Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 12:49 PM EST

PDB ID	:	4WEB
Title	:	Structure of the core ectodomain of the hepatitis C virus envelope glycoprotein 2
Authors	:	Khan, A.G.; Whidby, J.; Miller, M.T.; Scarborough, H.; Zatorski, A.V.; Cygan, A.; Price, A.A.; Yost, S.A.; Bohannon, C.D.; Jacob, J.; Grakoui, A.; Marcotrigiano, J.
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 (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:

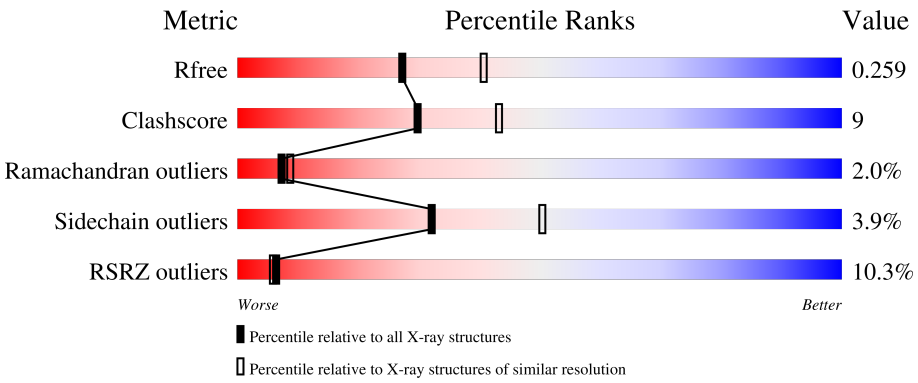
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	11% 37% 17% • 43%
2	H	467	3% 34% 11% • 54%
3	L	240	8% 74% 15% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	E	702	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	E	123	891	573	144	161	13	0	0	0

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

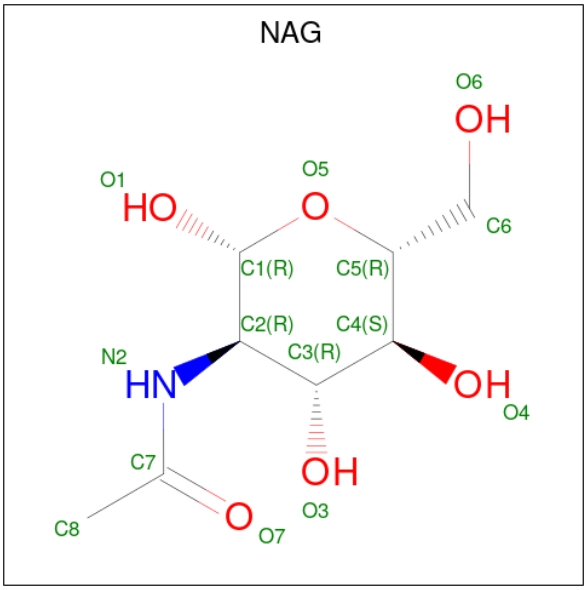
- Molecule 2 is a protein called Mouse Fab Heavy Chain.

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

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

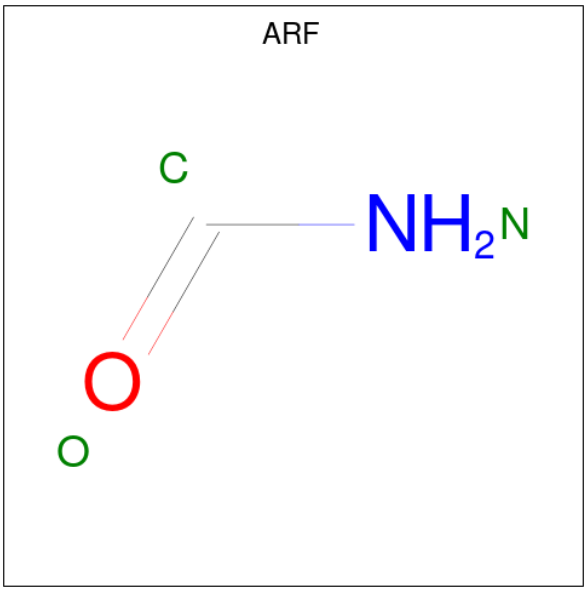
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	217	1648	1025	273	342	8	0	0	0

- 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
			Total	C	N	O		
4	E	1	14	8	1	5	0	0
4	E	1	14	8	1	5	0	0

- Molecule 5 is FORMAMIDE (three-letter code: ARF) (formula: CH_3NO).



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

- Molecule 6 is water.

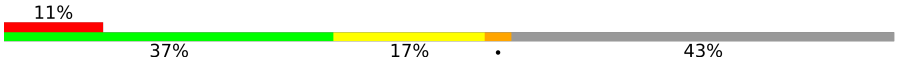
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	E	12	12	12	0	0
			Total	O		
6	H	61	61	61	0	0
			Total	O		
6	L	63	63	63	0	0

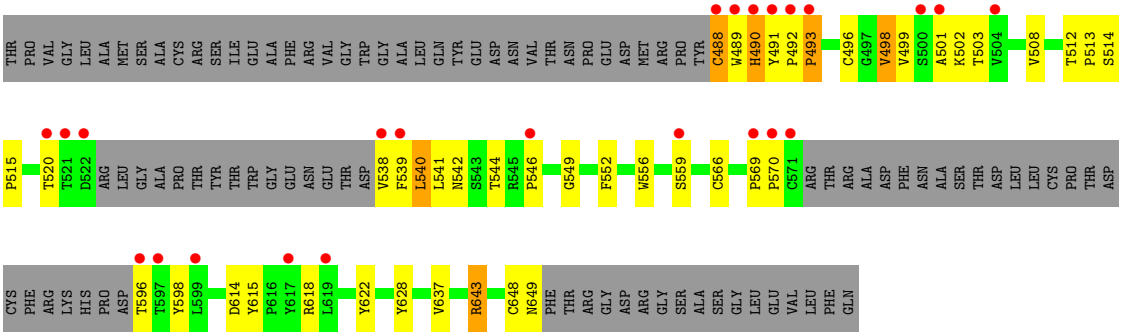
3 Residue-property plots (i)

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: hepatitis C virus envelope glycoprotein 2

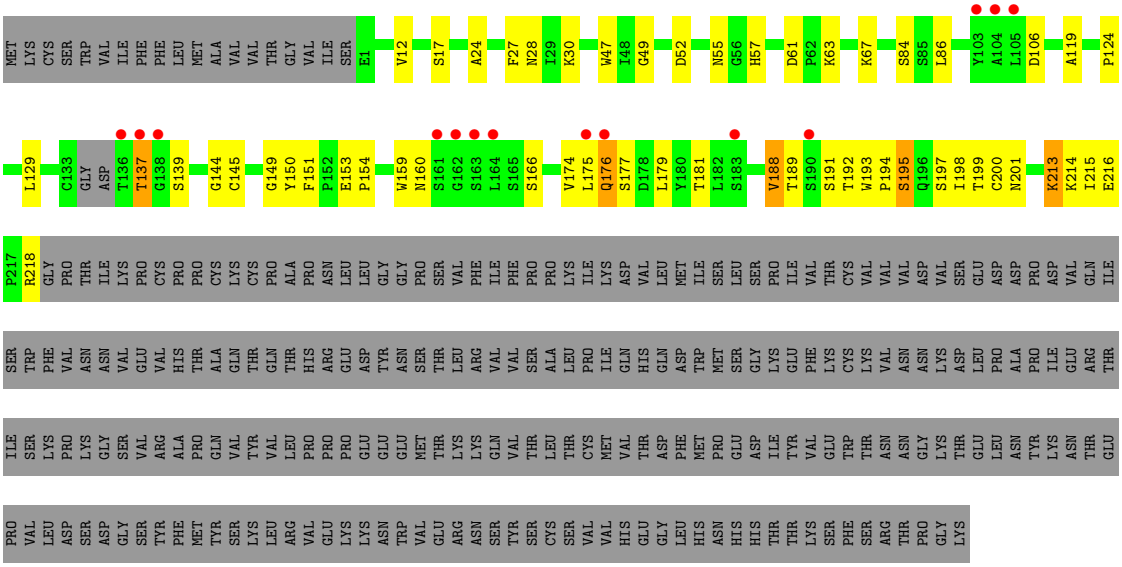
Chain E:





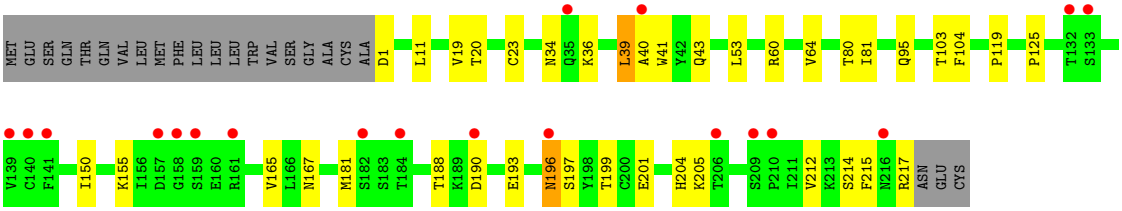
- Molecule 2: Mouse Fab Heavy Chain

Chain H:



- Molecule 3: Mouse Fab Light Chain

Chain L:


MET GLU SER GLN THR GLN VAL LEU MET PHE LEU LEU LEU TRP VAL SER GLY ALA CYS ALA D1 L11 V19 T20 C23 N34 Q35 K36 L39 A40 W41 Y42 Q43 L53 R60 V64 T80 I81 Q95 T103 F104 P119 P125 T132 S133
V139 C140 F141 I150 K155 I156 D157 G158 S159 E160 R161 V165 L166 N167 M181 S182 S183 T184 T188 K189 D190 E193 M196 S197 Y198 T199 C200 E201 H204 K205 T206 S209 P210 I211 V212 K213 S214 F215 N216 R217 ASN GLU CYS

4 Data and refinement statistics (i)

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 29.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.2 (24.69-2.40) 94.2 (29.91-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1690	Depositor
R, R_{free}	0.199 , 0.259 0.202 , 0.259	Depositor DCC
R_{free} test set	1999 reflections (8.21%)	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 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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 (i)

5.1 Standard geometry (i)

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	0.46	1/920 (0.1%)	0.72	2/1269 (0.2%)
2	H	0.48	0/1655	0.66	0/2268
3	L	0.46	0/1685	0.62	0/2295
All	All	0.47	1/4260 (0.0%)	0.66	2/5832 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	492	PRO	N-CD	5.02	1.54	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	643	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	E	493	PRO	CA-N-CD	-5.21	104.20	111.50

There are no chirality outliers.

There are no planarity outliers.

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	E	891	0	812	26	0
2	H	1616	0	1561	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1648	0	1535	19	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	77	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 9.

All (77) 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:520:THR:HG1	1:E:538:VAL:N	1.98	0.62
1:E:596:THR:HG22	1:E:598:TYR:H	1.64	0.61
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
1:E:643:ARG:HH22	2:H:106:ASP:CG	2.09	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
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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:189:THR:C	2:H:191:SER:H	2.17	0.47
2:H:129:LEU:HB2	2:H:144:GLY:C	2.35	0.47
2:H:197:SER:HB2	2:H:214:LYS:HE3	1.96	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
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
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
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.54	0.43
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
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
3:L:167:ASN:HB3	3:L:181:MET:HE2	2.00	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
2:H:199:THR:HG23	2:H:213:LYS:C	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	2 1
2	H	212/467 (45%)	196 (92%)	12 (6%)	4 (2%)	8 10
3	L	215/240 (90%)	205 (95%)	9 (4%)	1 (0%)	29 41
All	All	544/924 (59%)	498 (92%)	35 (6%)	11 (2%)	7 9

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (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	E	96/186 (52%)	92 (96%)	4 (4%)	30	47
2	H	185/420 (44%)	179 (97%)	6 (3%)	39	59
3	L	186/214 (87%)	178 (96%)	8 (4%)	29	46
All	All	467/820 (57%)	449 (96%)	18 (4%)	32	50

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	488	CYS
1	E	498	VAL
1	E	503	THR
1	E	544	THR
2	H	17	SER
2	H	166	SER
2	H	188	VAL
2	H	192	THR
2	H	201	ASN
2	H	213	LYS
3	L	20	THR
3	L	39	LEU
3	L	80	THR
3	L	103	THR
3	L	165	VAL
3	L	188	THR
3	L	205	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	214	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

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 monosaccharides 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	H	502	-	2,2,2	1.33	0	1,1,1	0.83	0
5	ARF	E	703	-	2,2,2	1.27	0	1,1,1	0.59	0
5	ARF	H	503	-	2,2,2	1.42	1 (50%)	1,1,1	0.39	0
5	ARF	L	301	-	2,2,2	1.28	0	1,1,1	0.66	0
4	NAG	E	702	1	14,14,15	0.40	0	17,19,21	0.39	0
5	ARF	H	501	-	2,2,2	1.36	0	1,1,1	0.56	0
4	NAG	E	701	1	14,14,15	0.33	0	17,19,21	0.43	0
5	ARF	L	302	-	2,2,2	1.54	1 (50%)	1,1,1	0.34	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	2.09	1.43	1.30
5	H	503	ARF	C-N	2.00	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.95	24 (19%)	1	0	34, 70, 97, 112	0
2	H	216/467 (46%)	0.10	14 (6%)	18	17	24, 40, 75, 102	0
3	L	217/240 (90%)	0.27	19 (8%)	10	9	24, 41, 77, 86	0
All	All	556/924 (60%)	0.35	57 (10%)	6	6	24, 45, 86, 112	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	538	VAL	6.9
1	E	491	TYR	6.6
1	E	539	PHE	5.3
1	E	596	THR	5.2
1	E	501	ALA	4.6
1	E	489	TRP	4.5
1	E	521	THR	4.4
1	E	571	CYS	4.3
1	E	500	SER	4.2
2	H	137	THR	4.2
1	E	522	ASP	4.1
3	L	132	THR	3.8
1	E	619	LEU	3.7
1	E	504	VAL	3.7
1	E	492	PRO	3.6
3	L	158	GLY	3.5
3	L	139	VAL	3.5
1	E	570	PRO	3.3
1	E	617	TYR	3.3
1	E	520	THR	3.2
3	L	209	SER	3.1
1	E	599	LEU	3.1
1	E	493	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	488	CYS	3.0
1	E	569	PRO	2.9
3	L	133	SER	2.9
2	H	136	THR	2.9
3	L	157	ASP	2.8
2	H	138	GLY	2.8
2	H	163	SER	2.8
1	E	490	HIS	2.7
3	L	40	ALA	2.7
2	H	161	SER	2.6
3	L	161	ARG	2.5
3	L	35	GLN	2.5
2	H	104	ALA	2.5
2	H	176	GLN	2.5
3	L	210	PRO	2.4
3	L	184	THR	2.4
3	L	206	THR	2.4
3	L	196	ASN	2.4
2	H	164	LEU	2.4
2	H	175	LEU	2.3
2	H	105	LEU	2.3
1	E	559	SER	2.3
2	H	162	GLY	2.2
3	L	216	ASN	2.2
3	L	140	CYS	2.2
3	L	141	PHE	2.1
2	H	183	SER	2.1
1	E	597	THR	2.1
2	H	190	SER	2.1
3	L	182	SER	2.1
3	L	159	SER	2.1
1	E	546	PRO	2.1
2	H	103	TYR	2.0
3	L	190	ASP	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	E	702	14/15	0.66	0.48	83,92,99,103	0
4	NAG	E	701	14/15	0.81	0.40	91,94,101,102	0
5	ARF	H	502	3/3	0.85	0.15	36,36,36,44	0
5	ARF	L	301	3/3	0.86	0.13	52,52,53,54	0
5	ARF	H	503	3/3	0.92	0.21	32,32,36,41	0
5	ARF	L	302	3/3	0.92	0.17	33,33,36,42	0
5	ARF	E	703	3/3	0.96	0.16	40,40,47,50	0
5	ARF	H	501	3/3	0.97	0.17	32,32,35,37	0

6.5 Other polymers (i)

There are no such residues in this entry.