18	1.24
3	F	102	ASN	C-O	-5.15	1.18	1.23
3	D	38	ARG	C-N	-5.15	1.26	1.33
1	B	111	PRO	C-O	-5.14	1.18	1.23
2	C	83	PHE	C-O	-5.14	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	GLN	C-O	-5.13	1.18	1.24
3	F	3	GLN	C-O	-5.12	1.17	1.23
1	A	59	TYR	CE2-CZ	-5.11	1.25	1.38
1	B	134	LYS	C-O	-5.10	1.18	1.24
2	C	13	ALA	C-O	-5.09	1.17	1.23
1	A	41	ILE	CA-CB	-5.09	1.49	1.55
1	A	60(G)	TYR	C-O	-5.08	1.17	1.24
2	E	24	ARG	C-O	-5.08	1.18	1.23
2	E	72	THR	C-O	-5.07	1.18	1.24
1	B	233	LEU	C-O	-5.06	1.17	1.24
1	A	82	GLU	CA-C	-5.05	1.46	1.52
1	B	185	LEU	C-O	-5.04	1.17	1.24
1	A	192	GLN	C-O	-5.04	1.17	1.23
1	B	117	MET	C-O	-5.03	1.17	1.24
2	C	170	ASP	C-O	-5.02	1.17	1.24
1	A	196	GLY	C-O	-5.02	1.17	1.24

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	43	LYS	O-C-N	-10.53	108.78	122.78
1	A	119[A]	ARG	CA-C-O	-10.29	110.36	119.72
1	A	119[B]	ARG	CA-C-O	-10.29	110.36	119.72
2	E	137	ASN	N-CA-C	9.11	123.75	108.90
2	E	205	VAL	CB-CA-C	-7.13	101.32	111.31
3	F	43	LYS	CA-C-N	6.95	129.15	122.27
3	F	43	LYS	C-N-CA	6.95	129.15	122.27
2	E	91	HIS	N-CA-C	6.87	120.33	112.57
3	F	193	THR	O-C-N	-6.85	115.41	123.22
2	E	106	ILE	N-CA-C	6.66	117.68	108.89
2	E	109	THR	N-CA-CB	6.46	119.46	109.97
2	E	113	PRO	O-C-N	6.39	130.64	122.91
2	C	146	VAL	N-CA-C	6.35	117.44	108.36
2	C	154	LEU	N-CA-C	-6.32	101.76	110.35
3	D	213	PRO	N-CA-C	-6.11	99.89	112.47
3	F	53	SER	N-CA-C	6.06	117.56	111.07
1	A	27	TRP	CA-C-N	6.05	126.16	119.87
1	A	27	TRP	C-N-CA	6.05	126.16	119.87
1	A	171	LEU	N-CA-C	6.01	118.61	111.33
3	F	163	VAL	N-CA-C	5.94	116.74	108.89
3	F	188	SER	CB-CA-C	-5.94	97.48	109.55
2	C	126	LYS	CB-CA-C	-5.94	102.89	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	54	GLY	N-CA-C	-5.90	107.24	114.92
1	A	41	ILE	CB-CA-C	-5.63	106.09	111.44
2	E	112	ALA	CA-C-N	5.60	125.91	119.92
2	E	112	ALA	C-N-CA	5.60	125.91	119.92
2	C	137	ASN	N-CA-C	5.55	117.57	108.52
2	E	113	PRO	CA-C-N	-5.53	115.25	123.11
2	E	113	PRO	C-N-CA	-5.53	115.25	123.11
3	F	31	SER	N-CA-C	5.45	119.55	113.01
1	A	195	SER	N-CA-C	5.39	118.28	110.42
3	D	30	SER	N-CA-C	5.36	119.31	112.34
1	A	59	TYR	CB-CA-C	5.33	118.55	111.14
3	F	52(A)	GLY	CA-C-N	5.30	127.33	120.44
3	F	52(A)	GLY	C-N-CA	5.30	127.33	120.44
1	A	59	TYR	N-CA-C	5.26	119.40	112.25
1	A	118	VAL	CA-C-N	5.22	132.74	122.40
1	A	118	VAL	C-N-CA	5.22	132.74	122.40
2	E	46	LEU	N-CA-C	5.20	116.63	109.15
3	F	189	LEU	N-CA-CB	-5.18	101.33	109.51
3	F	178	LEU	N-CA-C	5.17	116.14	108.86
3	D	163	VAL	N-CA-C	5.04	115.84	108.58
3	F	54	GLY	CA-C-N	5.02	125.52	120.00
3	F	54	GLY	C-N-CA	5.02	125.52	120.00
2	E	191	VAL	N-CA-C	5.01	115.30	107.99
3	D	87	THR	N-CA-C	5.01	117.81	110.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	126	LYS	Peptide
2	C	94	LEU	Peptide
3	D	100(A)	GLN	Peptide
3	D	125	ALA	Peptide
3	D	172	SER	Peptide
3	D	183	THR	Peptide
3	F	125	ALA	Peptide
3	F	188	SER	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	1891	0	1808	68	0
1	B	1882	0	1793	49	0
2	C	1593	0	1540	85	0
2	E	1609	0	1550	97	0
3	D	1575	0	1527	93	0
3	F	1667	0	1629	96	0
4	A	12	0	18	9	0
4	B	24	0	36	21	0
4	C	8	0	12	8	0
4	D	4	0	6	3	0
4	E	4	0	6	0	0
5	C	5	0	0	0	0
5	E	5	0	0	0	0
6	A	175	0	0	11	0
6	B	199	0	0	9	0
6	C	118	0	0	8	0
6	D	105	0	0	3	0
6	E	124	0	0	2	0
6	F	103	0	0	7	0
All	All	11103	0	9925	472	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (472) 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)
3:F:123:PRO:CG	3:F:209:LYS:HE2	1.35	1.54
2:E:187:GLU:C	2:E:211:ARG:NH1	1.74	1.46
3:F:123:PRO:HG3	3:F:209:LYS:CE	1.45	1.44
2:C:151:ASP:HA	2:C:191:VAL:CG2	1.46	1.42
3:F:122:PHE:HA	3:F:209:LYS:NZ	1.27	1.37
3:F:123:PRO:CD	3:F:209:LYS:NZ	1.88	1.36
3:F:123:PRO:HD3	3:F:209:LYS:NZ	1.05	1.36
2:E:195:GLU:CB	2:E:206:THR:HG22	1.56	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:123:PRO:CD	3:F:209:LYS:HZ3	1.44	1.23
2:C:151:ASP:CA	2:C:191:VAL:CG2	2.17	1.22
2:C:150:VAL:O	2:C:153:ALA:HB3	1.42	1.20
2:E:187:GLU:CA	2:E:211:ARG:NH1	2.04	1.20
2:E:195:GLU:HB2	2:E:206:THR:HG22	1.20	1.18
1:A:35:ALA:HB3	1:A:41:ILE:CD1	1.75	1.16
2:E:187:GLU:HA	2:E:211:ARG:NH1	1.62	1.12
2:E:195:GLU:HB2	2:E:206:THR:CG2	1.80	1.12
2:E:195:GLU:HG3	2:E:206:THR:CG2	1.79	1.11
2:E:189:HIS:O	2:E:211:ARG:NE	1.81	1.10
3:D:183:THR:HA	3:D:184:VAL:CG2	1.79	1.10
2:C:151:ASP:HA	2:C:191:VAL:HG22	1.10	1.10
2:E:116:PHE:CE1	3:F:137:ALA:HB2	1.86	1.09
1:A:35:ALA:HB3	1:A:41:ILE:HD11	1.34	1.08
3:F:185:PRO:HG2	3:F:188:SER:OG	1.51	1.08
3:F:140:CYS:SG	3:F:196:CYS:CB	2.42	1.08
3:D:183:THR:CA	3:D:184:VAL:HG23	1.85	1.07
2:E:187:GLU:O	2:E:211:ARG:NH1	1.86	1.06
3:F:122:PHE:CA	3:F:209:LYS:NZ	2.17	1.06
2:C:150:VAL:O	2:C:153:ALA:CB	2.03	1.05
1:A:35:ALA:CB	1:A:41:ILE:HD12	1.86	1.05
1:B:230:ARG:HD3	4:B:6:EDO:H12	1.33	1.04
1:A:91:HIS:NE2	4:A:13:EDO:H22	1.71	1.03
2:C:151:ASP:N	2:C:191:VAL:HG23	1.74	1.02
3:F:193:THR:HG23	3:F:210:LYS:HD2	1.06	1.02
2:E:151:ASP:OD2	2:E:189:HIS:CD2	2.14	1.01
2:E:195:GLU:CB	2:E:206:THR:CG2	2.37	1.01
2:C:125:LEU:O	2:C:183:LYS:HD3	1.59	1.01
2:E:205:VAL:HG12	2:E:205:VAL:O	1.56	1.01
3:F:193:THR:CG2	3:F:210:LYS:HD2	1.91	1.00
3:F:123:PRO:CG	3:F:209:LYS:CE	2.19	0.98
1:B:60:ILE:HD11	1:B:94:PHE:HE2	1.28	0.98
2:E:187:GLU:C	2:E:211:ARG:HH12	1.46	0.97
2:C:151:ASP:HA	2:C:191:VAL:HG21	1.46	0.97
3:F:122:PHE:CA	3:F:209:LYS:HZ3	1.73	0.97
2:E:195:GLU:CG	2:E:206:THR:CG2	2.43	0.96
2:E:187:GLU:CA	2:E:211:ARG:HH12	1.74	0.96
1:A:35:ALA:CB	1:A:41:ILE:CD1	2.41	0.96
2:E:195:GLU:CG	2:E:206:THR:HG22	1.96	0.95
2:C:94:LEU:CD2	2:C:96:TYR:CE1	2.50	0.94
2:C:197:THR:HG22	2:C:204:PRO:HG3	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:151:ASP:CG	2:E:189:HIS:CD2	2.47	0.92
2:C:151:ASP:H	2:C:191:VAL:HG23	1.28	0.92
2:C:100:ASP:HB2	6:C:405:HOH:O	1.68	0.92
2:E:116:PHE:CD1	3:F:137:ALA:HB3	2.05	0.91
3:F:193:THR:HG23	3:F:210:LYS:CD	1.99	0.91
3:F:123:PRO:HD3	3:F:209:LYS:CE	2.00	0.91
1:B:230:ARG:HB3	4:B:6:EDO:H11	1.50	0.91
2:C:151:ASP:CA	2:C:191:VAL:HG22	1.90	0.91
2:E:187:GLU:C	2:E:211:ARG:HH11	1.59	0.90
2:E:116:PHE:CE1	3:F:137:ALA:CB	2.55	0.90
3:F:123:PRO:N	3:F:209:LYS:HZ3	1.70	0.90
2:E:150:VAL:HG12	2:E:189:HIS:CD2	2.07	0.89
3:F:140:CYS:CB	3:F:196:CYS:SG	2.60	0.89
2:C:198:HIS:CD2	2:C:200:GLY:H	1.91	0.89
3:F:122:PHE:C	3:F:209:LYS:HZ3	1.81	0.88
3:F:123:PRO:CD	3:F:209:LYS:CE	2.45	0.88
2:C:151:ASP:N	2:C:191:VAL:CG2	2.36	0.87
2:C:146:VAL:CG2	2:C:196:VAL:HG22	2.05	0.87
1:B:60:ILE:HD11	1:B:94:PHE:CE2	2.10	0.87
3:D:155:ASN:HD21	3:D:194:TYR:HD1	1.16	0.87
2:E:188:LYS:O	2:E:188:LYS:HG3	1.74	0.86
2:E:195:GLU:HG3	2:E:206:THR:HG23	1.57	0.86
2:C:198:HIS:HD2	2:C:200:GLY:H	1.21	0.86
3:D:6:GLN:HE21	3:D:104:GLY:HA3	1.38	0.86
1:A:84:ARG:HG2	1:A:84:ARG:HH11	1.40	0.86
1:A:35:ALA:HB2	1:A:41:ILE:HD12	1.55	0.86
2:E:108:ARG:HD3	2:E:109:THR:O	1.76	0.85
2:E:116:PHE:CD1	3:F:137:ALA:CB	2.59	0.85
1:A:128:HIS:HD2	6:A:284:HOH:O	1.58	0.85
3:F:122:PHE:HA	3:F:209:LYS:HZ2	1.03	0.84
2:E:195:GLU:CA	2:E:206:THR:HG22	2.06	0.83
3:F:136:ALA:CB	3:F:189:LEU:HD11	2.09	0.83
3:F:33:ALA:H	3:F:100(F):GLN:HE22	1.25	0.83
3:D:43:LYS:HE2	6:D:289:HOH:O	1.78	0.82
3:F:96:TYR:HB2	3:F:101:ASP:HB3	1.62	0.82
3:D:138:LEU:HD12	3:D:139:GLY:O	1.79	0.81
2:E:108:ARG:HG2	2:E:109:THR:N	1.95	0.81
3:F:186:SER:O	3:F:189:LEU:HB2	1.80	0.81
3:D:143:LYS:HE3	3:D:171:GLN:HE22	1.46	0.81
2:C:94:LEU:HD23	2:C:96:TYR:CE1	2.13	0.81
1:A:60(F):ARG:HG2	1:A:60(I):ASP:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:117:LYS:HD3	3:D:175:LEU:CD2	2.11	0.80
2:C:146:VAL:HG22	2:C:196:VAL:HA	1.64	0.80
2:C:146:VAL:HG21	2:C:196:VAL:HG22	1.62	0.79
2:C:149:LYS:HA	2:C:153:ALA:O	1.83	0.79
1:A:60:ILE:HD11	1:A:94:PHE:HE2	1.47	0.79
3:F:33:ALA:H	3:F:100(F):GLN:NE2	1.81	0.78
2:E:189:HIS:O	2:E:211:ARG:CD	2.31	0.78
2:E:118:PHE:CD1	3:F:124:LEU:HB3	2.19	0.77
3:D:184:VAL:HB	3:D:185:PRO:HD3	1.65	0.77
3:D:183:THR:HA	3:D:184:VAL:HG23	0.89	0.77
2:C:46:LEU:HD23	2:C:55:GLN:HE21	1.50	0.76
3:D:155:ASN:HB2	3:D:158:ALA:HB3	1.68	0.76
1:A:185:LEU:H	4:A:2:EDO:H22	1.51	0.75
2:E:94:LEU:CD2	2:E:96:TYR:CE1	2.69	0.75
2:C:65:SER:OG	4:C:216:EDO:H12	1.87	0.75
3:F:121:VAL:O	3:F:209:LYS:HD2	1.86	0.75
6:B:346:HOH:O	3:D:100(C):ARG:HD3	1.88	0.74
3:F:185:PRO:CG	3:F:188:SER:OG	2.33	0.74
1:A:185:LEU:H	4:A:2:EDO:C2	2.00	0.74
3:D:124:LEU:HB2	3:D:139:GLY:HA2	1.70	0.73
2:E:210:ASN:O	2:E:211:ARG:C	2.30	0.73
1:A:119[A]:ARG:CG	1:A:119[A]:ARG:HH11	2.00	0.73
2:E:183:LYS:NZ	2:E:187:GLU:OE2	2.22	0.73
2:E:108:ARG:HG2	2:E:109:THR:H	1.53	0.72
3:D:124:LEU:H	3:D:139:GLY:HA3	1.54	0.72
6:B:346:HOH:O	3:D:100(C):ARG:CD	2.37	0.71
3:F:125:ALA:HA	3:F:126:PRO:C	2.15	0.71
1:B:207:ILE:CD1	4:B:7:EDO:H22	2.21	0.71
1:A:128:HIS:HE1	6:A:269:HOH:O	1.74	0.71
1:A:119[A]:ARG:HH11	1:A:119[A]:ARG:HG3	1.55	0.71
3:F:123:PRO:HD3	3:F:209:LYS:HZ1	0.89	0.70
3:D:82:MET:HB3	3:D:82(C):LEU:HD21	1.73	0.70
3:F:170:LEU:HD21	3:F:174:GLY:HA2	1.72	0.70
3:D:108[A]:MET:SD	3:D:149:PRO:HG3	2.31	0.70
2:E:184:ALA:O	6:E:444:HOH:O	2.10	0.69
1:A:28:PRO:HB2	1:A:119[A]:ARG:HB3	1.75	0.69
3:F:121:VAL:O	3:F:209:LYS:CD	2.41	0.68
1:B:105:LEU:HD13	1:B:242:THR:CG2	2.23	0.68
2:C:151:ASP:H	2:C:191:VAL:CG2	2.01	0.68
2:C:94:LEU:HD21	2:C:96:TYR:CE1	2.28	0.68
3:D:117:LYS:HD3	3:D:175:LEU:HD22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ASP:OD2	6:B:440:HOH:O	2.11	0.68
2:E:151:ASP:HB2	2:E:189:HIS:CD2	2.29	0.67
2:C:118:PHE:CD1	3:D:124:LEU:HB3	2.30	0.67
1:B:204(A):ASP:OD2	1:B:206:ARG:NE	2.27	0.67
1:A:204(A):ASP:C	1:A:204(A):ASP:OD1	2.30	0.67
1:A:86:LYS:HG2	1:A:86:LYS:O	1.92	0.67
1:B:128:HIS:HE1	6:B:341:HOH:O	1.78	0.67
3:D:119:PRO:HD2	3:D:205:THR:HG21	1.77	0.67
2:C:146:VAL:HG22	2:C:196:VAL:HG22	1.75	0.67
2:E:12[B]:SER:OG	2:E:107:LYS:HB2	1.94	0.66
1:A:28:PRO:HD2	1:A:29:TRP:CZ3	2.31	0.66
1:A:185:LEU:N	4:A:2:EDO:H22	2.09	0.66
3:D:194:TYR:O	3:D:211:VAL:HG22	1.96	0.66
1:A:60(C):ARG:HG2	3:F:28:THR:CG2	2.26	0.66
2:E:149:LYS:HG2	2:E:154:LEU:HD23	1.76	0.66
1:A:150[A]:THR:HG23	6:A:266:HOH:O	1.95	0.66
2:E:149:LYS:CG	2:E:154:LEU:HD23	2.25	0.66
3:F:140:CYS:CB	3:F:196:CYS:HG	2.01	0.66
2:E:198:HIS:HD2	2:E:200:GLY:H	1.43	0.66
3:D:100(C):ARG:CB	3:D:100(C):ARG:HH11	2.10	0.65
2:C:94:LEU:HD21	2:C:96:TYR:HE1	1.60	0.65
3:D:159:LEU:HD13	3:D:182:VAL:HG21	1.78	0.65
3:D:201:LYS:N	3:D:202:PRO:CD	2.60	0.65
3:D:124:LEU:HB2	3:D:139:GLY:CA	2.26	0.65
3:D:19:ARG:NH1	3:D:79:TYR:CD1	2.66	0.64
1:A:178:PRO:HG2	4:A:12:EDO:O2	1.97	0.64
1:A:60:ILE:HD11	1:A:94:PHE:CE2	2.32	0.64
2:E:187:GLU:CA	2:E:211:ARG:HH11	1.95	0.64
2:C:66:GLY:HA2	4:C:216:EDO:H11	1.79	0.64
3:F:100(H):VAL:O	3:F:100(H):VAL:CG1	2.44	0.64
2:E:140:TYR:CG	2:E:141:PRO:HA	2.33	0.64
1:A:91:HIS:HD1	1:A:93:PHE:H	1.46	0.64
2:E:151:ASP:CB	2:E:189:HIS:CD2	2.80	0.64
1:B:204(A):ASP:CG	1:B:206:ARG:HE	2.06	0.63
3:D:155:ASN:ND2	3:D:194:TYR:HD1	1.92	0.63
1:B:128:HIS:HD2	6:B:351:HOH:O	1.81	0.63
1:A:84:ARG:HH11	1:A:84:ARG:CG	2.11	0.63
2:C:21:ILE:HG12	2:C:102:THR:HG21	1.81	0.63
1:B:29:TRP:HH2	4:B:7:EDO:H21	1.64	0.62
2:C:115:VAL:HG22	2:C:136:LEU:HD22	1.80	0.62
2:C:150:VAL:O	2:C:153:ALA:HB2	1.94	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:123:PRO:HB3	3:D:211:VAL:HG12	1.81	0.62
2:C:66:GLY:CA	4:C:216:EDO:H11	2.29	0.62
2:E:125:LEU:O	2:E:183:LYS:HD2	2.00	0.62
2:E:195:GLU:HA	2:E:206:THR:HG22	1.82	0.62
3:D:182:VAL:O	3:D:184:VAL:HG22	1.99	0.61
2:E:195:GLU:HB2	2:E:206:THR:HG21	1.78	0.61
3:D:100(C):ARG:HH11	3:D:100(C):ARG:HB2	1.65	0.61
1:B:204(A):ASP:OD2	1:B:206:ARG:NH2	2.33	0.61
3:D:182:VAL:O	3:D:184:VAL:CG2	2.49	0.61
1:B:28:PRO:HD2	1:B:29:TRP:CZ3	2.36	0.60
3:F:121:VAL:O	3:F:121:VAL:HG12	1.99	0.60
3:D:100(I):SER:O	4:D:243:EDO:H12	2.01	0.60
2:C:151:ASP:OD1	2:C:191:VAL:HG22	2.02	0.60
1:A:150[B]:THR:HG22	6:A:266:HOH:O	2.01	0.60
2:E:152:ASN:OD1	2:E:152:ASN:O	2.19	0.60
2:E:189:HIS:O	2:E:211:ARG:HD2	2.00	0.60
3:F:122:PHE:CA	3:F:209:LYS:HZ2	1.96	0.60
2:C:198:HIS:HD2	2:C:200:GLY:N	1.98	0.60
2:E:55:GLN:HE21	2:E:56:SER:H	1.49	0.60
2:C:46:LEU:HD23	2:C:55:GLN:NE2	2.17	0.60
2:E:89:GLN:HE21	2:E:96:TYR:HB3	1.65	0.60
1:A:119[A]:ARG:HH11	1:A:119[A]:ARG:HB2	1.65	0.59
1:B:25:GLY:HA2	4:B:3:EDO:H22	1.83	0.59
2:C:11:LEU:C	2:C:11:LEU:HD12	2.27	0.59
2:C:65:SER:OG	4:C:216:EDO:C1	2.50	0.59
1:B:124:PRO:HD2	6:B:349:HOH:O	2.02	0.59
3:D:100(H):VAL:O	3:D:100(H):VAL:CG1	2.51	0.59
2:C:146:VAL:HG22	2:C:196:VAL:CA	2.32	0.59
1:A:165:GLN:NE2	6:A:346:HOH:O	2.33	0.59
1:A:121:ILE:HD13	1:A:209:GLN:HB2	1.83	0.59
2:E:11:LEU:HD12	2:E:11:LEU:C	2.28	0.59
1:B:135:ALA:H	4:B:8:EDO:H21	1.67	0.58
3:D:19:ARG:NH1	3:D:79:TYR:CE1	2.70	0.58
3:F:75:LYS:HE2	6:F:334:HOH:O	2.02	0.58
1:A:119[A]:ARG:HB2	1:A:119[A]:ARG:NH1	2.19	0.58
2:C:195:GLU:O	2:C:195:GLU:HG3	2.04	0.58
2:E:4:MET:HE1	2:E:25:ALA:HB2	1.85	0.58
1:A:28:PRO:HD2	1:A:29:TRP:CE3	2.39	0.58
1:B:230:ARG:CD	4:B:6:EDO:H12	2.23	0.57
1:B:234:PHE:CE1	4:B:1:EDO:H11	2.39	0.57
1:A:237:TRP:HB2	4:A:13:EDO:O2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:51:ILE:HD11	3:F:54:GLY:HA2	1.86	0.57
3:D:124:LEU:HD12	3:D:139:GLY:HA2	1.84	0.57
3:D:126:PRO:O	3:D:138:LEU:HB2	2.04	0.57
3:F:13:LYS:NZ	6:F:309:HOH:O	2.38	0.57
1:B:117:MET:HE2	6:B:357:HOH:O	2.03	0.57
2:E:188:LYS:O	2:E:188:LYS:CG	2.49	0.57
1:A:36:LEU:HD22	1:A:63:GLN:HA	1.87	0.56
3:D:182:VAL:HG22	3:D:183:THR:N	2.20	0.56
3:D:6:GLN:HE21	3:D:104:GLY:CA	2.16	0.56
2:E:94:LEU:HA	2:E:95:PRO:C	2.30	0.56
1:B:233:LEU:HG	4:B:6:EDO:O2	2.06	0.56
2:C:145:LYS:O	2:C:145:LYS:HG3	2.05	0.56
3:D:100(B):ARG:HD2	6:D:259:HOH:O	2.04	0.56
2:C:108:ARG:O	6:C:400:HOH:O	2.17	0.56
1:A:60(C):ARG:HG2	3:F:28:THR:HG23	1.88	0.56
1:B:230:ARG:HB3	4:B:6:EDO:C1	2.29	0.56
3:F:123:PRO:CD	3:F:209:LYS:HZ1	1.85	0.55
2:E:116:PHE:N	2:E:116:PHE:CD2	2.74	0.55
3:F:184:VAL:HB	3:F:185:PRO:HD2	1.88	0.55
2:E:138:ASN:OD1	2:E:138:ASN:N	2.39	0.55
3:D:64:LYS:HD2	3:D:65:GLY:N	2.21	0.55
1:A:165:GLN:NE2	1:A:230:ARG:HH21	2.05	0.55
1:B:124:PRO:O	1:B:235:ARG:HD3	2.07	0.55
1:A:119[A]:ARG:HH11	1:A:119[A]:ARG:CB	2.19	0.55
3:F:148:GLU:OE2	3:F:168:ALA:HB3	2.05	0.55
2:E:94:LEU:HD21	2:E:96:TYR:CE1	2.42	0.55
1:B:114:TYR:CZ	1:B:120:PRO:HG3	2.42	0.54
1:A:204(A):ASP:OD1	1:A:205:GLY:N	2.40	0.54
1:A:60(C):ARG:HG2	3:F:28:THR:HG21	1.90	0.54
3:D:100(I):SER:HB2	4:D:243:EDO:C1	2.37	0.54
2:C:150:VAL:HG23	2:C:155:GLN:NE2	2.23	0.54
2:C:191:VAL:HG23	2:C:191:VAL:O	2.08	0.54
3:F:160:THR:HG23	6:F:364:HOH:O	2.08	0.54
1:B:25:GLY:CA	4:B:3:EDO:H22	2.39	0.53
3:F:148:GLU:HG2	3:F:149:PRO:HA	1.90	0.53
3:F:162:GLY:HA3	3:F:182:VAL:HG23	1.90	0.53
2:C:143:GLU:H	2:C:143:GLU:CD	2.12	0.53
3:F:100(H):VAL:O	3:F:100(H):VAL:HG13	2.08	0.53
3:F:140:CYS:HG	3:F:196:CYS:CB	2.03	0.53
3:D:154:TRP:HZ2	3:D:180:SER:O	1.91	0.53
3:D:11:LEU:HD12	3:D:110:THR:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LYS:HE2	1:B:244:VAL:C	2.34	0.53
1:A:36:LEU:O	1:A:38:GLN:HG3	2.09	0.53
3:D:61:ASP:C	3:D:63:VAL:H	2.17	0.53
1:A:165:GLN:HE21	1:A:165:GLN:HA	1.73	0.53
1:A:95:ASN:ND2	3:F:56:SER:OG	2.42	0.52
2:C:151:ASP:CA	2:C:191:VAL:HG21	2.14	0.52
1:A:77:SER:HB2	6:A:304:HOH:O	2.08	0.52
2:C:89:GLN:HE21	2:C:96:TYR:HB3	1.74	0.52
2:E:141:PRO:HB2	2:E:143:GLU:OE1	2.10	0.52
3:D:184:VAL:CB	3:D:185:PRO:HD3	2.33	0.52
2:E:151:ASP:CG	2:E:189:HIS:HD2	2.11	0.52
2:C:125:LEU:O	2:C:183:LYS:CD	2.48	0.52
2:E:124:GLN:HE22	2:E:131:SER:HB2	1.74	0.51
1:B:105:LEU:HD13	1:B:242:THR:HG23	1.91	0.51
3:D:138:LEU:HD12	3:D:138:LEU:C	2.34	0.51
3:F:136:ALA:HB2	3:F:189:LEU:HD11	1.91	0.51
2:C:175:LEU:HD11	6:C:439:HOH:O	2.10	0.51
3:D:159:LEU:CD1	3:D:182:VAL:HG11	2.40	0.51
2:C:143:GLU:OE1	2:C:143:GLU:N	2.30	0.51
3:D:51:ILE:HD11	3:D:54:GLY:HA2	1.92	0.51
2:E:151:ASP:OD2	2:E:189:HIS:CG	2.62	0.51
3:F:18:LEU:HB3	3:F:82:MET:HE3	1.91	0.51
1:B:70:LEU:HD11	1:B:76:ARG:HG2	1.93	0.51
3:D:68:THR:HG21	3:F:173:SER:HA	1.92	0.51
1:A:185:LEU:N	4:A:2:EDO:C2	2.71	0.51
1:B:234:PHE:CD1	4:B:1:EDO:H11	2.46	0.51
1:B:73:GLN:HE21	1:B:141:TRP:CG	2.28	0.51
3:D:6:GLN:H	3:D:105:GLN:HE22	1.58	0.51
2:E:190:LYS:HA	2:E:211:ARG:HD2	1.91	0.51
1:B:28:PRO:HD2	1:B:29:TRP:CE3	2.46	0.51
2:C:5:THR:HG22	6:C:341:HOH:O	2.12	0.50
3:F:182:VAL:CG2	3:F:183:THR:N	2.74	0.50
3:F:193:THR:CG2	3:F:210:LYS:CD	2.75	0.50
3:F:201:LYS:N	3:F:202:PRO:CD	2.74	0.50
3:D:6:GLN:NE2	3:D:104:GLY:HA3	2.19	0.50
3:D:143:LYS:HE3	3:D:171:GLN:NE2	2.23	0.50
3:D:100(I):SER:HB2	4:D:243:EDO:H11	1.93	0.49
3:F:122:PHE:O	3:F:141:LEU:N	2.33	0.49
2:C:140:TYR:CG	2:C:141:PRO:HA	2.48	0.49
2:C:146:VAL:HG11	2:C:194:CYS:SG	2.52	0.49
2:E:151:ASP:HB2	2:E:189:HIS:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:61:ASP:O	3:D:63:VAL:N	2.46	0.49
2:E:55:GLN:HE21	2:E:56:SER:N	2.10	0.49
3:F:38:ARG:HD3	3:F:90:TYR:CE2	2.47	0.49
3:F:182:VAL:HG22	3:F:183:THR:N	2.28	0.49
3:F:185:PRO:HG2	3:F:188:SER:HG	1.70	0.49
2:C:111:ALA:HA	4:C:217:EDO:H12	1.93	0.49
1:A:86:LYS:HB2	1:A:109:GLU:HG2	1.94	0.49
2:E:108:ARG:CG	2:E:109:THR:N	2.69	0.49
3:F:178:LEU:HD12	3:F:179:SER:N	2.27	0.49
4:B:4:EDO:H22	6:B:508:HOH:O	2.13	0.49
2:E:198:HIS:CD2	2:E:200:GLY:H	2.26	0.49
1:B:27:TRP:C	4:B:3:EDO:H21	2.37	0.48
1:B:185:LEU:N	4:B:4:EDO:H11	2.28	0.48
2:E:115:VAL:HG22	2:E:136:LEU:HD22	1.95	0.48
3:D:100(C):ARG:HB2	3:D:100(C):ARG:NH1	2.29	0.48
1:A:38:GLN:NE2	6:A:353:HOH:O	2.45	0.48
3:F:156:SER:H	3:F:197:ASN:ND2	2.12	0.48
2:E:94:LEU:CD2	2:E:96:TYR:CZ	2.97	0.48
3:F:192:GLN:HG2	3:F:194:TYR:CZ	2.48	0.48
1:B:29:TRP:CH2	4:B:7:EDO:H21	2.46	0.48
3:D:165:THR:HG23	3:D:180:SER:HB2	1.95	0.48
2:E:116:PHE:CZ	3:F:137:ALA:HB2	2.45	0.47
2:C:163:VAL:HG22	2:C:175:LEU:HD12	1.96	0.47
2:E:105:GLU:HG2	2:E:106:ILE:N	2.28	0.47
2:E:124:GLN:HE22	2:E:131:SER:CB	2.27	0.47
2:C:175:LEU:HD23	2:C:176:SER:N	2.29	0.47
1:A:237:TRP:HB2	4:A:13:EDO:HO2	1.78	0.47
1:B:230:ARG:HH11	4:B:6:EDO:H12	1.79	0.47
1:B:185:LEU:H	4:B:4:EDO:H11	1.80	0.47
3:D:6:GLN:NE2	3:D:106:GLY:H	2.12	0.47
2:E:55:GLN:HE21	2:E:55:GLN:HA	1.79	0.47
2:C:69:THR:OG1	6:C:369:HOH:O	2.18	0.47
1:A:213:VAL:HG22	1:A:228:TYR:HE2	1.79	0.47
1:A:165:GLN:HE21	1:A:165:GLN:CA	2.27	0.47
2:E:150:VAL:H	2:E:155:GLN:HE21	1.61	0.47
3:F:96:TYR:HA	6:F:311:HOH:O	2.13	0.47
3:D:182:VAL:CG2	3:D:183:THR:N	2.78	0.47
2:C:175:LEU:CD1	6:C:439:HOH:O	2.62	0.46
2:E:125:LEU:HD21	2:E:186:TYR:CD2	2.50	0.46
3:F:195:ILE:HA	3:F:210:LYS:HA	1.97	0.46
2:E:149:LYS:HG3	2:E:154:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:33:ALA:N	3:F:100(F):GLN:HE22	2.04	0.46
1:A:128:HIS:CE1	6:A:269:HOH:O	2.58	0.46
2:E:49:TYR:CZ	2:E:53:SER:HB3	2.51	0.46
1:B:60(C):ARG:HG2	3:D:28:THR:HG23	1.97	0.46
3:D:139:GLY:O	3:D:154:TRP:HH2	1.98	0.46
3:D:159:LEU:HD13	3:D:182:VAL:HG11	1.96	0.46
1:A:171:LEU:C	1:A:173:PRO:HD3	2.40	0.46
1:A:184(A):PHE:HB3	4:A:2:EDO:H21	1.98	0.46
3:D:22:CYS:HB3	3:D:78:LEU:HB3	1.98	0.46
3:D:139:GLY:O	3:D:154:TRP:CH2	2.69	0.46
2:C:159:SER:HA	2:C:178:THR:O	2.16	0.46
3:D:207:VAL:HG12	3:D:208:ASP:H	1.80	0.46
2:C:89:GLN:HG3	2:C:98:PHE:CE1	2.52	0.45
2:C:192:TYR:O	2:C:208:SER:HB2	2.16	0.45
3:F:160:THR:CG2	6:F:364:HOH:O	2.63	0.45
3:D:64:LYS:CD	3:D:65:GLY:N	2.79	0.45
2:E:161:GLU:HA	2:E:176:SER:O	2.16	0.45
1:B:234:PHE:CD1	4:B:1:EDO:C1	3.00	0.45
3:F:12:VAL:HG21	3:F:82(C):LEU:HD13	1.98	0.45
2:C:66:GLY:N	4:C:216:EDO:H11	2.31	0.45
2:C:95:PRO:O	2:C:95:PRO:HG2	2.17	0.45
1:B:236:ASP:O	1:B:240:GLU:HB2	2.17	0.45
2:C:146:VAL:CG2	2:C:196:VAL:HG13	2.46	0.45
3:D:150:VAL:CG1	3:D:178:LEU:HD21	2.46	0.45
2:E:137:ASN:O	2:E:138:ASN:C	2.55	0.45
3:F:150:VAL:O	3:F:150:VAL:HG13	2.16	0.45
1:B:60(C):ARG:HG2	3:D:28:THR:CG2	2.46	0.45
1:A:50:ASN:HD21	1:A:111:PRO:HG3	1.82	0.45
1:A:84:ARG:CG	1:A:84:ARG:NH1	2.74	0.45
3:D:207:VAL:HG12	3:D:208:ASP:N	2.32	0.45
2:C:27:GLN:NE2	6:C:411:HOH:O	2.42	0.44
1:B:207:ILE:HD11	4:B:7:EDO:H22	1.96	0.44
3:F:100(C):ARG:NH2	6:F:352:HOH:O	2.50	0.44
3:F:156:SER:H	3:F:197:ASN:HD21	1.64	0.44
3:F:185:PRO:O	3:F:188:SER:CB	2.65	0.44
2:C:146:VAL:HG22	2:C:196:VAL:CG2	2.44	0.44
3:D:12:VAL:HG23	3:D:111:VAL:HG22	1.99	0.44
3:D:100(H):VAL:O	3:D:100(H):VAL:HG13	2.18	0.44
2:C:110:VAL:HG21	2:C:199:GLN:NE2	2.33	0.44
2:C:117:ILE:HG22	2:C:207:LYS:HD3	1.99	0.44
3:D:39:GLN:HG3	3:D:44:GLY:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:153:SER:OG	3:D:197:ASN:HB2	2.18	0.44
3:F:123:PRO:HA	3:F:140:CYS:HA	1.99	0.44
3:D:18:LEU:HB3	3:D:82:MET:CE	2.47	0.44
2:E:175:LEU:HD23	2:E:176:SER:N	2.33	0.44
3:F:72:ASP:OD1	3:F:72:ASP:C	2.60	0.44
1:A:171:LEU:HD22	1:A:223:ASN:HB3	2.00	0.44
1:A:128:HIS:CD2	6:A:284:HOH:O	2.47	0.44
1:B:204(A):ASP:OD2	1:B:206:ARG:CZ	2.65	0.43
3:D:150:VAL:HG13	3:D:178:LEU:HD21	2.00	0.43
1:B:203:GLU:OE1	1:B:203:GLU:HA	2.18	0.43
2:C:112:ALA:CB	4:C:217:EDO:H22	2.48	0.43
2:C:195:GLU:CB	2:C:206:THR:HB	2.48	0.43
3:D:184:VAL:H	3:D:185:PRO:CD	2.31	0.43
2:E:23:CYS:HB2	2:E:35:TRP:CH2	2.54	0.43
2:E:151:ASP:CB	2:E:189:HIS:HD2	2.31	0.43
3:F:5:VAL:O	3:F:5:VAL:HG12	2.16	0.43
2:C:118:PHE:HE1	3:D:138:LEU:HA	1.83	0.43
3:F:11:LEU:HD12	3:F:110:THR:O	2.19	0.43
2:E:94:LEU:HD22	2:E:96:TYR:CE1	2.53	0.43
3:F:82(A)[A]:SER:O	3:F:82(B):SER:C	2.60	0.43
2:E:201:LEU:HD12	2:E:201:LEU:HA	1.60	0.43
3:D:148:GLU:HB3	3:D:149:PRO:HA	2.01	0.43
2:E:89:GLN:HG3	2:E:98:PHE:CE1	2.54	0.43
1:A:60(C):ARG:NH2	6:A:343:HOH:O	2.52	0.43
2:E:118:PHE:HB2	2:E:133:VAL:HB	2.01	0.43
3:F:146:PHE:HA	3:F:147:PRO:HA	1.77	0.43
2:C:158:ASN:OD1	2:C:158:ASN:N	2.51	0.43
2:E:140:TYR:CD1	2:E:141:PRO:HA	2.54	0.43
3:F:82:MET:HB3	3:F:82(C):LEU:HD21	2.00	0.42
1:B:207:ILE:HD13	4:B:7:EDO:H22	1.96	0.42
1:A:204(A):ASP:OD2	1:A:206:ARG:NE	2.40	0.42
3:F:122:PHE:CD1	3:F:122:PHE:N	2.85	0.42
1:A:206:ARG:C	1:A:207:ILE:HG12	2.43	0.42
2:E:115:VAL:C	2:E:116:PHE:CD2	2.98	0.42
1:B:181:MET:HE2	1:B:183:VAL:HG22	2.02	0.42
3:D:138:LEU:HD12	3:D:139:GLY:N	2.35	0.42
1:A:235:ARG:HD2	1:A:235:ARG:HA	1.88	0.42
2:C:142:ARG:HD2	6:C:409:HOH:O	2.19	0.42
2:E:35:TRP:CE2	2:E:73:LEU:HB2	2.54	0.42
3:F:82(A)[B]:SER:O	3:F:82(B):SER:C	2.61	0.42
2:C:58:VAL:HA	2:C:59:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:117:LYS:HD3	3:D:175:LEU:HD21	1.96	0.42
2:E:124:GLN:HG2	2:E:129:THR:O	2.19	0.42
1:B:114:TYR:HA	1:B:118:VAL:O	2.19	0.42
2:C:195:GLU:HB2	2:C:206:THR:HB	2.02	0.42
3:D:61:ASP:C	3:D:63:VAL:N	2.77	0.42
3:D:201:LYS:N	3:D:202:PRO:HD3	2.35	0.42
2:C:78:LEU:HD21	2:C:106:ILE:CD1	2.50	0.41
3:D:6:GLN:N	3:D:105:GLN:HE22	2.18	0.41
2:E:118:PHE:CE1	3:F:124:LEU:HB3	2.52	0.41
3:F:185:PRO:O	3:F:188:SER:OG	2.38	0.41
2:C:143:GLU:CD	2:C:143:GLU:N	2.74	0.41
3:F:186:SER:C	3:F:188:SER:N	2.75	0.41
2:C:78:LEU:HD21	2:C:106:ILE:HD12	2.01	0.41
3:D:12:VAL:HG21	3:D:82(C):LEU:CD1	2.50	0.41
2:E:58:VAL:HA	2:E:59:PRO:HD3	1.90	0.41
2:E:203:SER:O	2:E:204:PRO:C	2.63	0.41
1:B:97:PHE:HB2	3:D:52:SER:HB3	2.02	0.41
3:D:182:VAL:HG22	3:D:183:THR:H	1.86	0.41
2:C:94:LEU:HD23	2:C:96:TYR:CZ	2.54	0.41
1:A:95:ASN:OD1	1:A:98:THR:N	2.45	0.41
1:A:177:THR:HB	1:A:178:PRO:HD2	2.02	0.41
2:E:194:CYS:O	2:E:206:THR:HA	2.21	0.41
3:D:11:LEU:HA	3:D:110:THR:O	2.20	0.41
3:D:154:TRP:HB2	3:D:159:LEU:HB2	2.03	0.41
2:C:114:SER:HB2	2:C:137:ASN:HB3	2.03	0.41
2:C:194:CYS:O	2:C:206:THR:HA	2.20	0.41
3:D:123:PRO:HA	3:D:140:CYS:CB	2.50	0.41
3:D:182:VAL:CG2	3:D:183:THR:H	2.33	0.41
1:A:231:LEU:HD23	1:A:231:LEU:HA	1.92	0.41
6:A:260:HOH:O	3:F:99:TYR:HB2	2.20	0.41
1:A:234:PHE:O	1:A:238:ILE:HG13	2.20	0.41
3:F:173:SER:N	6:F:385:HOH:O	2.53	0.41
1:B:117:MET:CE	6:B:357:HOH:O	2.65	0.41
2:C:58:VAL:HG13	2:C:59:PRO:HD2	2.02	0.41
1:A:165:GLN:NE2	1:A:230:ARG:NH2	2.68	0.41
2:E:14:SER:O	2:E:17:ASP:HB2	2.21	0.41
3:F:64:LYS:HB3	3:F:64:LYS:HE2	1.86	0.41
2:C:71:PHE:HA	4:C:216:EDO:O2	2.20	0.41
1:A:110:LYS:HB2	1:A:110:LYS:HE3	1.68	0.41
2:C:146:VAL:HG22	2:C:196:VAL:CB	2.51	0.40
3:D:12:VAL:HG21	3:D:82(C):LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:183:THR:CA	3:D:184:VAL:CG2	2.70	0.40
1:A:61:PRO:HG3	1:A:88:ILE:HG13	2.03	0.40
2:E:1:ASP:N	6:E:331:HOH:O	2.44	0.40
3:D:18:LEU:HD12	3:D:18:LEU:HA	1.89	0.40
3:F:185:PRO:CB	3:F:188:SER:OG	2.68	0.40
1:B:52:LEU:HD11	1:B:108:LEU:HD21	2.03	0.40
1:A:114:TYR:HA	1:A:118:VAL:O	2.21	0.40
3:F:123:PRO:HG3	3:F:209:LYS:HE2	0.51	0.40
3:F:178:LEU:HD12	3:F:178:LEU:C	2.46	0.40
2:C:150:VAL:CG2	2:C:155:GLN:NE2	2.84	0.40
2:E:55:GLN:HE21	2:E:55:GLN:CA	2.33	0.40
2:E:116:PHE:N	2:E:116:PHE:HD2	2.20	0.40
3:D:213:PRO:CD	6:D:319:HOH:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	243/241 (101%)	235 (97%)	8 (3%)	0	100	100
1	B	242/241 (100%)	237 (98%)	5 (2%)	0	100	100
2	C	208/214 (97%)	198 (95%)	9 (4%)	1 (0%)	24	25
2	E	210/214 (98%)	203 (97%)	5 (2%)	2 (1%)	12	10
3	D	206/257 (80%)	190 (92%)	14 (7%)	2 (1%)	12	10
3	F	221/257 (86%)	210 (95%)	10 (4%)	1 (0%)	24	25
All	All	1330/1424 (93%)	1273 (96%)	51 (4%)	6 (0%)	24	25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	184	VAL
3	D	62	SER
2	E	138	ASN
2	C	127	SER
3	F	123	PRO
2	E	29	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	201/197 (102%)	193 (96%)	8 (4%)	28	35
1	B	200/197 (102%)	193 (96%)	7 (4%)	32	40
2	C	181/186 (97%)	166 (92%)	15 (8%)	10	10
2	E	182/186 (98%)	164 (90%)	18 (10%)	7	6
3	D	174/210 (83%)	167 (96%)	7 (4%)	28	35
3	F	185/210 (88%)	170 (92%)	15 (8%)	11	11
All	All	1123/1186 (95%)	1053 (94%)	70 (6%)	16	17

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	48	SER
1	B	86	LYS
1	B	110	LYS
1	B	116	SER
1	B	129	VAL
1	B	195	SER
1	B	239	LYS
2	C	7	SER
2	C	12	SER
2	C	30	SER
2	C	33	LEU
2	C	56	SER
2	C	67	SER

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Mol	Chain	Res	Type
2	C	94	LEU
2	C	97	THR
2	C	126	LYS
2	C	127	SER
2	C	145	LYS
2	C	170	ASP
2	C	188	LYS
2	C	205	VAL
2	C	206	THR
3	D	21	SER
3	D	63	VAL
3	D	64	LYS
3	D	68	THR
3	D	181	VAL
3	D	183	THR
3	D	197	ASN
1	A	33	LEU
1	A	36	LEU
1	A	38	GLN
1	A	75	GLN
1	A	119[A]	ARG
1	A	119[B]	ARG
1	A	165	GLN
1	A	207	ILE
2	E	22	THR
2	E	24	ARG
2	E	30	SER
2	E	33	LEU
2	E	48	ILE
2	E	56	SER
2	E	93	ASN
2	E	108	ARG
2	E	110	VAL
2	E	116	PHE
2	E	136	LEU
2	E	138	ASN
2	E	169	LYS
2	E	170	ASP
2	E	185	ASP
2	E	201	LEU
2	E	205	VAL
2	E	207	LYS

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Mol	Chain	Res	Type
3	F	1	GLN
3	F	63	VAL
3	F	85	GLU
3	F	113	SER
3	F	122	PHE
3	F	138	LEU
3	F	143	LYS
3	F	161	SER
3	F	170	LEU
3	F	186	SER
3	F	187	SER
3	F	188	SER
3	F	195	ILE
3	F	201	LYS
3	F	207	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	128	HIS
1	B	192	GLN
2	C	55	GLN
2	C	79	GLN
2	C	93	ASN
2	C	198	HIS
2	C	199	GLN
3	D	6	GLN
3	D	76	ASN
3	D	171	GLN
1	A	38	GLN
1	A	50	ASN
1	A	128	HIS
1	A	165	GLN
1	A	174	GLN
1	A	175	GLN
1	A	223	ASN
2	E	55	GLN
2	E	124	GLN
2	E	137	ASN
2	E	189	HIS
2	E	198	HIS
3	F	1	GLN

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Mol	Chain	Res	Type
3	F	81	GLN
3	F	100(F)	GLN
3	F	164	HIS
3	F	171	GLN
3	F	197	ASN
3	F	199	ASN

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 ⓘ

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	A	13	-	3,3,3	0.41	0	2,2,2	0.38	0
4	EDO	A	2	-	3,3,3	0.39	0	2,2,2	0.97	0
4	EDO	B	8	-	3,3,3	0.31	0	2,2,2	0.18	0
5	SO4	E	215	-	4,4,4	0.24	0	6,6,6	0.15	0
4	EDO	B	7	-	3,3,3	0.26	0	2,2,2	0.32	0
4	EDO	E	216	-	3,3,3	0.20	0	2,2,2	1.13	0
4	EDO	C	217	-	3,3,3	0.40	0	2,2,2	0.45	0
4	EDO	B	4	-	3,3,3	0.30	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	1	-	3,3,3	0.45	0	2,2,2	0.14	0
4	EDO	D	243	-	3,3,3	0.19	0	2,2,2	1.02	0
4	EDO	B	6	-	3,3,3	0.41	0	2,2,2	0.56	0
5	SO4	C	215	-	4,4,4	0.24	0	6,6,6	0.11	0
4	EDO	A	12	-	3,3,3	0.28	0	2,2,2	0.54	0
4	EDO	B	3	-	3,3,3	0.55	0	2,2,2	0.52	0
4	EDO	C	216	-	3,3,3	0.45	0	2,2,2	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	13	-	-	1/1/1/1	-
4	EDO	A	2	-	-	1/1/1/1	-
4	EDO	B	8	-	-	1/1/1/1	-
4	EDO	B	7	-	-	0/1/1/1	-
4	EDO	E	216	-	-	0/1/1/1	-
4	EDO	C	217	-	-	1/1/1/1	-
4	EDO	B	4	-	-	1/1/1/1	-
4	EDO	B	1	-	-	0/1/1/1	-
4	EDO	D	243	-	-	1/1/1/1	-
4	EDO	B	6	-	-	0/1/1/1	-
4	EDO	A	12	-	-	1/1/1/1	-
4	EDO	B	3	-	-	0/1/1/1	-
4	EDO	C	216	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	217	EDO	O1-C1-C2-O2
4	A	2	EDO	O1-C1-C2-O2
4	B	4	EDO	O1-C1-C2-O2
4	B	8	EDO	O1-C1-C2-O2
4	A	12	EDO	O1-C1-C2-O2
4	A	13	EDO	O1-C1-C2-O2
4	D	243	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	13	EDO	3	0
4	A	2	EDO	5	0
4	B	8	EDO	1	0
4	B	7	EDO	5	0
4	C	217	EDO	2	0
4	B	4	EDO	3	0
4	B	1	EDO	3	0
4	D	243	EDO	3	0
4	B	6	EDO	6	0
4	A	12	EDO	1	0
4	B	3	EDO	3	0
4	C	216	EDO	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	43:LYS	C	44:GLY	N	1.20

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	241/241 (100%)	-0.16	2 (0%) 82 82	11, 30, 47, 74	5 (2%)
1	B	241/241 (100%)	-0.34	3 (1%) 76 76	11, 26, 44, 63	4 (1%)
2	C	210/214 (98%)	0.88	58 (27%) 1 1	16, 37, 122, 138	0
2	E	211/214 (98%)	0.49	27 (12%) 7 6	15, 37, 90, 110	1 (0%)
3	D	211/257 (82%)	0.83	42 (19%) 3 2	17, 42, 95, 111	1 (0%)
3	F	224/257 (87%)	0.65	31 (13%) 6 6	19, 44, 83, 108	1 (0%)
All	All	1338/1424 (93%)	0.37	163 (12%) 8 7	11, 33, 95, 138	12 (0%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	189	LEU	7.5
3	D	138	LEU	6.3
3	D	185	PRO	5.9
3	D	126	PRO	5.8
3	D	125	ALA	5.7
3	D	195	ILE	5.7
2	C	209	PHE	5.5
2	C	184	ALA	5.4
3	D	158	ALA	5.3
3	D	184	VAL	5.1
3	D	193	THR	5.0
2	C	125	LEU	5.0
2	C	192	TYR	4.9
2	C	146	VAL	4.8
2	C	119	PRO	4.5
3	D	157	GLY	4.4
2	C	201	LEU	4.3
2	C	154	LEU	4.2
2	C	181	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
2	C	132	VAL	4.2
3	F	195	ILE	4.2
2	C	121	SER	4.1
2	C	133	VAL	4.1
2	C	191	VAL	4.1
2	C	117	ILE	4.0
3	F	214	LYS	4.0
2	E	148	TRP	3.9
2	E	125	LEU	3.8
2	C	205	VAL	3.8
3	F	191	THR	3.8
3	D	122	PHE	3.7
3	D	182	VAL	3.7
2	C	120	PRO	3.7
3	D	213	PRO	3.7
3	D	124	LEU	3.6
3	D	139	GLY	3.6
3	D	214	LYS	3.6
3	D	210	LYS	3.6
3	F	209	LYS	3.6
2	C	179	LEU	3.5
2	C	157	GLY	3.5
2	C	150	VAL	3.4
2	C	153	ALA	3.4
3	F	188	SER	3.4
2	C	210	ASN	3.4
2	E	121	SER	3.4
3	D	159	LEU	3.4
2	C	180	THR	3.3
2	C	206	THR	3.3
3	F	185	PRO	3.3
2	C	186	TYR	3.3
3	D	172	SER	3.2
3	F	132	SER	3.2
2	E	146	VAL	3.2
2	E	191	VAL	3.2
2	E	192	TYR	3.2
2	C	148	TRP	3.1
2	E	153	ALA	3.1
3	D	211	VAL	3.1
2	C	131	SER	3.1
2	E	154	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	194	TYR	3.0
3	F	126	PRO	3.0
2	C	203	SER	3.0
2	E	126	LYS	3.0
3	D	123	PRO	3.0
2	C	149	LYS	3.0
2	C	118	PHE	3.0
3	D	121	VAL	3.0
3	F	190	GLY	3.0
3	D	208	ASP	2.9
3	D	120	SER	2.9
3	D	155	ASN	2.9
3	F	207	VAL	2.9
1	B	204(A)	ASP	2.9
2	C	194	CYS	2.9
2	E	185	ASP	2.8
2	E	117	ILE	2.8
2	C	122	ASP	2.8
3	D	156	SER	2.8
1	A	24	GLU	2.8
2	C	188	LYS	2.8
2	C	156	SER	2.7
2	E	118	PHE	2.7
2	C	190	LYS	2.7
3	F	158	ALA	2.6
2	C	116	PHE	2.6
2	E	206	THR	2.6
2	E	209	PHE	2.6
2	E	150	VAL	2.6
2	E	152	ASN	2.6
3	F	136	ALA	2.6
2	C	151	ASP	2.6
2	C	207	LYS	2.6
3	D	209	LYS	2.6
2	E	202	SER	2.6
2	C	128	GLY	2.6
3	F	193	THR	2.6
2	E	119	PRO	2.6
3	F	213	PRO	2.6
3	D	173	SER	2.6
2	C	187	GLU	2.5
3	F	208	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	36	LEU	2.5
3	D	154	TRP	2.5
2	C	196	VAL	2.5
3	D	163	VAL	2.5
3	D	212	GLU	2.5
3	F	133	GLY	2.5
2	C	130	ALA	2.5
2	E	193	ALA	2.5
2	C	135	LEU	2.5
2	C	189	HIS	2.5
2	C	200	GLY	2.5
2	C	152	ASN	2.5
2	E	184	ALA	2.4
2	E	122	ASP	2.4
2	C	134	CYS	2.4
2	E	194	CYS	2.4
3	D	140	CYS	2.4
2	C	127	SER	2.4
3	D	153	SER	2.4
3	F	123	PRO	2.4
2	C	147	GLN	2.4
2	C	185	ASP	2.4
2	E	205	VAL	2.4
2	C	60	SER	2.3
3	F	160	THR	2.3
2	E	115	VAL	2.3
3	D	181	VAL	2.3
3	F	150	VAL	2.3
2	C	155	GLN	2.3
2	C	112	ALA	2.3
2	C	182	SER	2.3
3	F	140	CYS	2.3
1	B	204	ALA	2.3
2	C	193	ALA	2.3
3	F	53	SER	2.2
2	C	204	PRO	2.2
3	F	184	VAL	2.2
2	E	186	TYR	2.2
3	F	194	TYR	2.2
2	C	202	SER	2.2
3	D	199	ASN	2.2
3	D	161	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	120	SER	2.2
3	F	211	VAL	2.2
3	D	17	SER	2.2
3	F	161	SER	2.2
2	E	210	ASN	2.2
3	D	160	THR	2.2
3	F	122	PHE	2.1
1	B	79	GLY	2.1
2	E	203	SER	2.1
3	F	124	LEU	2.1
3	D	12	VAL	2.1
3	D	170	LEU	2.1
3	F	210	LYS	2.1
3	F	125	ALA	2.1
3	D	207	VAL	2.0
2	C	159	SER	2.0
2	C	24	ARG	2.0
3	D	174	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	12	4/4	0.76	0.17	59,60,61,65	0
4	EDO	A	13	4/4	0.83	0.17	33,39,45,54	0
4	EDO	C	216	4/4	0.88	0.21	44,46,53,53	0
4	EDO	A	2	4/4	0.89	0.12	40,42,42,54	0
4	EDO	B	7	4/4	0.89	0.19	47,53,61,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	4	4/4	0.89	0.13	40,45,48,52	0
4	EDO	B	8	4/4	0.90	0.10	42,42,53,61	0
4	EDO	B	3	4/4	0.92	0.13	21,38,41,47	0
4	EDO	B	1	4/4	0.92	0.14	55,60,61,63	0
4	EDO	D	243	4/4	0.93	0.23	58,61,64,64	0
4	EDO	B	6	4/4	0.93	0.12	23,27,31,32	0
5	SO4	C	215	5/5	0.93	0.10	60,64,70,77	0
4	EDO	C	217	4/4	0.94	0.10	42,43,44,48	0
4	EDO	E	216	4/4	0.95	0.10	48,51,51,55	0
5	SO4	E	215	5/5	0.95	0.12	51,57,63,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.