



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:33 PM UTC

PDB ID : 4WEB / pdb_00004web
Title : Structure of the core ectodomain of the hepatitis C virus envelope glycoprotein 2
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Deposited on : 2014-09-09
Resolution : 2.40 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

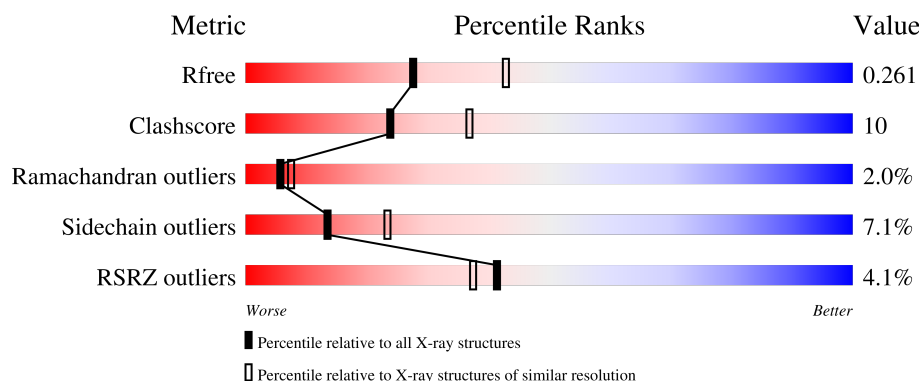
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	E	217	<div> <div>8%</div> <div>35% 17% 5% 43%</div> </div>
2	H	467	<div> <div>%</div> <div>34% 10% 54%</div> </div>
3	L	240	<div> <div></div> <div>72% 18% 10%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4337 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 hepatitis C virus envelope glycoprotein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	123	Total	C	N	O	S	0	0	0
			891	573	144	161	13			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	450	THR	-	expression tag	UNP Q9QF35
E	451	PRO	-	expression tag	UNP Q9QF35
E	452	VAL	-	expression tag	UNP Q9QF35
E	453	GLY	-	expression tag	UNP Q9QF35
E	454	LEU	-	expression tag	UNP Q9QF35
E	455	ALA	-	expression tag	UNP Q9QF35
E	656	GLY	-	expression tag	UNP Q9QF35
E	657	SER	-	expression tag	UNP Q9QF35
E	658	ALA	-	expression tag	UNP Q9QF35
E	659	SER	-	expression tag	UNP Q9QF35
E	660	GLY	-	expression tag	UNP Q9QF35
E	661	LEU	-	expression tag	UNP Q9QF35
E	662	GLU	-	expression tag	UNP Q9QF35
E	663	VAL	-	expression tag	UNP Q9QF35
E	664	LEU	-	expression tag	UNP Q9QF35
E	665	PHE	-	expression tag	UNP Q9QF35
E	666	GLN	-	expression tag	UNP Q9QF35

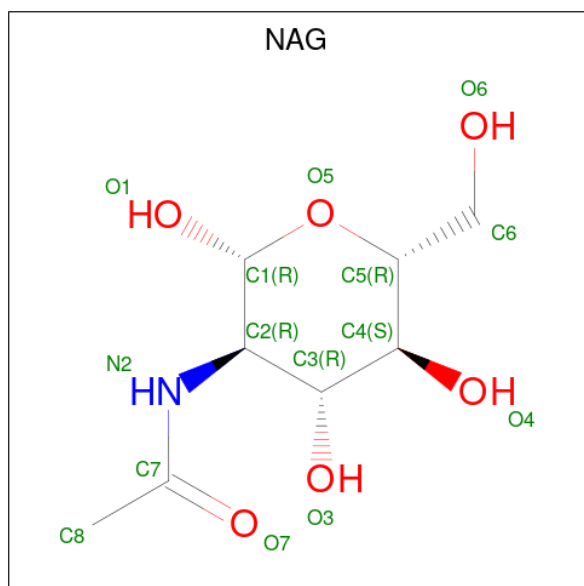
- Molecule 2 is a protein called Mouse Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1616	1015	264	332	5			

- Molecule 3 is a protein called Mouse Fab Light Chain.

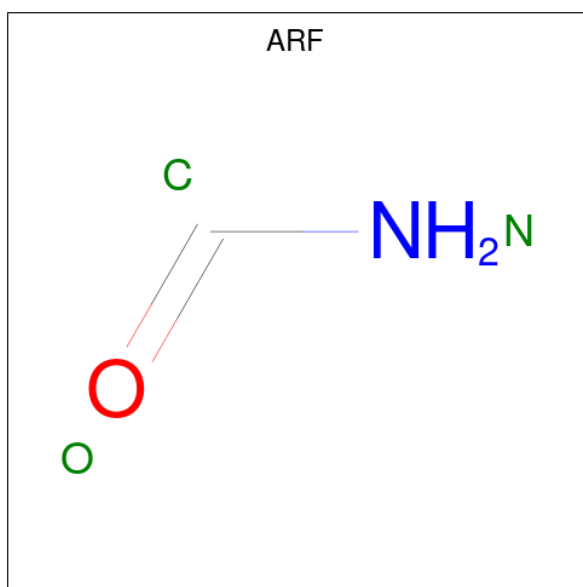
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	217	Total 1648	C 1025	N 273	O 342	S 8	0	0	0

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



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

- Molecule 5 is FORMAMIDE (CCD ID: ARF) (formula: CH_3NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	N	O	0	0
			3	1	1	1		
5	H	1	Total	C	N	O	0	0
			3	1	1	1		
5	H	1	Total	C	N	O	0	0
			3	1	1	1		
5	H	1	Total	C	N	O	0	0
			3	1	1	1		
5	L	1	Total	C	N	O	0	0
			3	1	1	1		
5	L	1	Total	C	N	O	0	0
			3	1	1	1		

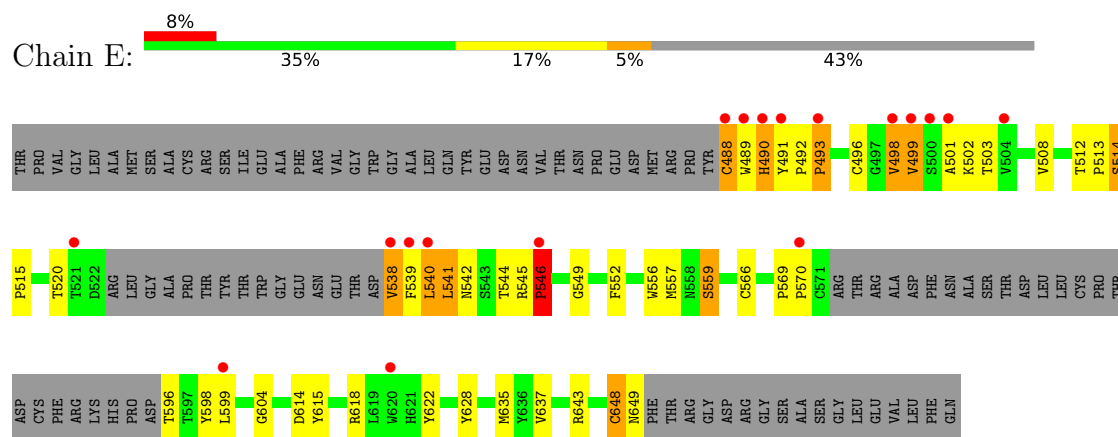
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	12	Total	O	0	0
			12	12		
6	H	61	Total	O	0	0
			61	61		
6	L	63	Total	O	0	0
			63	63		

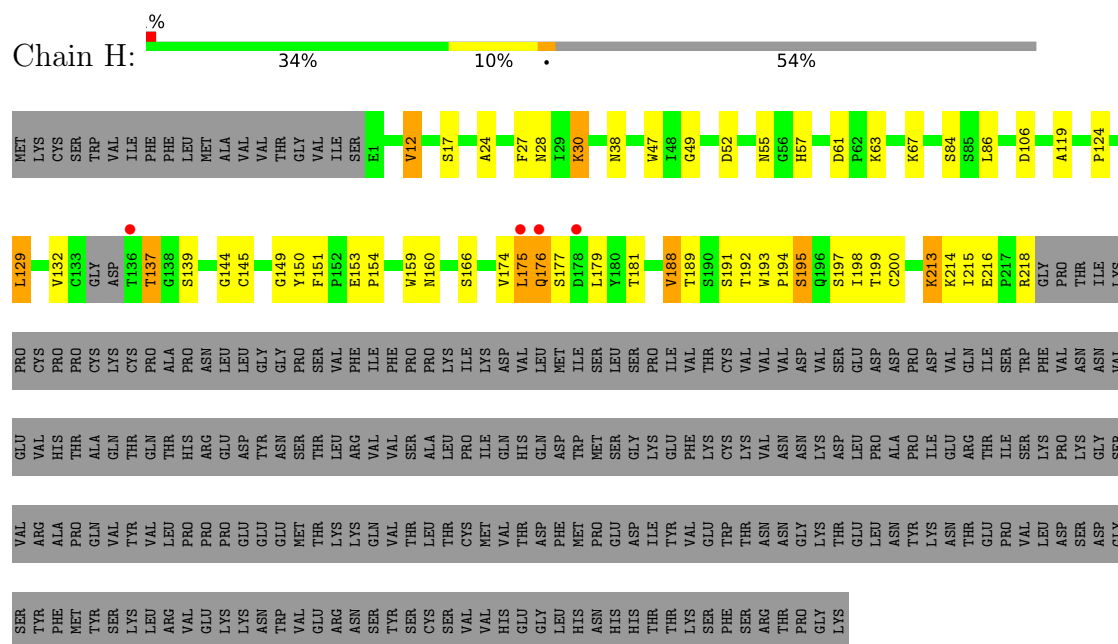
3 Residue-property plots

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: hepatitis C virus envelope glycoprotein 2

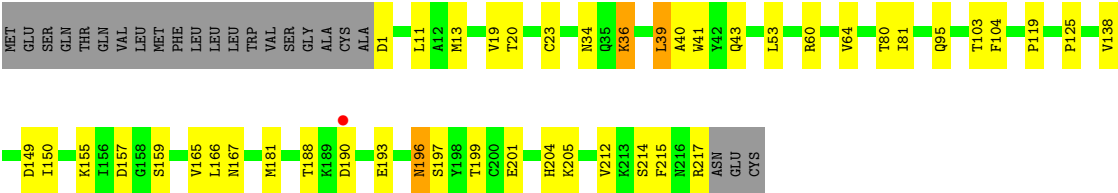


- Molecule 2: Mouse Fab Heavy Chain



- Molecule 3: Mouse Fab Light Chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.96Å 194.57Å 37.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.69 – 2.40 24.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.2 (24.69-2.40) 94.1 (24.69-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1690	Depositor
R, R_{free}	0.199 , 0.259 0.204 , 0.261	Depositor DCC
R_{free} test set	1999 reflections (7.73%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4337	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	E	0.57	1/920 (0.1%)	1.18	11/1269 (0.9%)
2	H	0.58	1/1655 (0.1%)	0.93	2/2268 (0.1%)
3	L	0.55	0/1685	0.90	0/2295
All	All	0.56	2/4260 (0.0%)	0.98	13/5832 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	38	ASN	CG-OD1	5.83	1.34	1.23
1	E	492	PRO	N-CD	5.09	1.54	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	546	PRO	N-CA-C	9.21	121.94	110.70
1	E	546	PRO	CA-C-N	-8.98	109.41	119.28
1	E	546	PRO	C-N-CA	-8.98	109.41	119.28
1	E	545	ARG	CA-C-N	8.81	129.45	120.38
1	E	545	ARG	C-N-CA	8.81	129.45	120.38
2	H	175	LEU	CA-C-N	6.42	133.25	121.70
2	H	175	LEU	C-N-CA	6.42	133.25	121.70
1	E	493	PRO	CA-N-CD	-5.57	104.20	112.00
1	E	604	GLY	CA-C-N	5.52	125.35	119.28
1	E	604	GLY	C-N-CA	5.52	125.35	119.28
1	E	648	CYS	CB-CA-C	-5.07	109.14	116.54
1	E	514	SER	CA-C-N	5.00	126.09	119.84
1	E	514	SER	C-N-CA	5.00	126.09	119.84

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	E	891	0	812	29	0
2	H	1616	0	1561	35	0
3	L	1648	0	1535	20	0
4	E	28	0	26	1	0
5	E	3	0	3	1	0
5	H	9	0	9	0	0
5	L	6	0	6	0	0
6	E	12	0	0	2	0
6	H	61	0	0	0	0
6	L	63	0	0	1	0
All	All	4337	0	3952	82	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 10.

All (82) 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:H:124:PRO:HB3	2:H:150:TYR:HB3	1.70	0.74
1:E:499:VAL:O	1:E:539:PHE:HB3	1.91	0.69
1:E:501:ALA:HB2	1:E:539:PHE:HE2	1.59	0.68
2:H:55:ASN:HB3	2:H:57:HIS:H	1.60	0.67
1:E:501:ALA:HB2	1:E:539:PHE:CE2	2.30	0.66
3:L:43:GLN:HB2	3:L:53:LEU:HD11	1.76	0.66
1:E:488:CYS:N	1:E:489:TRP:HA	2.11	0.65
3:L:1:ASP:OD2	6:L:401:HOH:O	2.15	0.62
1:E:596:THR:HG22	1:E:598:TYR:H	1.64	0.61
1:E:643:ARG:HH22	2:H:106:ASP:CG	2.09	0.61
1:E:520:THR:HG1	1:E:538:VAL:N	2.00	0.60
3:L:201:GLU:HG2	3:L:212:VAL:HG12	1.82	0.60
1:E:546:PRO:HA	1:E:549:GLY:O	2.03	0.58
5:E:703:ARF:H	6:E:807:HOH:O	2.03	0.58
1:E:643:ARG:HD2	6:E:806:HOH:O	2.05	0.56
2:H:218:ARG:CZ	3:L:125:PRO:HG2	2.35	0.56
1:E:496:CYS:HB3	1:E:541:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:149:GLY:HA2	2:H:179:LEU:HB3	1.88	0.55
1:E:508:VAL:HG22	1:E:556:TRP:HB3	1.89	0.55
2:H:175:LEU:HB3	2:H:176:GLN:HB2	1.89	0.54
3:L:167:ASN:HB3	3:L:181:MET:HE2	1.91	0.53
2:H:137:THR:HG22	2:H:139:SER:H	1.73	0.53
1:E:513:PRO:HD3	1:E:637:VAL:HG21	1.90	0.53
2:H:52:ASP:HB3	2:H:55:ASN:HB2	1.91	0.52
2:H:189:THR:C	2:H:191:SER:H	2.17	0.52
2:H:129:LEU:HB2	2:H:144:GLY:C	2.35	0.52
2:H:194:PRO:O	2:H:195:SER:OG	2.14	0.52
3:L:34:ASN:OD1	3:L:36:LYS:HB2	2.11	0.51
1:E:643:ARG:NH2	2:H:106:ASP:OD1	2.43	0.51
2:H:61:ASP:OD1	2:H:63:LYS:HG2	2.10	0.50
1:E:496:CYS:HA	1:E:566:CYS:HB2	1.93	0.50
2:H:67:LYS:HG2	2:H:84:SER:O	2.11	0.50
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.47	0.50
3:L:150:ILE:HD12	3:L:204:HIS:HD2	1.77	0.49
2:H:28:ASN:OD1	2:H:30:LYS:HB2	2.12	0.49
3:L:196:ASN:ND2	3:L:217:ARG:O	2.44	0.49
1:E:540:LEU:HD11	1:E:542:ASN:ND2	2.29	0.48
2:H:197:SER:HB2	2:H:214:LYS:HE3	1.96	0.47
1:E:596:THR:HG21	1:E:635:MET:HE3	1.97	0.47
2:H:159:TRP:CZ3	2:H:200:CYS:HB3	2.50	0.47
1:E:648:CYS:HB3	1:E:649:ASN:H	1.55	0.47
1:E:488:CYS:HB3	1:E:490:HIS:H	1.80	0.46
2:H:214:LYS:HE2	2:H:216:GLU:OE1	2.15	0.46
1:E:540:LEU:HD12	1:E:540:LEU:HA	1.64	0.46
3:L:190:ASP:HA	3:L:193:GLU:HB2	1.97	0.46
3:L:197:SER:HB2	3:L:215:PHE:O	2.16	0.46
2:H:153:GLU:HG3	2:H:154:PRO:HA	1.99	0.45
2:H:199:THR:HG23	2:H:213:LYS:C	2.41	0.45
1:E:628:TYR:CG	1:E:648:CYS:O	2.69	0.45
2:H:119:ALA:HB3	2:H:151:PHE:CE2	2.52	0.45
2:H:175:LEU:CG	2:H:176:GLN:HA	2.47	0.45
3:L:39:LEU:HG	3:L:40:ALA:N	2.31	0.45
2:H:12:VAL:HG21	2:H:86:LEU:HD12	2.00	0.43
2:H:191:SER:C	2:H:193:TRP:H	2.26	0.43
3:L:155:LYS:N	3:L:199:THR:O	2.50	0.43
2:H:160:ASN:OD1	2:H:198:ILE:HA	2.19	0.43
1:E:540:LEU:HD11	1:E:542:ASN:CG	2.43	0.43
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:150:ILE:HD12	3:L:204:HIS:CD2	2.52	0.43
1:E:546:PRO:HG2	1:E:552:PHE:CD2	2.53	0.43
1:E:569:PRO:HA	1:E:570:PRO:HD3	1.78	0.43
3:L:23:CYS:HB2	3:L:41:TRP:CH2	2.53	0.42
2:H:175:LEU:HB3	2:H:176:GLN:CB	2.49	0.42
2:H:198:ILE:O	2:H:215:ILE:HG12	2.18	0.42
3:L:157:ASP:C	3:L:159:SER:H	2.27	0.42
2:H:145:CYS:HB2	2:H:159:TRP:CH2	2.54	0.42
2:H:197:SER:CB	2:H:214:LYS:HE3	2.49	0.42
1:E:618:ARG:O	1:E:622:TYR:N	2.51	0.42
3:L:95:GLN:HB2	3:L:104:PHE:CD1	2.55	0.41
1:E:514:SER:HA	1:E:515:PRO:HD3	1.83	0.41
1:E:559:SER:HB2	4:E:701:NAG:H82	2.02	0.41
2:H:179:LEU:HD23	2:H:179:LEU:HA	1.90	0.41
3:L:19:VAL:HB	3:L:81:ILE:HB	2.02	0.41
3:L:60:ARG:HD3	3:L:64:VAL:O	2.20	0.41
3:L:119:PRO:HG3	3:L:150:ILE:HD11	2.03	0.41
1:E:498:VAL:HB	1:E:540:LEU:HD13	2.03	0.40
1:E:598:TYR:CD2	1:E:635:MET:HE1	2.56	0.40
2:H:193:TRP:HA	2:H:194:PRO:HA	1.89	0.40
2:H:174:VAL:O	2:H:181:THR:N	2.44	0.40
2:H:188:VAL:HG22	2:H:189:THR:H	1.85	0.40
3:L:11:LEU:HA	3:L:11:LEU:HD23	1.78	0.40
1:E:614:ASP:OD1	1:E:615:TYR:N	2.55	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	E	117/217 (54%)	97 (83%)	14 (12%)	6 (5%)	1 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	212/467 (45%)	196 (92%)	12 (6%)	4 (2%)	6	8
3	L	215/240 (90%)	205 (95%)	9 (4%)	1 (0%)	24	37
All	All	544/924 (59%)	498 (92%)	35 (6%)	11 (2%)	6	7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	502	LYS
1	E	540	LEU
2	H	177	SER
2	H	176	GLN
2	H	195	SER
3	L	196	ASN
1	E	490	HIS
1	E	491	TYR
1	E	493	PRO
2	H	137	THR
1	E	512	THR

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	E	96/186 (52%)	85 (88%)	11 (12%)	5	8
2	H	185/420 (44%)	176 (95%)	9 (5%)	22	39
3	L	186/214 (87%)	173 (93%)	13 (7%)	14	24
All	All	467/820 (57%)	434 (93%)	33 (7%)	13	23

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	488	CYS
1	E	498	VAL
1	E	499	VAL

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Mol	Chain	Res	Type
1	E	503	THR
1	E	538	VAL
1	E	541	LEU
1	E	544	THR
1	E	546	PRO
1	E	557	MET
1	E	559	SER
1	E	599	LEU
2	H	12	VAL
2	H	17	SER
2	H	30	LYS
2	H	129	LEU
2	H	132	VAL
2	H	166	SER
2	H	188	VAL
2	H	192	THR
2	H	213	LYS
3	L	13	MET
3	L	20	THR
3	L	36	LYS
3	L	39	LEU
3	L	80	THR
3	L	103	THR
3	L	138	VAL
3	L	149	ASP
3	L	165	VAL
3	L	166	LEU
3	L	188	THR
3	L	205	LYS
3	L	214	SER

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

Mol	Chain	Res	Type
3	L	85	GLN
3	L	167	ASN

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](#)

8 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
5	ARF	E	703	-	2,2,2	1.31	0	1,1,1	0.60	0
5	ARF	H	503	-	2,2,2	1.47	1 (50%)	1,1,1	0.39	0
5	ARF	H	501	-	2,2,2	1.40	0	1,1,1	0.57	0
5	ARF	H	502	-	2,2,2	1.37	0	1,1,1	0.85	0
5	ARF	L	301	-	2,2,2	1.32	0	1,1,1	0.68	0
5	ARF	L	302	-	2,2,2	1.58	1 (50%)	1,1,1	0.34	0
4	NAG	E	702	1	14,14,15	0.42	0	17,19,21	0.41	0
4	NAG	E	701	1	14,14,15	0.35	0	17,19,21	0.45	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	NAG	E	702	1	-	0/6/23/26	0/1/1/1
4	NAG	E	701	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	302	ARF	C-N	2.15	1.43	1.30
5	H	503	ARF	C-N	2.06	1.43	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	701	NAG	O5-C5-C6-O6
4	E	701	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	703	ARF	1	0
4	E	701	NAG	1	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	E	123/217 (56%)	0.84	18 (14%) 6 4	34, 70, 97, 112	0
2	H	216/467 (46%)	-0.18	4 (1%) 66 62	24, 40, 75, 102	0
3	L	217/240 (90%)	-0.15	1 (0%) 87 85	24, 41, 77, 86	0
All	All	556/924 (60%)	0.05	23 (4%) 41 37	24, 45, 86, 112	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	538	VAL	4.7
1	E	489	TRP	4.1
1	E	501	ALA	3.8
1	E	539	PHE	3.8
2	H	175	LEU	3.7
1	E	521	THR	3.3
1	E	491	TYR	3.3
1	E	488	CYS	2.8
1	E	490	HIS	2.8
1	E	493	PRO	2.7
1	E	500	SER	2.6
1	E	570	PRO	2.6
3	L	190	ASP	2.5
1	E	499	VAL	2.4
2	H	178	ASP	2.4
1	E	498	VAL	2.3
1	E	540	LEU	2.2
1	E	504	VAL	2.2
1	E	620	TRP	2.1
2	H	136	THR	2.1
1	E	599	LEU	2.1
2	H	176	GLN	2.0
1	E	546	PRO	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(\AA^2)	Q<0.9
4	NAG	E	702	14/15	0.55	0.15	83,92,99,103	0
4	NAG	E	701	14/15	0.70	0.12	91,94,101,102	0
5	ARF	L	301	3/3	0.80	0.13	52,52,53,54	0
5	ARF	L	302	3/3	0.84	0.15	33,33,36,42	0
5	ARF	E	703	3/3	0.86	0.14	40,40,47,50	0
5	ARF	H	502	3/3	0.89	0.11	36,36,36,44	0
5	ARF	H	503	3/3	0.91	0.09	32,32,36,41	0
5	ARF	H	501	3/3	0.95	0.09	32,32,35,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.