Full wwPDB X-ray Structure Validation Report (i)

Jan 21, 2024 – 12:06 PM EST

PDB ID	:	8VIS
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 (i) 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 (i)) were used in the production of this report:

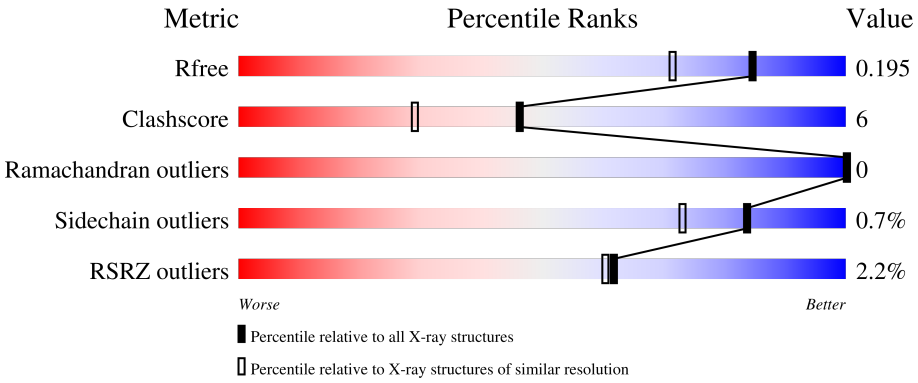
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 <=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	8% · 90%
1	C	145	14% · 85%
1	E	145	3% 12% · 86%
1	G	145	2% 13% · 86%
2	B	244	83% 12% ·

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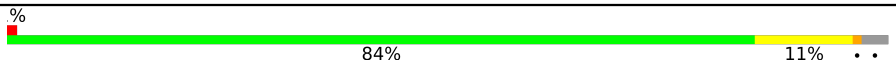
Mol	Chain	Length	Quality of chain
2	D	244	
2	F	244	
2	H	244	

2 Entry composition (i)

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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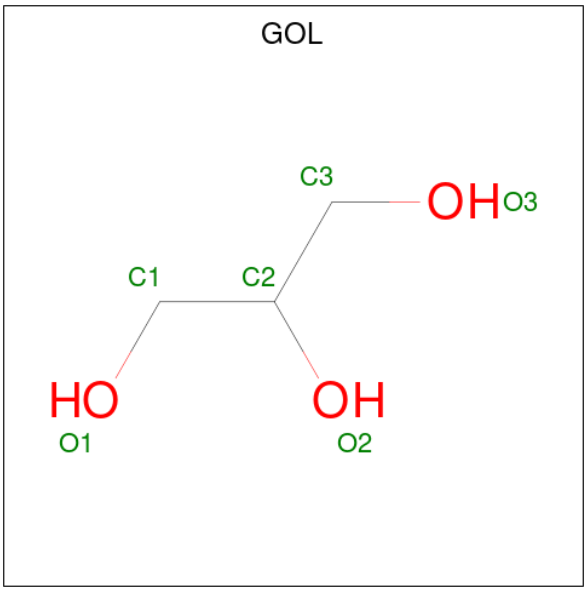
Chain	Residue	Modelled	Actual	Comment	Reference
D	426	HIS	-	expression tag	UNP O60235
D	427	HIS	-	expression tag	UNP O60235
D	428	HIS	-	expression tag	UNP O60235
D	429	HIS	-	expression tag	UNP O60235
D	430	HIS	-	expression tag	UNP O60235
F	419	GLU	-	expression tag	UNP O60235
F	420	PHE	-	expression tag	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 (three-letter code: MG) (formula: Mg).

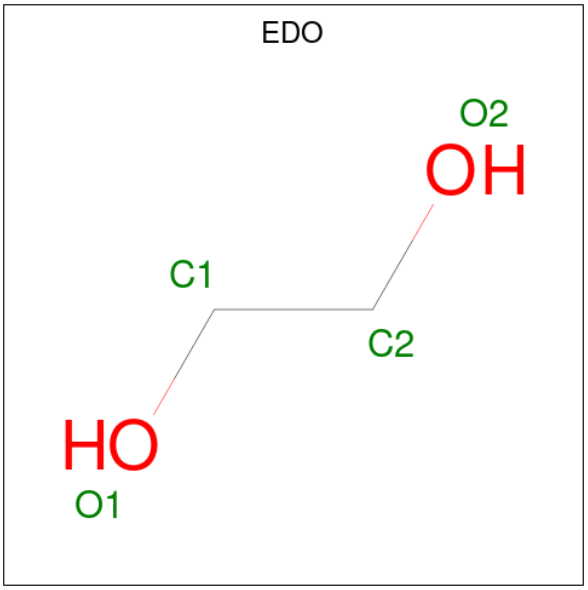
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

- Molecule 7 is water.

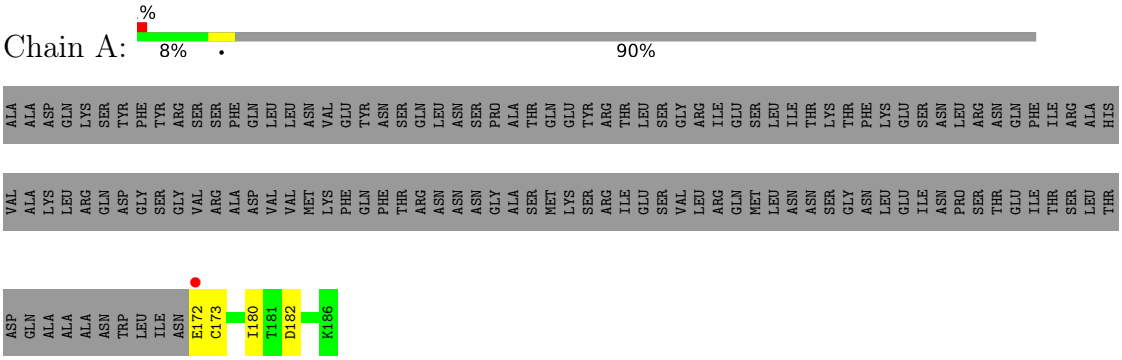
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	25	Total O 25 25	0	0
7	B	256	Total O 256 256	0	0
7	C	43	Total O 43 43	0	0
7	D	267	Total O 267 267	0	0
7	E	27	Total O 27 27	0	0
7	F	270	Total O 270 270	0	0
7	G	16	Total O 16 16	0	0
7	H	245	Total O 245 245	0	0

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.

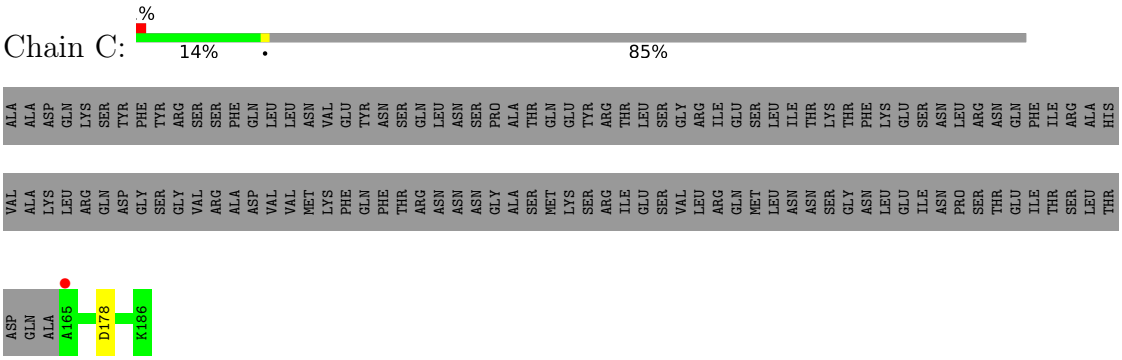
• Molecule 1: Transmembrane protease serine 11D non-catalytic chain

Chain A:



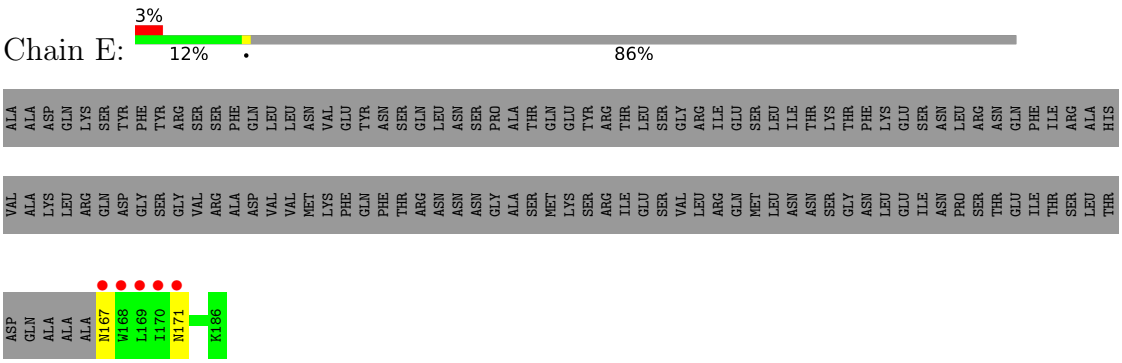
• Molecule 1: Transmembrane protease serine 11D non-catalytic chain

Chain C:



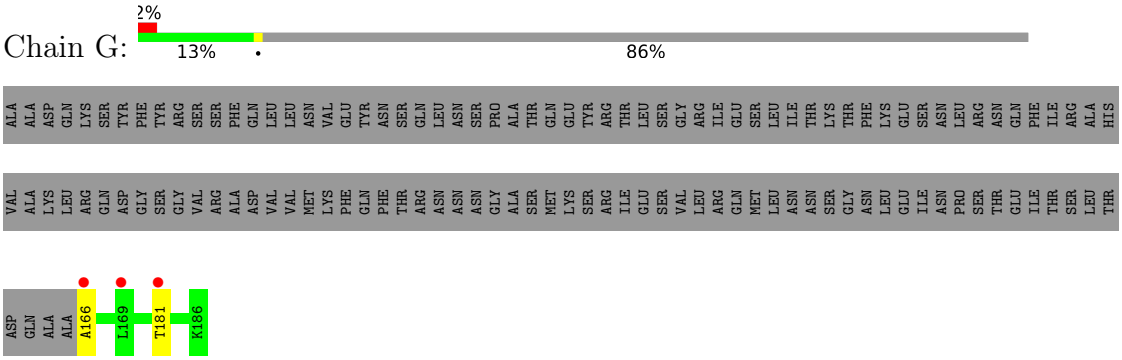
• Molecule 1: Transmembrane protease serine 11D non-catalytic chain

Chain E:



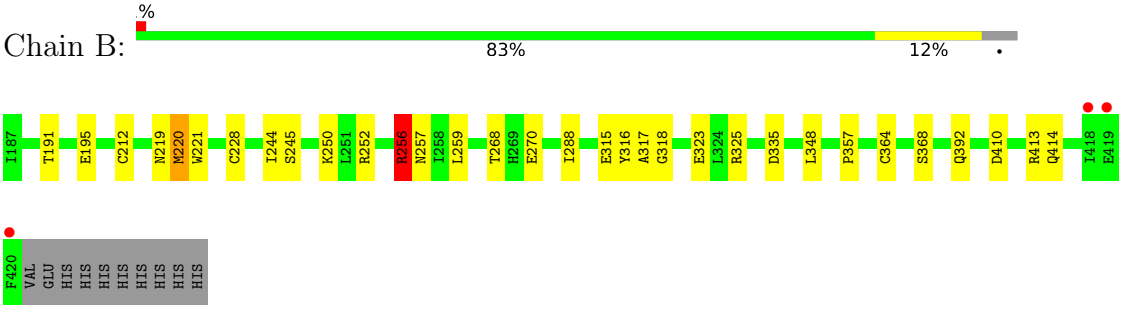
• Molecule 1: Transmembrane protease serine 11D non-catalytic chain

Chain G:



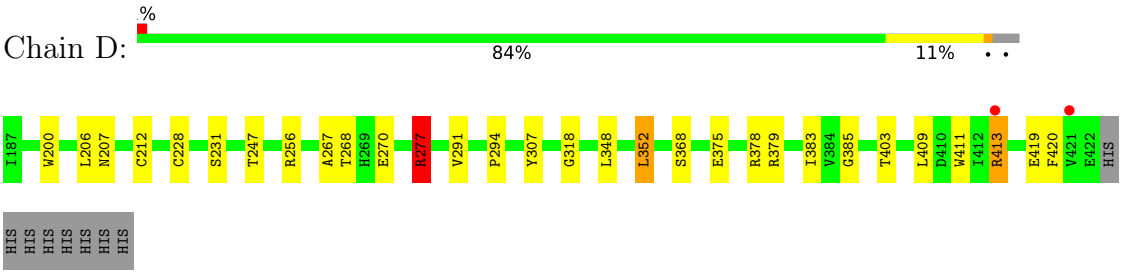
• Molecule 2: Transmembrane protease serine 11D catalytic chain

Chain B:



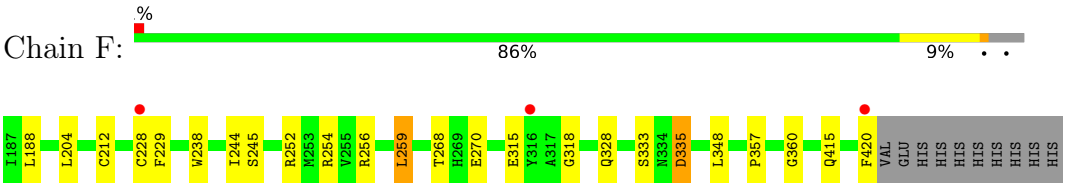
• Molecule 2: Transmembrane protease serine 11D catalytic chain

Chain D:



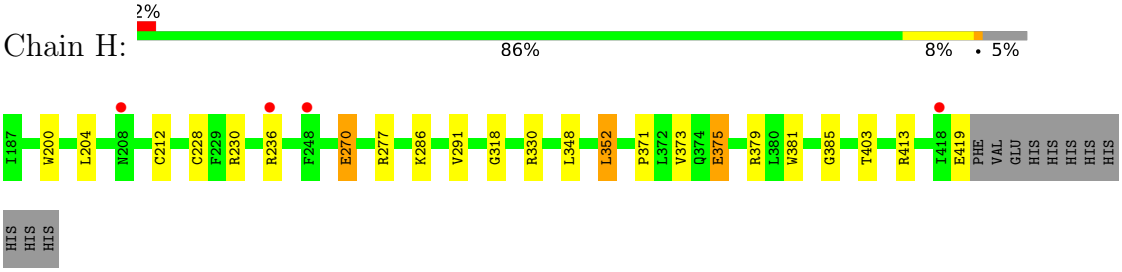
• Molecule 2: Transmembrane protease serine 11D catalytic chain

Chain F:



• Molecule 2: Transmembrane protease serine 11D catalytic chain

Chain H:



4 Data and refinement statistics (i)

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 49.72 – 1.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.77-1.59) 100.0 (49.72-1.59)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 1.59Å)	Xtriage
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	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9337	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, UNX, MG, 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	0.65	0/108	0.97	0/144
1	C	0.57	0/166	0.88	0/225
1	E	0.49	0/153	0.89	0/207
1	G	0.52	0/161	0.89	0/218
2	B	0.55	0/1975	0.95	6/2695 (0.2%)
2	D	0.54	0/1981	0.89	8/2701 (0.3%)
2	F	0.54	0/2021	0.89	5/2754 (0.2%)
2	H	0.59	3/1977 (0.2%)	0.82	0/2692
All	All	0.55	3/8542 (0.0%)	0.89	19/11636 (0.2%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	270[A]	GLU	CD-OE1	6.16	1.32	1.25
2	H	270[B]	GLU	CD-OE1	6.16	1.32	1.25
2	H	375	GLU	CD-OE2	-5.29	1.19	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	256[A]	ARG	NE-CZ-NH1	-13.39	113.61	120.30
2	B	256[B]	ARG	NE-CZ-NH1	-13.39	113.61	120.30
2	B	256[A]	ARG	NE-CZ-NH2	8.08	124.34	120.30
2	B	256[B]	ARG	NE-CZ-NH2	8.08	124.34	120.30
2	B	325	ARG	NE-CZ-NH2	-6.76	116.92	120.30
2	D	307	TYR	CB-CG-CD2	-6.39	117.16	121.00
2	B	325	ARG	NE-CZ-NH1	6.19	123.40	120.30
2	D	413[A]	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	D	413[B]	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	D	413[C]	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	F	335[B]	ASP	CB-CG-OD1	5.50	123.25	118.30
2	F	335[C]	ASP	CB-CG-OD1	5.50	123.25	118.30
2	D	277	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	F	335[B]	ASP	CA-CB-CG	5.12	124.66	113.40
2	F	335[C]	ASP	CA-CB-CG	5.12	124.66	113.40
2	D	413[A]	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	D	413[B]	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	D	413[C]	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	F	256	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	28	0
2	D	1893	0	1844	31	0
2	F	1923	0	1871	18	0
2	H	1878	0	1840	19	0
3	A	1	0	0	0	0
3	E	1	0	0	0	0
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	3	1
7	E	27	0	0	0	0
7	F	270	0	0	4	0
7	G	16	0	0	2	0
7	H	245	0	0	3	0
All	All	9337	0	7911	98	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 (98) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:328[B]:GLN:OE1	7:F:601:HOH:O	1.92	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: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: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:F:259[A]:LEU:C	2:F:259[A]:LEU:HD23	2.22	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	0.57
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:244:ILE:HD12	2:F:244:ILE:C	2.34	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
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:B:212[B]:CYS:HG	2:B:228:CYS:CB	2.25	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
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: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:D:352:LEU:C	2:D:352:LEU:HD23	2.38	0.43
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: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
2:B:244:ILE:HD12	2:B:244:ILE:C	2.40	0.41
1:C:178:ASP:OD2	2:D:375:GLU:OE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:H:352:LEU:HD23	2:H:352:LEU:C	2.42	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%)	12 (100%)	0	100	100
1	C	17/127 (13%)	17 (100%)	0	100	100
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%)	88	80
2	D	207/203 (102%)	206 (100%)	1 (0%)	88	80
2	F	212/203 (104%)	208 (98%)	4 (2%)	57	34
2	H	204/203 (100%)	202 (99%)	2 (1%)	76	61
All	All	891/1320 (68%)	883 (99%)	8 (1%)	84	65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	280	ASN
2	B	392	GLN
2	H	319	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

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	0.81	0
5	EDO	H	502	-	3,3,3	0.11	0	2,2,2	0.10	0
4	GOL	B	501	-	5,5,5	0.14	0	5,5,5	0.40	0
4	GOL	D	500	-	5,5,5	0.11	0	5,5,5	0.36	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	-
5	EDO	H	502	-	-	1/1/1/1	-
4	GOL	B	501	-	-	0/4/4/4	-
4	GOL	D	500	-	-	2/4/4/4	-

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
5	B	502	EDO	O1-C1-C2-O2
4	D	500	GOL	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, 95^{th} 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%)	0.11	1 (6%)	17	16	11, 14, 31, 49	0
1	C	22/145 (15%)	0.08	1 (4%)	33	30	10, 17, 23, 43	0
1	E	20/145 (13%)	1.38	5 (25%)	0	0	12, 16, 50, 55	0
1	G	21/145 (14%)	0.96	3 (14%)	2	2	14, 26, 39, 41	0
2	B	234/244 (95%)	-0.22	3 (1%)	77	77	7, 12, 25, 65	0
2	D	236/244 (96%)	-0.28	2 (0%)	86	86	8, 14, 27, 50	0
2	F	234/244 (95%)	-0.13	3 (1%)	77	77	8, 13, 26, 50	0
2	H	233/244 (95%)	-0.17	4 (1%)	70	69	8, 15, 30, 58	0
All	All	1015/1556 (65%)	-0.13	22 (2%)	62	60	7, 14, 29, 65	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	170	ILE	8.2
1	E	168	TRP	6.3
1	E	169	LEU	5.5
1	C	165	ALA	4.3
1	E	167	ASN	4.3
1	E	171	ASN	4.2
2	F	420	PHE	4.1
2	B	419	GLU	3.9
2	F	228[A]	CYS	3.8
2	H	248	PHE	3.4
1	G	181	THR	3.2
2	D	413[A]	ARG	3.0
2	H	418	ILE	2.6
1	G	166	ALA	2.5
2	B	420	PHE	2.5
1	A	172	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	208	ASN	2.3
2	D	421	VAL	2.3
1	G	169	LEU	2.3
2	F	316[A]	TYR	2.1
2	B	418	ILE	2.0
2	H	236[A]	ARG	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 monosaccharides 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, 95^{th} 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	0.47	0.29	20,20,20,20	0
6	UNX	H	501	1/1	0.60	0.21	20,20,20,20	0
6	UNX	F	501	1/1	0.81	0.14	35,35,35,35	0
6	UNX	D	502	1/1	0.82	0.19	20,20,20,20	0
5	EDO	H	502	4/4	0.82	0.37	20,20,20,20	0
4	GOL	B	501	6/6	0.83	0.28	41,56,63,65	0
4	GOL	D	500	6/6	0.87	0.23	30,35,43,49	0
5	EDO	B	502	4/4	0.94	0.27	29,34,36,41	0
6	UNX	D	501	1/1	0.94	0.10	20,20,20,20	0
3	MG	E	500	1/1	0.99	0.06	12,12,12,12	0
3	MG	H	500	1/1	1.00	0.04	13,13,13,13	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.