



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:25 AM UTC

PDB ID : 8VIS / pdb_00008vis
Title : Human TMPRSS11D complexed with a disulfide-linked autoinhibitory DDDDK peptide
Authors : Fraser, B.J.; Dong, A.; Ilyassov, O.; Kenney, T.; Li, Y.Y.; Seitova, A.; Li, Y.; Hejazi, Z.; Edwards, A.; Benard, F.; Arrowsmith, C.
Deposited on : 2024-01-05
Resolution : 1.59 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

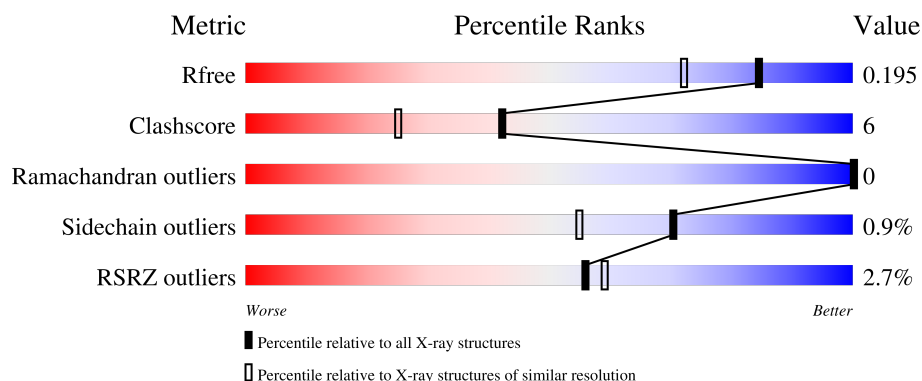
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	145	
1	C	145	
1	E	145	
1	G	145	
2	B	244	

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Mol	Chain	Length	Quality of chain
2	D	244	84% 11%
2	F	244	2% 86% 9%
2	H	244	2% 86% 9% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9337 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 Transmembrane protease serine 11D non-catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	15	Total	C	N	O	S	0	0	0
			108	62	16	29	1			
1	C	22	Total	C	N	O	S	0	0	0
			164	99	26	38	1			
1	E	20	Total	C	N	O	S	0	0	0
			151	90	24	36	1			
1	G	21	Total	C	N	O	S	0	0	0
			159	96	25	37	1			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ALA	-	expression tag	UNP O60235
A	43	ALA	-	expression tag	UNP O60235
A	182	ASP	LEU	engineered mutation	UNP O60235
A	183	ASP	SER	engineered mutation	UNP O60235
A	184	ASP	GLU	engineered mutation	UNP O60235
A	185	ASP	GLN	engineered mutation	UNP O60235
A	186	LYS	ARG	engineered mutation	UNP O60235
C	42	ALA	-	expression tag	UNP O60235
C	43	ALA	-	expression tag	UNP O60235
C	182	ASP	LEU	engineered mutation	UNP O60235
C	183	ASP	SER	engineered mutation	UNP O60235
C	184	ASP	GLU	engineered mutation	UNP O60235
C	185	ASP	GLN	engineered mutation	UNP O60235
C	186	LYS	ARG	engineered mutation	UNP O60235
E	42	ALA	-	expression tag	UNP O60235
E	43	ALA	-	expression tag	UNP O60235
E	182	ASP	LEU	engineered mutation	UNP O60235
E	183	ASP	SER	engineered mutation	UNP O60235
E	184	ASP	GLU	engineered mutation	UNP O60235
E	185	ASP	GLN	engineered mutation	UNP O60235
E	186	LYS	ARG	engineered mutation	UNP O60235

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Chain	Residue	Modelled	Actual	Comment	Reference
G	42	ALA	-	expression tag	UNP O60235
G	43	ALA	-	expression tag	UNP O60235
G	182	ASP	LEU	engineered mutation	UNP O60235
G	183	ASP	SER	engineered mutation	UNP O60235
G	184	ASP	GLU	engineered mutation	UNP O60235
G	185	ASP	GLN	engineered mutation	UNP O60235
G	186	LYS	ARG	engineered mutation	UNP O60235

- Molecule 2 is a protein called Transmembrane protease serine 11D catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	19	1
			1884	1186	333	354	11			
2	D	236	Total	C	N	O	S	0	14	0
			1893	1189	340	352	12			
2	F	234	Total	C	N	O	S	0	23	0
			1923	1209	340	362	12			
2	H	233	Total	C	N	O	S	0	17	0
			1878	1180	343	344	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	419	GLU	-	expression tag	UNP O60235
B	420	PHE	-	expression tag	UNP O60235
B	421	VAL	-	expression tag	UNP O60235
B	422	GLU	-	expression tag	UNP O60235
B	423	HIS	-	expression tag	UNP O60235
B	424	HIS	-	expression tag	UNP O60235
B	425	HIS	-	expression tag	UNP O60235
B	426	HIS	-	expression tag	UNP O60235
B	427	HIS	-	expression tag	UNP O60235
B	428	HIS	-	expression tag	UNP O60235
B	429	HIS	-	expression tag	UNP O60235
B	430	HIS	-	expression tag	UNP O60235
D	419	GLU	-	expression tag	UNP O60235
D	420	PHE	-	expression tag	UNP O60235
D	421	VAL	-	expression tag	UNP O60235
D	422	GLU	-	expression tag	UNP O60235
D	423	HIS	-	expression tag	UNP O60235
D	424	HIS	-	expression tag	UNP O60235
D	425	HIS	-	expression tag	UNP O60235

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Chain	Residue	Modelled	Actual	Comment	Reference
D	426	HIS	-	expression tag	UNP O60235
D	427	HIS	-	expression tag	UNP O60235
D	428	HIS	-	expression tag	UNP O60235
D	429	HIS	-	expression tag	UNP O60235
D	430	HIS	-	expression tag	UNP O60235
F	419	GLU	-	expression tag	UNP O60235
F	420	PHE	-	expression tag	UNP O60235
F	421	VAL	-	expression tag	UNP O60235
F	422	GLU	-	expression tag	UNP O60235
F	423	HIS	-	expression tag	UNP O60235
F	424	HIS	-	expression tag	UNP O60235
F	425	HIS	-	expression tag	UNP O60235
F	426	HIS	-	expression tag	UNP O60235
F	427	HIS	-	expression tag	UNP O60235
F	428	HIS	-	expression tag	UNP O60235
F	429	HIS	-	expression tag	UNP O60235
F	430	HIS	-	expression tag	UNP O60235
H	419	GLU	-	expression tag	UNP O60235
H	420	PHE	-	expression tag	UNP O60235
H	421	VAL	-	expression tag	UNP O60235
H	422	GLU	-	expression tag	UNP O60235
H	423	HIS	-	expression tag	UNP O60235
H	424	HIS	-	expression tag	UNP O60235
H	425	HIS	-	expression tag	UNP O60235
H	426	HIS	-	expression tag	UNP O60235
H	427	HIS	-	expression tag	UNP O60235
H	428	HIS	-	expression tag	UNP O60235
H	429	HIS	-	expression tag	UNP O60235
H	430	HIS	-	expression tag	UNP O60235

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

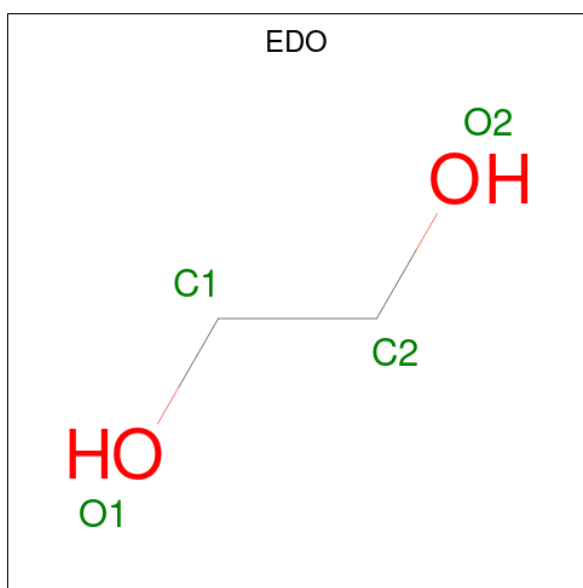
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total 2	X 2	0	0
6	F	1	Total 1	X 1	0	0
6	H	2	Total 2	X 2	0	0

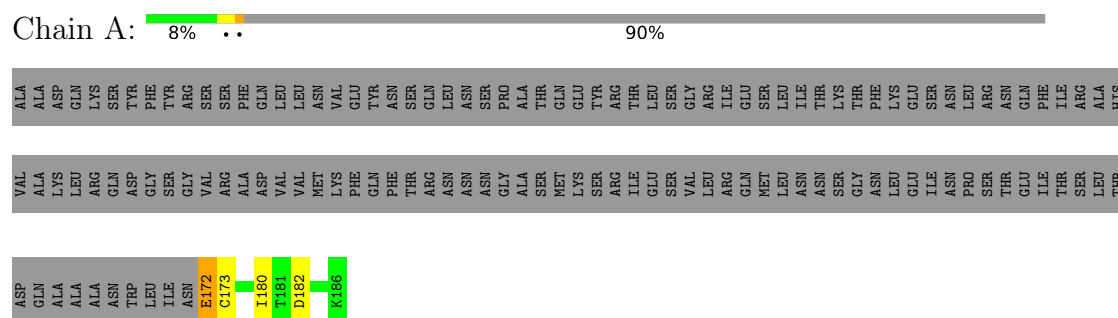
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	25	Total 25	O 25	0	0
7	B	256	Total 256	O 256	0	0
7	C	43	Total 43	O 43	0	0
7	D	267	Total 267	O 267	0	0
7	E	27	Total 27	O 27	0	0
7	F	270	Total 270	O 270	0	0
7	G	16	Total 16	O 16	0	0
7	H	245	Total 245	O 245	0	0

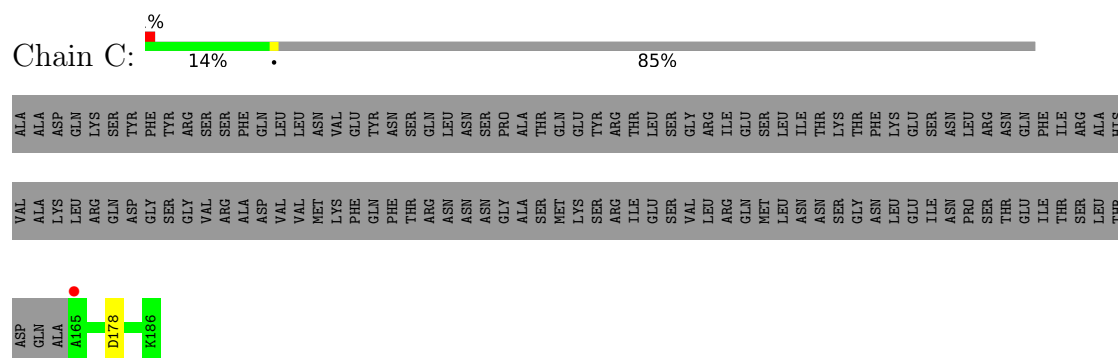
3 Residue-property plots

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.

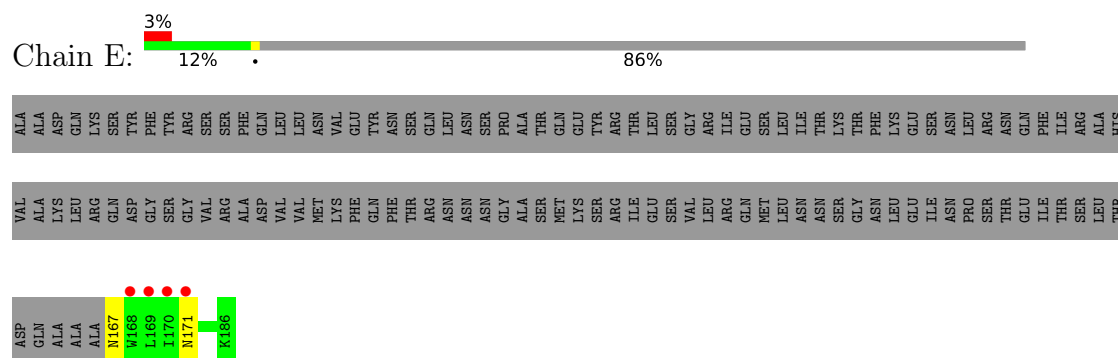
- Molecule 1: Transmembrane protease serine 11D non-catalytic chain



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- Molecule 1: Transmembrane protease serine 11D non-catalytic chain

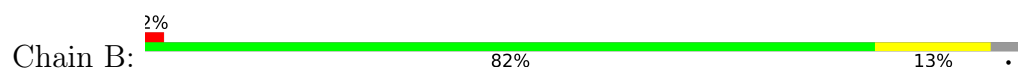


ALA ALA ASP GLN LYS SER TYR PHE TYR ARG SER SER PHE GLN LEU LEU VAL ASN VAL GLU TYR ASN SER PRO GLY THR THR THR SER SER SER GLY ARG ILE GLU MET SER LEU LEU ILE THR LYS THR PHE LYS GLU SER ASN LEU ARG ASN ARG PHE ILE THR

VAL ALA LYS LEU ARG GLN ASP GLY SER GLY VAL ARG ALA ASP VAL VAL MET MET PHE GLN PHE THR ARG ASN ASN ASN GLY ALA ALA MET MET LYS SER ARG VAL LEU ARG GLN MET SER ASN SER GLY ASN LEU ILE ASN PRO SER THR GLU THR THR SER LEU THR ARG THR

ASP GLN ALA A166 L169 I179 T180 T181 K186

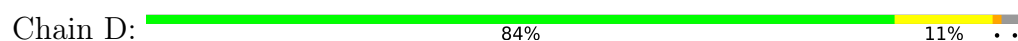
- Molecule 2: Transmembrane protease serine 11D catalytic chain



I187 T191 E196 C212 N219 M220 W221 C228 T244 S245 K250 L251 R252 R256 I258 L259 T268 H269 E270 L288 E315 Y316 A317 G318 E323 D336 L348 L352 P357 D362 A363 C364 S368 Q392 D410 R413 Q414

G417 I418 E419 F420 VAL GLU HIS HIS HIS HIS HIS HIS HIS

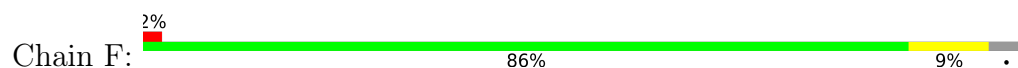
- Molecule 2: Transmembrane protease serine 11D catalytic chain



I187 W200 L204 C212 N207 M220 C228 S231 T247 R256 A267 T268 H269 E270 R277 V291 P294 P301 G318 L348 L352 S368 E375 R378 R379 I383 V384 G385 T403 L409 D410 W411 I412 R413 E419 F420 V421

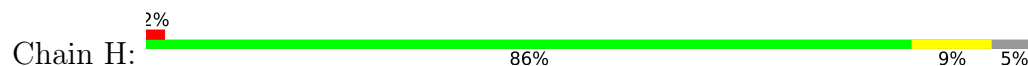
E422 HIS HIS HIS HIS HIS HIS HIS

- Molecule 2: Transmembrane protease serine 11D catalytic chain



I187 L188 L204 C212 C228 F229 W238 L244 S245 R252 R253 R254 L259 T268 H269 E270 E315 T316 A317 G318 S333 V334 D336 L348 P357 Q358 Q359 G360 V361 D362 P396 Q415 F420 VAL GLU HIS HIS HIS HIS HIS HIS HIS

- Molecule 2: Transmembrane protease serine 11D catalytic chain



I187 W200 L204 C212 C228 F229 R230 R236 F248 E270 R277 L278 E279 K286 V291 G318 R330 L348 L352 P371 L372 V373 Q374 E375 R379 L380 W381 G385 P396 T403 R413 I418 E419 PHE VAL GLU HIS HIS HIS HIS

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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.68Å 119.68Å 134.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.77 – 1.59 49.77 – 1.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.77-1.59) 100.0 (49.77-1.59)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.59Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.155 , 0.187 0.168 , 0.195	Depositor DCC
R_{free} test set	1331 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.7	Xtrriage
Anisotropy	0.066	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9337	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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 21.87 % 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 6.4028e-03. 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.73	0/108	1.08	0/144
1	C	0.68	0/166	1.06	0/225
1	E	0.65	0/153	1.02	0/207
1	G	0.64	0/161	1.06	0/218
2	B	0.67	0/1975	0.93	3/2695 (0.1%)
2	D	0.67	0/1981	0.94	2/2701 (0.1%)
2	F	0.66	0/2021	0.95	1/2754 (0.0%)
2	H	0.68	0/1977	0.91	3/2692 (0.1%)
All	All	0.67	0/8542	0.94	9/11636 (0.1%)

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	B	0	5
2	D	0	2
2	F	0	2
2	H	0	3
All	All	0	12

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	207	ASN	CA-CB-CG	8.09	120.69	112.60
2	D	301	PRO	N-CA-CB	6.01	106.34	103.22
2	B	362	ASP	CA-CB-CG	5.80	118.40	112.60
2	B	256[A]	ARG	NE-CZ-NH2	5.71	124.34	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	256[B]	ARG	NE-CZ-NH2	5.71	124.34	119.20
2	F	362	ASP	CA-CB-CG	5.29	117.89	112.60
2	H	279[A]	GLU	CA-C-O	5.06	125.78	120.42
2	H	279[B]	GLU	CA-C-O	5.06	125.78	120.42
2	H	279[C]	GLU	CA-C-O	5.06	125.78	120.42

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	252[A]	ARG	Sidechain
2	B	252[C]	ARG	Sidechain
2	B	256[A]	ARG	Sidechain
2	B	256[B]	ARG	Sidechain
2	B	413	ARG	Sidechain
2	D	277	ARG	Sidechain
2	D	378	ARG	Sidechain
2	F	252[A]	ARG	Sidechain
2	F	252[B]	ARG	Sidechain
2	H	330[A]	ARG	Sidechain
2	H	330[B]	ARG	Sidechain
2	H	413	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	108	0	88	4	0
1	C	164	0	143	2	0
1	E	151	0	123	1	0
1	G	159	0	138	2	0
2	B	1884	0	1836	29	0
2	D	1893	0	1844	32	0
2	F	1923	0	1871	17	0
2	H	1878	0	1840	19	0
3	A	1	0	0	0	0
3	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1	0	0	0	0
4	B	6	0	8	0	0
4	D	6	0	8	2	0
5	B	4	0	6	1	0
5	H	4	0	6	0	0
6	D	2	0	0	0	0
6	F	1	0	0	0	0
6	H	2	0	0	0	0
7	A	25	0	0	1	0
7	B	256	0	0	4	1
7	C	43	0	0	0	0
7	D	267	0	0	4	1
7	E	27	0	0	0	0
7	F	270	0	0	3	0
7	G	16	0	0	2	0
7	H	245	0	0	3	0
All	All	9337	0	7911	99	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 6.

All (99) 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:B:219[B]:ASN:ND2	7:B:601:HOH:O	1.76	1.15
2:H:230[B]:ARG:HH21	2:H:230[B]:ARG:HG2	1.22	0.99
2:B:191[B]:THR:HG21	2:D:231:SER:O	1.66	0.94
2:F:259[A]:LEU:HD11	2:F:415:GLN:OE1	1.73	0.89
2:D:413[A]:ARG:HD2	2:D:419:GLU:OE2	1.75	0.87
2:D:270[B]:GLU:HG2	2:D:348:LEU:HD12	1.57	0.86
2:F:420:PHE:HB2	7:F:628:HOH:O	1.77	0.85
2:B:256[B]:ARG:HD2	2:B:257:ASN:OD1	1.78	0.83
2:B:270[B]:GLU:HG2	2:B:348:LEU:HD12	1.69	0.75
2:B:392:GLN:NE2	7:B:605:HOH:O	2.23	0.70
2:D:220:MET:HE3	7:D:609:HOH:O	1.91	0.69
2:B:195[B]:GLU:OE1	7:B:602:HOH:O	2.11	0.67
2:B:323:GLU:OE1	7:B:603:HOH:O	2.12	0.67
2:F:228[B]:CYS:SG	2:F:238:TRP:CH2	2.88	0.67
1:A:172:GLU:O	7:A:601:HOH:O	2.13	0.67
2:H:277[B]:ARG:NH1	7:H:601:HOH:O	2.29	0.65
2:F:259[A]:LEU:C	2:F:259[A]:LEU:HD23	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:270[B]:GLU:HG2	2:F:348:LEU:HD12	1.80	0.62
2:B:410[B]:ASP:OD2	2:B:414:GLN:NE2	2.33	0.61
2:D:207:ASN:ND2	7:D:601:HOH:O	2.23	0.60
2:B:256[B]:ARG:CD	2:B:257:ASN:OD1	2.50	0.60
2:B:315:GLU:OE2	2:B:318[B]:GLY:HA3	2.02	0.59
2:F:228[B]:CYS:SG	2:F:229:PHE:CE1	2.96	0.59
2:B:212[B]:CYS:HB2	2:B:368:SER:O	2.03	0.58
2:H:230[B]:ARG:HG2	2:H:230[B]:ARG:NH2	2.00	0.58
2:D:268:THR:OG1	2:D:270[B]:GLU:HG3	2.04	0.58
2:B:316[B]:TYR:O	2:B:317[B]:ALA:HB3	2.04	0.56
2:B:335:ASP:OD2	2:F:333[B]:SER:HB2	2.04	0.56
2:D:411:TRP:HB2	4:D:500:GOL:H32	1.86	0.56
2:B:195[B]:GLU:OE2	2:B:250:LYS:HD2	2.06	0.56
2:B:268:THR:OG1	2:B:270[B]:GLU:HG3	2.06	0.56
2:F:357:PRO:HB3	2:H:318:GLY:O	2.06	0.56
2:B:191[B]:THR:CG2	2:D:231:SER:O	2.50	0.56
2:F:254[A]:ARG:NH1	7:F:606:HOH:O	2.38	0.56
1:A:173:CYS:HB3	5:B:502:EDO:H21	1.87	0.56
2:F:315:GLU:OE2	2:F:318[A]:GLY:HA3	2.06	0.56
2:H:204:LEU:HB2	2:H:212[B]:CYS:SG	2.47	0.55
2:D:413[C]:ARG:HH11	2:D:413[C]:ARG:HG2	1.70	0.55
2:B:270[B]:GLU:HG2	2:B:348:LEU:CD1	2.36	0.55
2:D:413[C]:ARG:HG2	2:D:413[C]:ARG:NH1	2.21	0.55
2:H:379[B]:ARG:HG3	2:H:379[B]:ARG:HH11	1.73	0.53
2:H:270[B]:GLU:HG2	2:H:348:LEU:HD12	1.88	0.53
2:D:277:ARG:NH2	7:D:607:HOH:O	2.41	0.53
2:F:244:ILE:HD12	2:F:244:ILE:C	2.34	0.52
2:H:286[B]:LYS:CG	7:H:785:HOH:O	2.57	0.52
2:D:212[B]:CYS:HB2	2:D:368:SER:O	2.11	0.51
2:F:188:LEU:HD23	2:F:360:GLY:O	2.11	0.50
2:D:277:ARG:HH11	2:D:277:ARG:HG2	1.75	0.50
2:F:244:ILE:HD12	2:F:245:SER:N	2.26	0.49
1:A:180:ILE:HD12	1:A:182:ASP:HB2	1.95	0.49
2:H:212[B]:CYS:CB	2:H:228:CYS:SG	3.01	0.48
2:D:409:LEU:O	2:D:413[C]:ARG:HG2	2.13	0.48
2:D:352:LEU:C	2:D:352:LEU:HD23	2.38	0.48
1:E:167:ASN:O	1:E:171:ASN:ND2	2.44	0.48
2:D:270[B]:GLU:HG2	2:D:348:LEU:CD1	2.38	0.47
2:H:230[B]:ARG:HH21	2:H:230[B]:ARG:CG	2.10	0.47
2:B:244:ILE:HD12	2:B:245:SER:N	2.30	0.47
2:D:411:TRP:HB2	4:D:500:GOL:C3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:PRO:HB3	2:D:318:GLY:O	2.14	0.47
2:F:259[A]:LEU:HD23	2:F:259[A]:LEU:O	2.14	0.47
2:H:212[B]:CYS:SG	2:H:228:CYS:SG	3.12	0.47
2:D:413[C]:ARG:CZ	2:D:420:PHE:HB2	2.46	0.46
1:A:180:ILE:HD13	2:D:267:ALA:HA	1.98	0.46
2:B:244:ILE:HD12	2:B:244:ILE:C	2.40	0.46
1:G:181:THR:HG23	7:G:202:HOH:O	2.15	0.45
2:H:230[B]:ARG:NH1	7:H:607:HOH:O	2.50	0.45
2:H:352:LEU:C	2:H:352:LEU:HD23	2.42	0.45
2:D:413[C]:ARG:NE	2:D:420:PHE:HB2	2.32	0.45
2:D:247[B]:THR:HG21	7:D:682:HOH:O	2.15	0.45
2:D:212[B]:CYS:CB	2:D:228:CYS:SG	3.05	0.45
1:G:166:ALA:N	7:G:203:HOH:O	2.50	0.44
2:D:294:PRO:HD3	2:D:383:ILE:O	2.18	0.44
2:B:212[B]:CYS:CB	2:B:228:CYS:SG	3.03	0.44
2:F:268:THR:OG1	2:F:270[B]:GLU:HG3	2.18	0.43
2:D:256[B]:ARG:HE	2:D:277:ARG:HD3	1.84	0.43
2:D:413[C]:ARG:HD2	2:D:419:GLU:HA	2.00	0.43
2:H:375:GLU:HB3	2:H:381:TRP:CE2	2.54	0.42
2:F:204:LEU:HB2	2:F:212[B]:CYS:SG	2.60	0.42
2:H:371:PRO:HB2	2:H:373:VAL:HG13	2.00	0.42
2:F:228[B]:CYS:SG	2:F:229:PHE:CZ	3.13	0.42
2:H:385:GLY:HA2	2:H:403:THR:O	2.20	0.42
1:C:178:ASP:O	2:D:379:ARG:HD3	2.20	0.42
2:B:258:ILE:C	2:B:259[A]:LEU:HD12	2.45	0.41
2:B:212[B]:CYS:SG	2:B:228:CYS:HB3	2.61	0.41
2:H:200:TRP:CG	2:H:291:VAL:HB	2.56	0.41
2:H:236[A]:ARG:HB3	2:H:236[A]:ARG:NH1	2.35	0.41
2:B:259[A]:LEU:HD12	2:B:259[A]:LEU:N	2.36	0.41
2:B:316[A]:TYR:CD1	2:B:392:GLN:HA	2.55	0.41
1:C:178:ASP:OD2	2:D:375:GLU:OE2	2.38	0.41
2:D:200:TRP:CG	2:D:291:VAL:HB	2.56	0.41
2:D:206:LEU:O	2:D:207:ASN:HB2	2.20	0.41
2:D:256[B]:ARG:NE	2:D:277:ARG:HD3	2.36	0.41
2:H:379[B]:ARG:HG3	2:H:379[B]:ARG:NH1	2.35	0.41
2:B:352:LEU:C	2:B:352:LEU:HD12	2.46	0.41
2:D:385:GLY:HA2	2:D:403:THR:O	2.22	0.40
2:B:220:MET:HG3	2:B:221:TRP:CD1	2.57	0.40
2:B:316[A]:TYR:HA	2:B:364:CYS:SG	2.61	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)
7:B:603:HOH:O	7:D:755:HOH:O[4_555]	1.98	0.22

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	13/145 (9%)	12 (92%)	1 (8%)	0	100	100
1	C	20/145 (14%)	19 (95%)	1 (5%)	0	100	100
1	E	18/145 (12%)	17 (94%)	1 (6%)	0	100	100
1	G	19/145 (13%)	19 (100%)	0	0	100	100
2	B	251/244 (103%)	245 (98%)	6 (2%)	0	100	100
2	D	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
2	F	255/244 (104%)	251 (98%)	4 (2%)	0	100	100
2	H	249/244 (102%)	246 (99%)	3 (1%)	0	100	100
All	All	1074/1556 (69%)	1053 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	12/127 (9%)	11 (92%)	1 (8%)	10	1
1	C	17/127 (13%)	17 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	16/127 (13%)	16 (100%)	0	100	100
1	G	17/127 (13%)	17 (100%)	0	100	100
2	B	206/203 (102%)	205 (100%)	1 (0%)	81	70
2	D	207/203 (102%)	206 (100%)	1 (0%)	81	70
2	F	212/203 (104%)	208 (98%)	4 (2%)	50	27
2	H	204/203 (100%)	202 (99%)	2 (1%)	68	50
All	All	891/1320 (68%)	882 (99%)	9 (1%)	70	50

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	GLU
2	B	220	MET
2	D	352	LEU
2	F	259[A]	LEU
2	F	259[B]	LEU
2	F	335[B]	ASP
2	F	335[C]	ASP
2	H	352	LEU
2	H	419	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	271	ASN
2	B	392	GLN
2	D	271	ASN
2	F	271	ASN
2	H	271	ASN
2	H	319	HIS
2	H	374	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic and 5 are unknown - leaving 4 for Mogul analysis.

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	$\# Z > 2$
5	EDO	B	502	-	3,3,3	0.21	0	2,2,2	0.72	0
4	GOL	D	500	-	5,5,5	0.11	0	5,5,5	0.37	0
5	EDO	H	502	-	3,3,3	0.11	0	2,2,2	0.04	0
4	GOL	B	501	-	5,5,5	0.14	0	5,5,5	0.40	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
5	EDO	B	502	-	-	1/1/1/1	-
4	GOL	D	500	-	-	2/4/4/4	-
5	EDO	H	502	-	-	1/1/1/1	-
4	GOL	B	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	500	GOL	O1-C1-C2-C3
4	D	500	GOL	O1-C1-C2-O2
5	B	502	EDO	O1-C1-C2-O2
5	H	502	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	EDO	1	0
4	D	500	GOL	2	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

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	15/145 (10%)	0.13	0 100 100	11, 14, 31, 49	0
1	C	22/145 (15%)	0.34	1 (4%) 38 40	10, 17, 23, 43	0
1	E	20/145 (13%)	0.57	4 (20%) 3 2	12, 16, 50, 55	0
1	G	21/145 (14%)	1.37	5 (23%) 2 1	14, 26, 39, 41	0
2	B	234/244 (95%)	-0.21	5 (2%) 63 67	5, 12, 25, 65	19 (8%)
2	D	236/244 (96%)	-0.15	1 (0%) 88 91	8, 13, 27, 50	14 (5%)
2	F	234/244 (95%)	-0.11	6 (2%) 57 60	6, 13, 25, 50	23 (9%)
2	H	233/244 (95%)	-0.05	5 (2%) 63 67	6, 14, 29, 58	17 (7%)
All	All	1015/1556 (65%)	-0.07	27 (2%) 56 59	5, 13, 28, 65	73 (7%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	420	PHE	6.4
1	C	165	ALA	4.8
2	F	420	PHE	4.5
2	D	421	VAL	4.1
2	B	419	GLU	4.0
2	F	317[A]	ALA	4.0
1	E	168	TRP	3.7
1	E	170	ILE	3.6
2	B	317[A]	ALA	3.5
1	G	181	THR	3.5
1	G	170	ILE	3.1
1	G	169	LEU	3.0
2	F	228[A]	CYS	2.9
1	E	169	LEU	2.6
2	H	418	ILE	2.5
1	G	166	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	419	GLU	2.4
2	B	417	GLY	2.4
1	G	180	ILE	2.4
2	F	318[A]	GLY	2.3
2	B	418	ILE	2.2
2	H	396	PRO	2.2
2	F	396	PRO	2.1
2	H	212[A]	CYS	2.1
2	F	358[A]	GLN	2.1
2	H	248	PHE	2.0
1	E	171	ASN	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
6	UNX	H	503	1/1	0.66	0.17	20,20,20,20	0
6	UNX	H	501	1/1	0.69	0.19	20,20,20,20	0
4	GOL	B	501	6/6	0.72	0.21	41,56,63,65	0
6	UNX	D	502	1/1	0.76	0.12	20,20,20,20	0
5	EDO	H	502	4/4	0.77	0.24	20,20,20,20	0
6	UNX	F	501	1/1	0.79	0.18	35,35,35,35	0
5	EDO	B	502	4/4	0.88	0.11	29,34,36,41	0
4	GOL	D	500	6/6	0.88	0.13	30,35,43,49	0
6	UNX	D	501	1/1	0.91	0.10	20,20,20,20	0
3	MG	H	500	1/1	0.99	0.05	13,13,13,13	0
3	MG	E	500	1/1	0.99	0.05	12,12,12,12	0
3	MG	A	500	1/1	1.00	0.04	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.