Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2021 – 11:13 am GMT

PDB ID	:	7A3Q
Title	:	Crystal structure of dengue 4 virus envelope glycoprotein in complex with the scFv fragment of the broadly neutralizing human antibody EDE1 C10
Authors	:	Sharma, A.; Vaney, M.C.; Guardado-Calvo, P.; Duquerroy, S.; Rouvinski, A.; Rey, F.A.
Deposited on	:	2020-08-18
Resolution	:	2.70 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 following versions of software and data (see references (i)) were used in the production of this report:

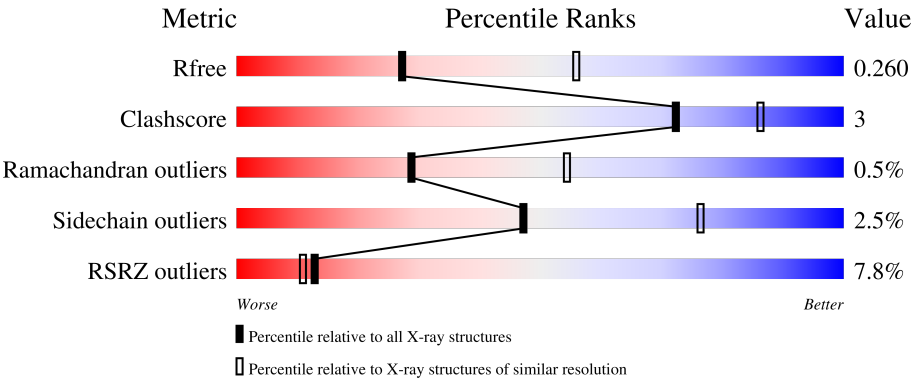
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	395	9% 84% 10% • 6%
1	B	395	8% 81% 11% • 7%
2	H	144	3% 76% 11% • 12%
2	I	144	10% 80% 8% 12%
3	L	154	% 64% 7% 29%

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Mol	Chain	Length	Quality of chain
3	M	154	3% 66% 6% 28%

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
5	3CX	H	500	X	-	-	-
5	3CX	I	500	X	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9449 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2878	1816	499	538	25			
1	B	366	Total	C	N	O	S	0	0	0
			2827	1785	487	530	25			

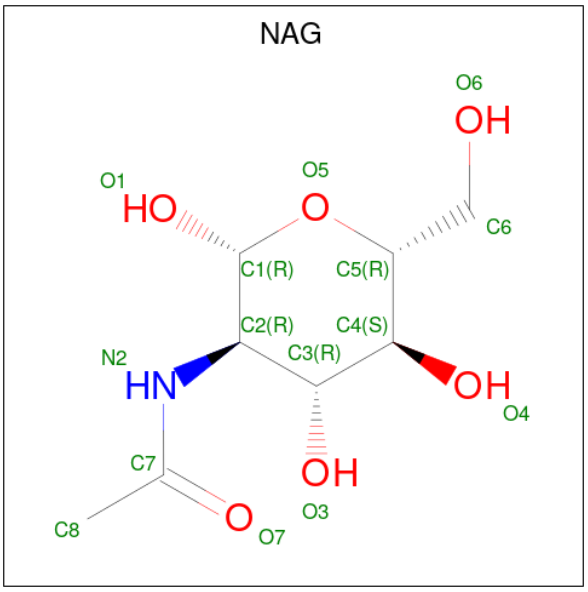
- Molecule 2 is a protein called Single Chain Variable Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	127	Total	C	N	O	S	0	0	0
			1021	650	169	197	5			
2	I	126	Total	C	N	O	S	0	0	0
			1015	647	168	195	5			

- Molecule 3 is a protein called Single Chain Variable Fragment.

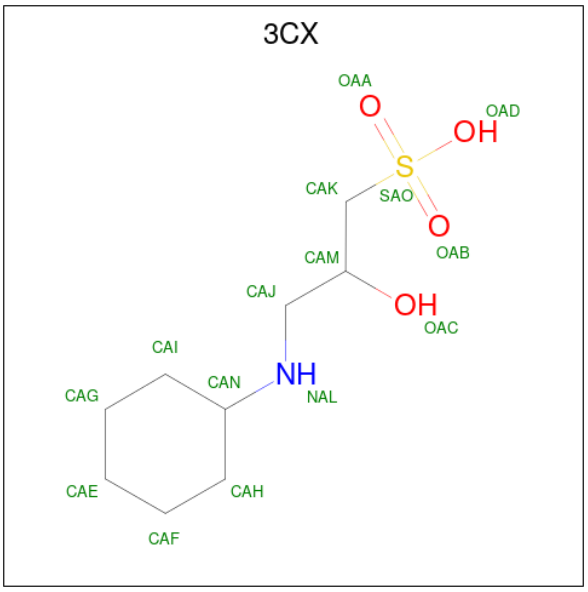
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	110	Total	C	N	O	S	0	0	0
			802	496	137	166	3			
3	M	111	Total	C	N	O	S	0	0	0
			808	499	138	168	3			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is (2S)-3-(cyclohexylamino)-2-hydroxypropane-1-sulfonic acid (three-letter code: 3CX) (formula: $C_9H_{19}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C N O S 15 9 1 4 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	I	1	Total	C	N	O	S	0	0
			15	9	1	4	1		

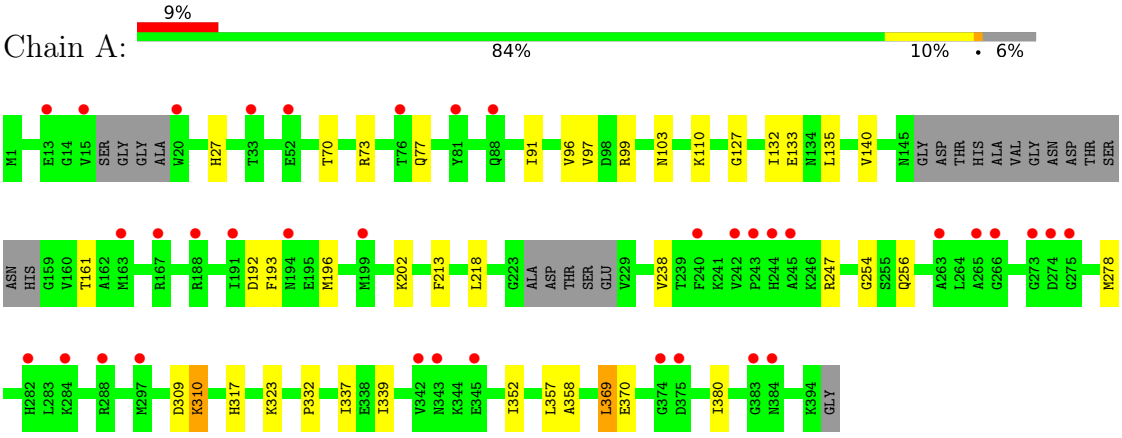
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total	O	0	0
			16	16		
6	B	10	Total	O	0	0
			10	10		
6	H	8	Total	O	0	0
			8	8		
6	I	3	Total	O	0	0
			3	3		
6	L	3	Total	O	0	0
			3	3		

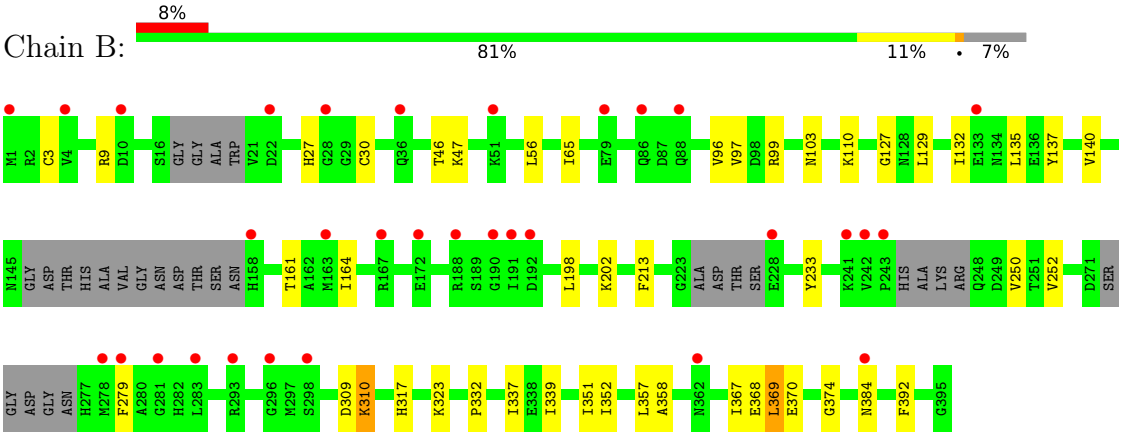
3 Residue-property plots (i)

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.

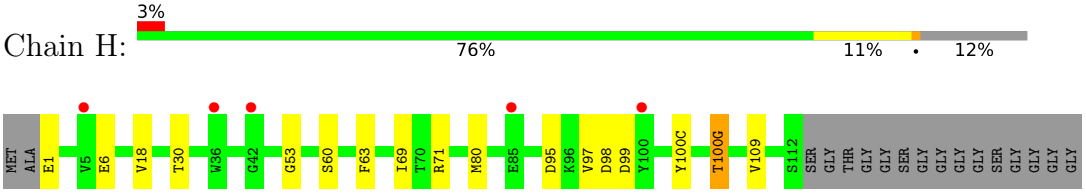
• Molecule 1: Envelope protein E



• Molecule 1: Envelope protein E

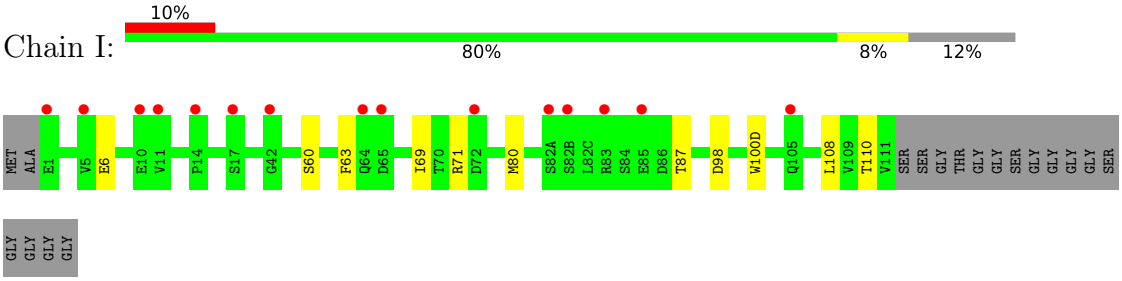


• Molecule 2: Single Chain Variable Fragment



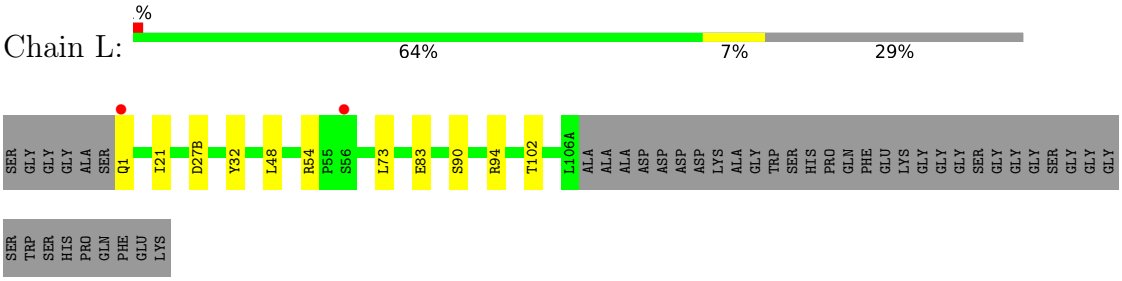
• Molecule 2: Single Chain Variable Fragment

Chain I:



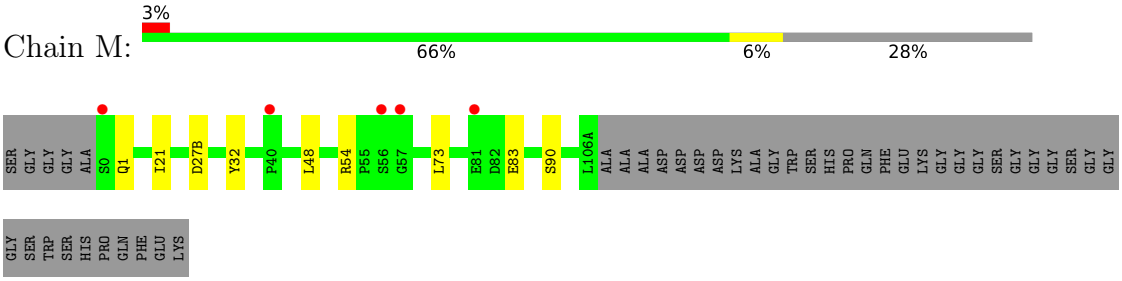
• Molecule 3: Single Chain Variable Fragment

Chain L:



• Molecule 3: Single Chain Variable Fragment

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.98Å 133.18Å 93.54Å 90.00° 92.15° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.70) 99.0 (19.96-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.71Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.216 , 0.239 0.238 , 0.260	Depositor DCC
R_{free} test set	2204 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	65.9	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9449	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 3CX, NAG

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	0.36	0/2933	0.57	0/3963
1	B	0.37	0/2878	0.56	0/3886
2	H	0.34	0/1050	0.59	0/1427
2	I	0.34	0/1044	0.56	0/1419
3	L	0.34	0/820	0.54	0/1113
3	M	0.33	0/826	0.55	0/1121
All	All	0.35	0/9551	0.56	0/12929

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2878	0	2877	17	1
1	B	2827	0	2824	27	2
2	H	1021	0	960	7	0
2	I	1015	0	955	4	0
3	L	802	0	766	7	1
3	M	808	0	771	4	0
4	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	13	0	0
5	H	15	0	18	0	0
5	I	15	0	18	0	0
6	A	16	0	0	0	0
6	B	10	0	0	0	0
6	H	8	0	0	0	0
6	I	3	0	0	0	0
6	L	3	0	0	0	0
All	All	9449	0	9215	63	2

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 3.

All (63) 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:L:21:ILE:HG21	3:L:102:THR:HG21	1.55	0.87
1:A:337:ILE:HD12	1:A:380:ILE:HG12	1.64	0.78
3:M:48:LEU:HD23	3:M:54:ARG:HB3	1.69	0.75
1:B:337:ILE:HD13	1:B:367:ILE:HG21	1.70	0.73
3:L:48:LEU:HD23	3:L:54:ARG:HB3	1.69	0.72
1:B:198:LEU:HD13	1:B:279:PHE:CE1	2.24	0.72
3:L:21:ILE:CG2	3:L:102:THR:HG21	2.25	0.66
1:B:46:THR:HG23	2:H:99:ASP:HB3	1.78	0.65
1:B:337:ILE:CD1	1:B:367:ILE:HG21	2.30	0.60
1:B:97:VAL:HG11	2:I:100(D):TRP:CH2	2.42	0.55
3:L:48:LEU:CD2	3:L:54:ARG:HB3	2.37	0.54
3:M:48:LEU:CD2	3:M:54:ARG:HB3	2.37	0.54
2:H:69:ILE:HG12	2:H:80:MET:HG2	1.91	0.52
1:B:198:LEU:HD13	1:B:279:PHE:CZ	2.44	0.52
2:I:69:ILE:HG12	2:I:80:MET:HG2	1.91	0.52
1:B:137:TYR:HB2	1:B:164:ILE:HB	1.90	0.52
1:B:337:ILE:HD11	1:B:351:ILE:HG21	1.91	0.52
2:I:87:THR:HG23	2:I:110:THR:HA	1.92	0.51
1:B:65:ILE:HD13	1:B:250:VAL:HG23	1.92	0.51
1:B:309:ASP:HB3	1:B:323:LYS:HB3	1.92	0.50
1:A:310:LYS:HB3	1:A:323:LYS:HB2	1.92	0.50
2:H:95:ASP:OD1	2:H:100(G):THR:HG22	2.11	0.50
1:B:99:ARG:HA	1:B:103:ASN:HD22	1.76	0.50
2:H:18:VAL:HG11	2:H:109:VAL:HG11	1.94	0.49
1:A:70:THR:O	3:L:94:ARG:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ILE:HG13	1:B:135:LEU:HD12	1.96	0.48
1:B:310:LYS:CB	1:B:323:LYS:HB2	2.44	0.47
1:B:310:LYS:HB2	1:B:323:LYS:HB2	1.96	0.47
1:B:339:ILE:HD11	1:B:369:LEU:HB3	1.96	0.47
2:H:97:VAL:HG23	2:H:100(C):TYR:HB2	1.97	0.47
1:A:99:ARG:HA	1:A:103:ASN:HD22	1.80	0.47
1:A:193:PHE:HA	1:A:196:MET:HB2	1.96	0.46
1:A:309:ASP:HB3	1:A:323:LYS:HB3	1.97	0.46
1:A:132:ILE:HG13	1:A:135:LEU:HD12	1.97	0.46
3:L:21:ILE:HD12	3:L:73:LEU:HD23	1.98	0.46
1:A:96:VAL:HG22	1:A:110:LYS:HB3	1.98	0.46
1:A:339:ILE:HD11	1:A:369:LEU:HB3	1.97	0.46
3:M:21:ILE:HD12	3:M:73:LEU:HD23	1.98	0.45
1:B:198:LEU:HD13	1:B:279:PHE:HE1	1.77	0.45
1:A:127:GLY:HA3	1:A:213:PHE:CZ	2.53	0.44
1:A:337:ILE:HD12	1:A:380:ILE:CG1	2.41	0.44
1:B:3:CYS:HB3	1:B:9:ARG:HG3	1.97	0.44
1:B:374:GLY:HA2	1:B:392:PHE:CE1	2.52	0.44
2:I:60:SER:HB3	2:I:63:PHE:HD2	1.82	0.44
1:A:352:ILE:HD11	1:A:370:GLU:HB2	1.99	0.44
2:H:60:SER:HB3	2:H:63:PHE:HD2	1.83	0.44
1:B:352:ILE:HD11	1:B:370:GLU:HB2	1.99	0.43
1:A:332:PRO:HA	1:A:358:ALA:O	2.19	0.42
3:L:32:TYR:O	3:L:90:SER:HA	2.19	0.42
1:B:27:HIS:HE1	1:B:47:LYS:HA	1.84	0.42
1:B:332:PRO:HA	1:B:358:ALA:O	2.20	0.42
1:B:96:VAL:HB	1:B:110:LYS:HB3	2.01	0.42
1:B:337:ILE:HD12	1:B:369:LEU:HD21	2.01	0.42
3:M:32:TYR:O	3:M:90:SER:HA	2.20	0.42
1:A:140:VAL:HG22	1:A:161:THR:HG22	2.01	0.42
1:A:97:VAL:HG11	1:A:247:ARG:HD2	2.02	0.41
1:B:352:ILE:HD13	1:B:368:GLU:HG2	2.03	0.41
1:B:140:VAL:HG22	1:B:161:THR:HG22	2.02	0.41
1:B:127:GLY:HA3	1:B:213:PHE:CZ	2.56	0.40
1:B:56:LEU:HD13	1:B:129:LEU:HD11	2.01	0.40
2:H:30:THR:HG23	2:H:53:GLY:HA2	2.02	0.40
1:A:91:ILE:HG21	1:A:238:VAL:HG21	2.03	0.40
1:A:218:LEU:HD21	1:A:256:GLN:HG3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:TYR:OH	3:L:1:GLN:OE1[1_455]	1.89	0.31
1:A:133:GLU:CG	1:B:384:ASN:OD1[2_10411]	1.95	0.25

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	364/395 (92%)	346 (95%)	15 (4%)	3 (1%)	19	43
1	B	354/395 (90%)	337 (95%)	16 (4%)	1 (0%)	41	66
2	H	125/144 (87%)	122 (98%)	3 (2%)	0	100	100
2	I	124/144 (86%)	120 (97%)	4 (3%)	0	100	100
3	L	108/154 (70%)	103 (95%)	4 (4%)	1 (1%)	17	40
3	M	109/154 (71%)	104 (95%)	4 (4%)	1 (1%)	17	40
All	All	1184/1386 (85%)	1132 (96%)	46 (4%)	6 (0%)	29	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ASP
1	A	254	GLY
1	A	202	LYS
1	B	202	LYS
3	L	83	GLU
3	M	83	GLU

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	318/333 (96%)	310 (98%)	8 (2%)	47 76
1	B	313/333 (94%)	307 (98%)	6 (2%)	57 82
2	H	107/112 (96%)	102 (95%)	5 (5%)	26 54
2	I	106/112 (95%)	102 (96%)	4 (4%)	33 62
3	L	90/116 (78%)	89 (99%)	1 (1%)	73 90
3	M	91/116 (78%)	89 (98%)	2 (2%)	52 79
All	All	1025/1122 (91%)	999 (98%)	26 (2%)	47 76

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	73	ARG
1	A	77	GLN
1	A	278	MET
1	A	310	LYS
1	A	317	HIS
1	A	357	LEU
1	A	369	LEU
1	B	30	CYS
1	B	252	VAL
1	B	310	LYS
1	B	317	HIS
1	B	357	LEU
1	B	369	LEU
2	H	1	GLU
2	H	6	GLU
2	H	71	ARG
2	H	98	ASP
2	H	100(G)	THR
2	I	6	GLU
2	I	71	ARG
2	I	98	ASP
2	I	108	LEU
3	L	27(B)	ASP
3	M	1	GLN
3	M	27(B)	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	B	103	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 monosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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	3CX	H	500	-	1/1/3/4	-	-
5	3CX	I	500	-	1/1/3/4	-	-

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	H	500	3CX	CAM
5	I	500	3CX	CAM

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	372/395 (94%)	0.49	36 (9%) 7 6	52, 78, 113, 129	0
1	B	366/395 (92%)	0.63	32 (8%) 10 8	47, 80, 119, 141	0
2	H	127/144 (88%)	0.32	5 (3%) 39 38	37, 70, 95, 114	0
2	I	126/144 (87%)	0.87	15 (11%) 4 3	60, 100, 137, 154	0
3	L	110/154 (71%)	0.07	2 (1%) 68 70	40, 58, 92, 110	0
3	M	111/154 (72%)	0.26	5 (4%) 33 31	57, 74, 102, 117	0
All	All	1212/1386 (87%)	0.50	95 (7%) 13 11	37, 78, 120, 154	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	384	ASN	7.5
1	A	244	HIS	6.3
1	B	279	PHE	5.8
1	B	191	ILE	5.5
1	A	15	VAL	5.4
1	B	167	ARG	5.2
1	A	191	ILE	5.1
1	A	384	ASN	4.9
1	B	241	LYS	4.9
1	B	243	PRO	4.6
2	I	64	GLN	4.4
1	A	240	PHE	4.2
2	I	1	GLU	4.1
1	B	278	MET	4.1
1	A	375	ASP	4.0
1	B	228	GLU	4.0
1	A	243	PRO	3.8
2	I	5	VAL	3.7
3	L	1	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	20	TRP	3.6
1	B	36	GLN	3.6
1	A	274	ASP	3.6
1	B	190	GLY	3.4
1	B	296	GLY	3.4
3	L	56	SER	3.4
1	B	86	GLN	3.3
1	A	282	HIS	3.3
1	B	281	GLY	3.3
3	M	40	PRO	3.3
1	A	273	GLY	3.2
3	M	81	GLU	3.2
2	I	17	SER	3.1
1	A	374	GLY	3.1
2	I	82(A)	SER	3.1
1	A	167	ARG	3.1
1	B	188	ARG	3.0
1	A	88	GLN	3.0
1	B	51	LYS	3.0
1	B	283	LEU	3.0
1	A	76	THR	2.9
2	I	72	ASP	2.9
1	A	266	GLY	2.9
1	B	158	HIS	2.9
3	M	0	SER	2.8
2	I	65	ASP	2.8
1	A	265	ALA	2.8
1	B	293	ARG	2.8
1	B	22	ASP	2.7
1	A	194	ASN	2.7
2	H	42	GLY	2.7
2	I	85	GLU	2.7
1	A	81	TYR	2.7
1	B	298	SER	2.7
1	A	188	ARG	2.6
1	B	192	ASP	2.6
1	B	242	VAL	2.6
2	H	85	GLU	2.6
1	A	245	ALA	2.5
1	B	4	VAL	2.5
2	H	100	TYR	2.5
2	I	10	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	28	GLY	2.5
1	A	343	ASN	2.5
1	B	10	ASP	2.5
1	B	133	GLU	2.5
2	I	42	GLY	2.4
2	I	82(B)	SER	2.4
1	A	345	GLU	2.4
2	I	11	VAL	2.3
1	A	284	LYS	2.3
2	I	105	GLN	2.3
1	A	297	MET	2.3
1	B	79	GLU	2.3
1	A	275	GLY	2.2
3	M	57	GLY	2.2
1	A	13	GLU	2.2
1	A	52	GLU	2.2
1	B	172	GLU	2.2
1	B	163	MET	2.2
2	I	14	PRO	2.2
2	H	36	TRP	2.2
1	A	342	VAL	2.1
1	A	33	THR	2.1
1	A	288	ARG	2.1
2	I	83	ARG	2.1
1	A	263	ALA	2.1
1	A	199	MET	2.1
1	B	1	MET	2.1
1	A	242	VAL	2.1
2	H	5	VAL	2.1
1	A	163	MET	2.1
1	B	362	ASN	2.1
1	A	383	GLY	2.1
1	B	88	GLN	2.0
3	M	56	SER	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
5	3CX	I	500	15/15	0.59	0.45	108,112,122,122	0
5	3CX	H	500	15/15	0.72	0.35	93,99,112,113	0
4	NAG	A	1001	14/15	0.77	0.38	109,111,112,112	0
4	NAG	B	1001	14/15	0.77	0.30	112,114,115,115	0

6.5 Other polymers (i)

There are no such residues in this entry.