Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 09:16 PM EDT

PDB ID	:	6WEX
Title	:	Crystal Structure of Broadly Neutralizing Antibody 3I14-D93N Mutant Bound to the Influenza A H6 Hemagglutinin
Authors	:	Harshbarger, W.D.; Lockbaum, G.J.; Deming, D.T.; Attatippaholkun, N.; Schiffer, C.A.; Marasco, W.A.
Deposited on	:	2020-04-03
Resolution	:	3.49 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:

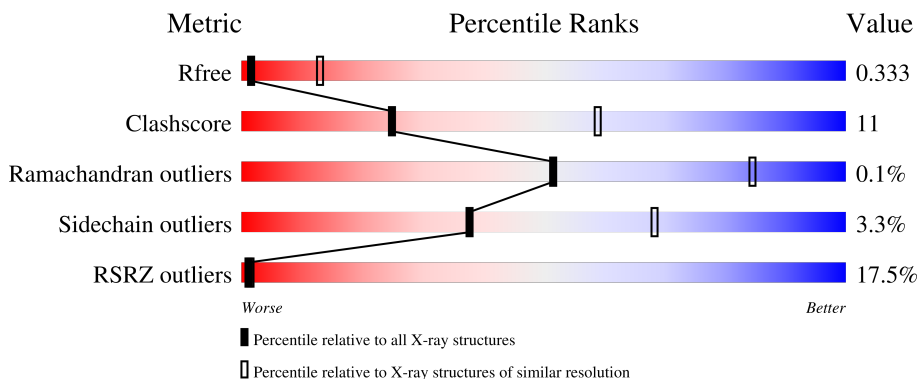|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.49 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	Percentile Ranks	Value
Rfree		0.333
Clashscore		11
Ramachandran outliers		0.1%
Sidechain outliers		3.3%
RSRZ outliers		17.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	325	6% — 76% / 23% / •
2	F	220	6% — 68% / 10% / 22%
3	H	235	33% — 65% / 29% / • 5%
4	L	213	24% — 73% / 24% / •

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 7123 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	325	Total 2565	C 1627	N 437	O 488	S 13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	9	PRO	-	expression tag	UNP A0A0M3KL64
E	10	GLY	-	expression tag	UNP A0A0M3KL64
E	?	-	THR	deletion	UNP A0A0M3KL64
E	?	-	ASN	deletion	UNP A0A0M3KL64

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	172	Total 1385	C 862	N 243	O 273	S 7	0	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	182	GLY	-	expression tag	UNP A0A0J9X245
F	183	SER	-	expression tag	UNP A0A0J9X245
F	184	PRO	-	expression tag	UNP A0A0J9X245
F	185	GLY	-	expression tag	UNP A0A0J9X245
F	186	SER	-	expression tag	UNP A0A0J9X245
F	187	GLY	-	expression tag	UNP A0A0J9X245
F	188	TYR	-	expression tag	UNP A0A0J9X245
F	189	ILE	-	expression tag	UNP A0A0J9X245
F	190	PRO	-	expression tag	UNP A0A0J9X245
F	191	GLU	-	expression tag	UNP A0A0J9X245
F	192	ALA	-	expression tag	UNP A0A0J9X245
F	193	PRO	-	expression tag	UNP A0A0J9X245

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Chain	Residue	Modelled	Actual	Comment	Reference
F	194	ARG	-	expression tag	UNP A0A0J9X245
F	195	ASP	-	expression tag	UNP A0A0J9X245
F	196	GLY	-	expression tag	UNP A0A0J9X245
F	197	GLN	-	expression tag	UNP A0A0J9X245
F	198	ALA	-	expression tag	UNP A0A0J9X245
F	199	TYR	-	expression tag	UNP A0A0J9X245
F	200	VAL	-	expression tag	UNP A0A0J9X245
F	201	ARG	-	expression tag	UNP A0A0J9X245
F	202	LYS	-	expression tag	UNP A0A0J9X245
F	203	ASP	-	expression tag	UNP A0A0J9X245
F	204	GLY	-	expression tag	UNP A0A0J9X245
F	205	GLU	-	expression tag	UNP A0A0J9X245
F	206	TRP	-	expression tag	UNP A0A0J9X245
F	207	VAL	-	expression tag	UNP A0A0J9X245
F	208	LEU	-	expression tag	UNP A0A0J9X245
F	209	LEU	-	expression tag	UNP A0A0J9X245
F	210	SER	-	expression tag	UNP A0A0J9X245
F	211	THR	-	expression tag	UNP A0A0J9X245
F	212	PHE	-	expression tag	UNP A0A0J9X245
F	213	LEU	-	expression tag	UNP A0A0J9X245
F	214	GLY	-	expression tag	UNP A0A0J9X245
F	215	HIS	-	expression tag	UNP A0A0J9X245
F	216	HIS	-	expression tag	UNP A0A0J9X245
F	217	HIS	-	expression tag	UNP A0A0J9X245
F	218	HIS	-	expression tag	UNP A0A0J9X245
F	219	HIS	-	expression tag	UNP A0A0J9X245
F	220	HIS	-	expression tag	UNP A0A0J9X245

- Molecule 3 is a protein called heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	223	1693	1083	285	319	6	0	0	0

- Molecule 4 is a protein called light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	213	1466	916	247	298	5	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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NAG

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
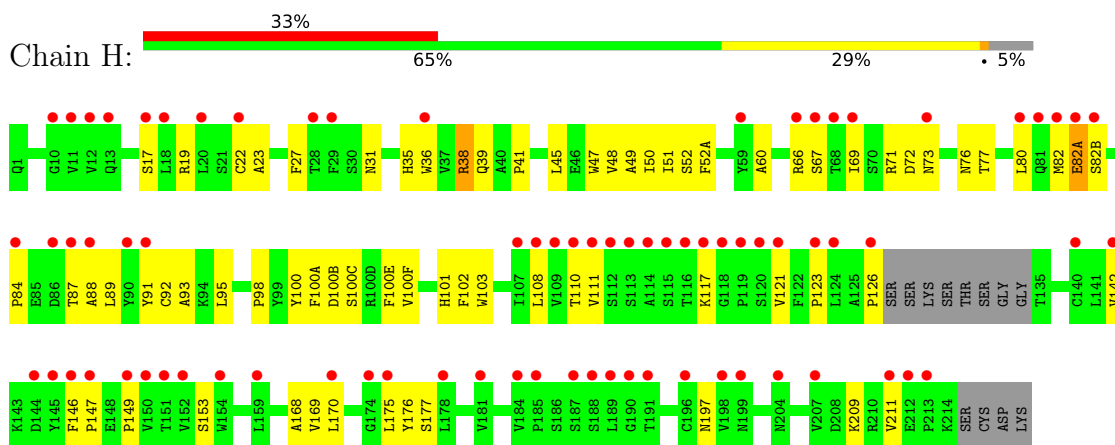
- Molecule 1: Hemagglutinin
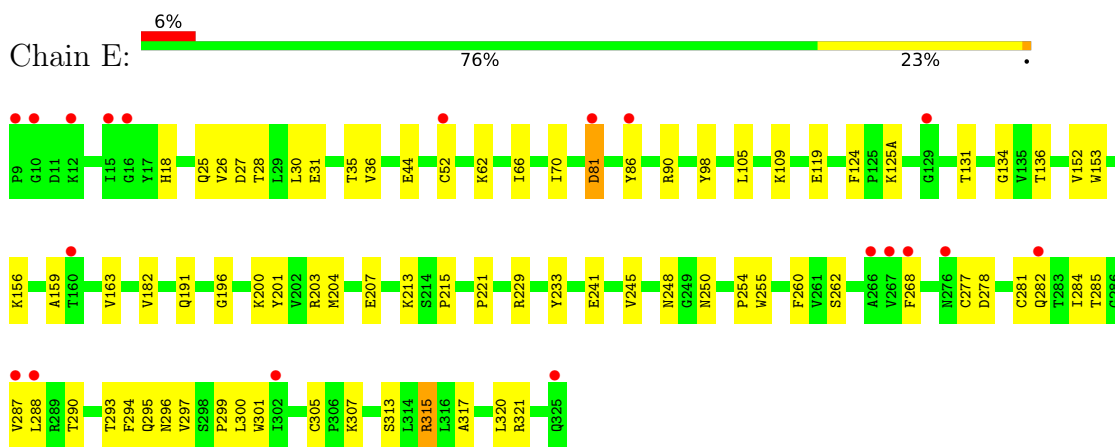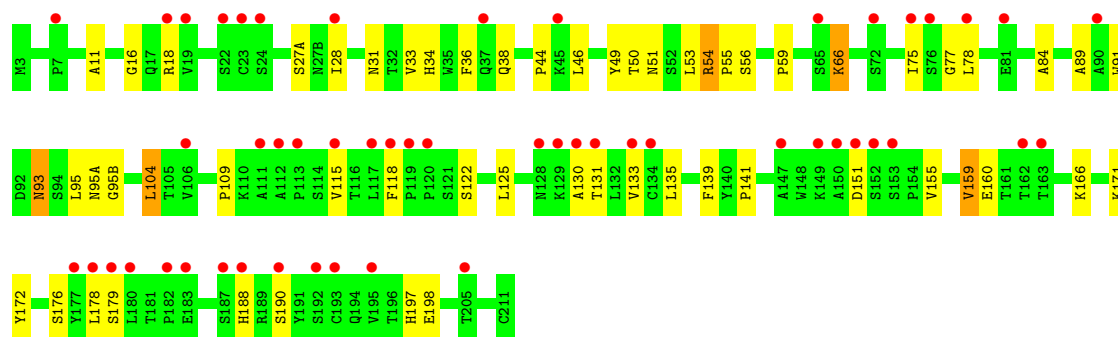

- Molecule 2: Hemagglutinin HA2 chain
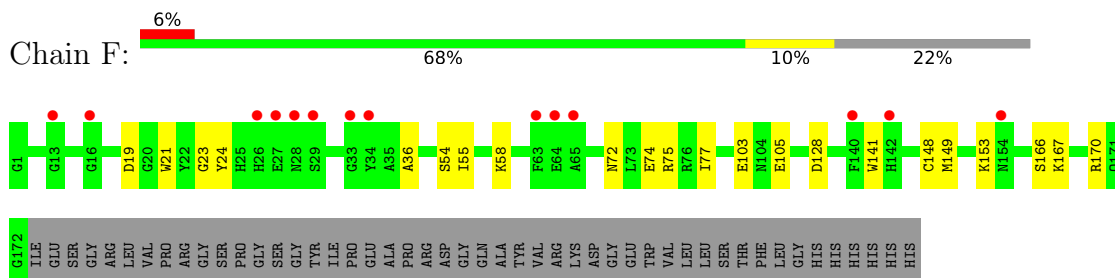
- Molecule 3: heavy chain

• Molecule 4: light chain

Chain L:

24%

73%

24%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	117.81Å 117.81Å 438.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.26 – 3.49 48.26 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.26-3.49) 95.4 (48.26-3.49)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.276 , 0.333 0.276 , 0.333	Depositor DCC
R_{free} test set	1530 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	96.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 91.3	EDS
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	7123	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 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	E	0.24	0/2627	0.46	0/3573
2	F	0.25	0/1413	0.38	0/1902
3	H	0.26	0/1739	0.49	0/2368
4	L	0.26	0/1496	0.54	0/2036
All	All	0.25	0/7275	0.47	0/9879

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	E	2565	0	2514	49	0
2	F	1385	0	1298	13	0
3	H	1693	0	1667	59	0
4	L	1466	0	1303	44	0
5	E	14	0	13	0	0
All	All	7123	0	6795	150	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 11.

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All (150) 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)
1:E:156:LYS:HD2	1:E:159:ALA:HA	1.67	0.75
1:E:315:ARG:HD3	1:E:315:ARG:H	1.51	0.75
3:H:35:HIS:HB2	3:H:93:ALA:O	1.87	0.74
3:H:101:HIS:ND1	3:H:101:HIS:O	2.22	0.73
4:L:160:GLU:OE1	4:L:160:GLU:N	2.21	0.72
3:H:101:HIS:NE2	4:L:56:SER:OG	2.23	0.71
1:E:288:LEU:HD21	1:E:297:VAL:HG21	1.74	0.69
2:F:128:ASP:HB2	2:F:170:ARG:HH22	1.58	0.68
4:L:50:THR:HB	4:L:53:LEU:HD23	1.76	0.67
1:E:313:SER:OG	1:E:315:ARG:NH1	2.28	0.66
2:F:167:LYS:HA	2:F:170:ARG:HD2	1.77	0.66
3:H:87:THR:HG23	3:H:110:THR:HA	1.76	0.66
4:L:131:THR:HG1	4:L:179:SER:HG	1.44	0.66
2:F:74:GLU:HG2	2:F:77:ILE:HD12	1.77	0.65
3:H:52(A):PHE:O	3:H:73:ASN:ND2	2.29	0.65
4:L:54:ARG:HB2	4:L:59:PRO:HD2	1.77	0.65
1:E:200:LYS:HB2	1:E:215:PRO:HG3	1.78	0.65
3:H:101:HIS:CD2	4:L:55:PRO:HB2	2.34	0.63
3:H:66:ARG:NH1	3:H:82(B):SER:O	2.32	0.63
3:H:123:PRO:HB2	3:H:211:VAL:HG13	1.81	0.62
1:E:26:VAL:HG21	1:E:317:ALA:HB2	1.82	0.62
4:L:18:ARG:HA	4:L:75:ILE:O	1.99	0.61
3:H:170:LEU:HD22	3:H:176:TYR:HE1	1.66	0.61
4:L:115:VAL:HA	4:L:135:LEU:O	2.00	0.61
3:H:170:LEU:HD22	3:H:176:TYR:CE1	2.37	0.60
3:H:103:TRP:CZ3	4:L:44:PRO:HB2	2.37	0.59
1:E:28:THR:HG22	1:E:30:LEU:H	1.67	0.59
3:H:35:HIS:CD2	3:H:95:LEU:HB2	2.39	0.58
1:E:27:ASP:OD2	1:E:315:ARG:NH2	2.36	0.58
1:E:207:GLU:HB2	1:E:241:GLU:HG2	1.85	0.58
4:L:33:VAL:N	4:L:51:ASN:OD1	2.33	0.57
1:E:284:ILE:HG23	1:E:285:THR:HG23	1.86	0.57
3:H:17:SER:HB3	3:H:82(A):GLU:HG2	1.85	0.57
4:L:95:LEU:HD13	4:L:95(A):ASN:N	2.19	0.57
3:H:93:ALA:HB1	3:H:103:TRP:HA	1.86	0.57
1:E:52:CYS:N	1:E:282:GLN:OE1	2.34	0.57
3:H:47:TRP:HZ3	3:H:60:ALA:HA	1.69	0.57
1:E:105:LEU:HD11	1:E:109:LYS:HE3	1.87	0.56
1:E:191:GLN:OE1	1:E:250:ASN:ND2	2.36	0.56
1:E:293:THR:HG23	1:E:294:PHE:HD1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:67:SER:OG	3:H:82:MET:SD	2.58	0.56
4:L:95:LEU:HD13	4:L:95(A):ASN:H	1.71	0.56
4:L:95:LEU:HD13	4:L:95(B):GLY:H	1.70	0.55
1:E:27:ASP:HB2	1:E:315:ARG:HH21	1.71	0.55
4:L:95:LEU:HD22	4:L:95(A):ASN:H	1.71	0.55
1:E:260:PHE:CE2	1:E:262:SER:HB2	2.42	0.55
1:E:25:GLN:HG2	1:E:35:THR:HG22	1.88	0.55
1:E:268:PHE:HB3	1:E:284:ILE:HD12	1.89	0.54
1:E:221:PRO:O	1:E:229:ARG:NH2	2.40	0.54
3:H:23:ALA:HB2	3:H:77:THR:HG23	1.89	0.54
4:L:95:LEU:HD13	4:L:95(B):GLY:N	2.22	0.54
1:E:28:THR:HG23	2:F:105:GLU:HB2	1.90	0.53
3:H:47:TRP:CZ3	4:L:95(B):GLY:HA3	2.44	0.53
1:E:213:LYS:NZ	1:E:233:TYR:OH	2.39	0.53
1:E:31:GLU:OE1	1:E:321:ARG:NH2	2.41	0.52
3:H:69:ILE:HG22	3:H:80:LEU:HB2	1.91	0.52
3:H:146:PHE:HB3	3:H:147:PRO:HD3	1.91	0.52
3:H:168:ALA:HB1	3:H:176:TYR:HB3	1.92	0.52
3:H:47:TRP:CH2	4:L:95(B):GLY:HA3	2.44	0.52
3:H:147:PRO:HG2	3:H:149:PRO:HG3	1.92	0.52
2:F:128:ASP:O	2:F:170:ARG:NH2	2.43	0.52
3:H:103:TRP:HZ3	4:L:36:PHE:HB3	1.75	0.52
1:E:204:MET:HG2	1:E:245:VAL:HG22	1.92	0.51
3:H:103:TRP:CZ3	4:L:36:PHE:HB3	2.46	0.51
3:H:121:VAL:HG22	3:H:142:VAL:HG22	1.93	0.51
3:H:101:HIS:HD2	4:L:55:PRO:HB2	1.74	0.51
1:E:52:CYS:SG	1:E:287:VAL:HG21	2.51	0.51
4:L:27(A):SER:O	4:L:93:ASN:N	2.43	0.51
2:F:23:GLY:HA3	2:F:36:ALA:HA	1.94	0.50
3:H:36:TRP:HB2	3:H:49:ALA:HB3	1.92	0.50
3:H:41:PRO:HD3	3:H:88:ALA:HA	1.93	0.50
1:E:201:TYR:HD2	1:E:203:ARG:HG3	1.75	0.50
3:H:38:ARG:O	3:H:45:LEU:HD23	2.11	0.49
4:L:141:PRO:HG2	4:L:197:HIS:NE2	2.27	0.49
4:L:49:TYR:HD2	4:L:50:THR:HG1	1.61	0.49
3:H:52:SER:O	3:H:71:ARG:NH1	2.46	0.48
4:L:166:LYS:HB3	4:L:171:LYS:H	1.77	0.48
1:E:296:ASN:OD1	1:E:296:ASN:N	2.46	0.48
1:E:18:HIS:N	2:F:21:TRP:O	2.46	0.48
4:L:11:ALA:HB3	4:L:104:LEU:HB3	1.95	0.48
1:E:301:TRP:CD2	1:E:305:CYS:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:SER:O	1:E:315:ARG:NH1	2.46	0.48
1:E:196:GLY:O	1:E:200:LYS:NZ	2.46	0.47
3:H:169:VAL:N	3:H:177:SER:O	2.42	0.47
1:E:44:GLU:HG2	1:E:290:THR:HG21	1.95	0.47
3:H:67:SER:HB3	3:H:80:LEU:HD11	1.95	0.47
4:L:34:HIS:CD2	4:L:89:ALA:HB3	2.49	0.47
4:L:197:HIS:CD2	4:L:198:GLU:H	2.33	0.47
1:E:182:VAL:HG21	1:E:213:LYS:HB3	1.95	0.47
3:H:101:HIS:HB2	4:L:46:LEU:HB3	1.97	0.47
3:H:153:SER:OG	3:H:197:ASN:HB2	2.14	0.47
4:L:28:ILE:O	4:L:66:LYS:NZ	2.47	0.47
1:E:36:VAL:HG21	1:E:317:ALA:HB1	1.98	0.46
3:H:69:ILE:HG23	3:H:80:LEU:HD13	1.97	0.46
3:H:147:PRO:C	3:H:149:PRO:HD3	2.36	0.46
2:F:149:MET:O	2:F:153:LYS:HG3	2.15	0.46
4:L:16:GLY:HA2	4:L:77:GLY:HA2	1.97	0.46
1:E:62:LYS:HA	1:E:90:ARG:HG3	1.96	0.46
3:H:48:VAL:O	3:H:60:ALA:HB2	2.15	0.46
1:E:52:CYS:O	1:E:86:TYR:OH	2.24	0.45
4:L:122:SER:HA	4:L:125:LEU:HD23	1.99	0.45
3:H:98:PRO:HG2	4:L:91:TRP:CE2	2.51	0.45
3:H:50:ILE:HG12	3:H:100(A):PHE:CE2	2.51	0.45
4:L:155:VAL:HG11	4:L:178:LEU:HD11	1.99	0.45
1:E:295:GLN:OE1	1:E:297:VAL:N	2.48	0.45
1:E:81:ASP:HA	1:E:119:GLU:HA	1.99	0.45
4:L:38:GLN:O	4:L:84:ALA:HB1	2.17	0.45
1:E:66:ILE:O	1:E:70:ILE:HG13	2.16	0.45
2:F:55:ILE:HD11	2:F:103:GLU:HG3	1.98	0.45
3:H:47:TRP:HZ2	3:H:50:ILE:HB	1.80	0.45
3:H:51:ILE:HD13	3:H:69:ILE:HD13	1.98	0.44
1:E:124:PHE:HB2	1:E:254:PRO:O	2.16	0.44
3:H:170:LEU:HD13	3:H:176:TYR:HD1	1.82	0.44
2:F:54:SER:O	2:F:58:LYS:HG2	2.17	0.44
3:H:103:TRP:CH2	4:L:44:PRO:HB2	2.53	0.44
3:H:123:PRO:HD3	3:H:209:LYS:HG2	1.98	0.44
4:L:151:ASP:OD1	4:L:190:SER:N	2.48	0.44
1:E:98:TYR:HD2	1:E:136:THR:HG21	1.82	0.44
2:F:141:TRP:HA	2:F:141:TRP:CE3	2.53	0.44
3:H:39:GLN:O	3:H:88:ALA:HB1	2.18	0.44
4:L:38:GLN:HA	4:L:44:PRO:HB3	1.98	0.44
3:H:72:ASP:O	3:H:76:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:VAL:HG22	1:E:248:ASN:HD22	1.81	0.44
3:H:31:ASN:N	3:H:31:ASN:OD1	2.49	0.44
4:L:16:GLY:N	4:L:77:GLY:O	2.51	0.44
1:E:125(A):LYS:HB3	1:E:131:THR:HG21	2.00	0.43
1:E:18:HIS:O	1:E:320:LEU:HD11	2.19	0.43
4:L:130:ALA:O	4:L:179:SER:HA	2.19	0.43
3:H:117:LYS:HG3	3:H:175:LEU:HD11	2.01	0.43
1:E:207:GLU:OE1	1:E:207:GLU:N	2.52	0.43
3:H:89:LEU:HG	3:H:108:LEU:HD13	2.01	0.43
1:E:81:ASP:OD1	1:E:81:ASP:N	2.52	0.42
3:H:84:PRO:HA	3:H:111:VAL:HG23	2.01	0.42
3:H:209:LYS:HD2	3:H:209:LYS:HA	1.88	0.42
4:L:139:PHE:O	4:L:172:TYR:HB2	2.20	0.42
1:E:307:LYS:HB2	1:E:307:LYS:HE3	1.80	0.42
3:H:100(C):SER:HB3	3:H:100(F):VAL:HG22	2.01	0.42
1:E:134:GLY:HA3	1:E:153:TRP:HB3	2.02	0.41
1:E:152:VAL:HG23	1:E:255:TRP:HB2	2.03	0.41
3:H:100(B):ASP:N	3:H:100(B):ASP:OD1	2.54	0.41
2:F:72:ASN:OD1	2:F:72:ASN:N	2.45	0.41
4:L:133:VAL:HA	4:L:176:SER:O	2.21	0.41
1:E:299:PRO:HG2	1:E:300:LEU:HD12	2.03	0.41
3:H:126:PRO:HA	4:L:118:PHE:CE1	2.55	0.41
4:L:31:ASN:OD1	4:L:93:ASN:HB2	2.21	0.41
3:H:36:TRP:CZ2	3:H:92:CYS:HB3	2.55	0.40
3:H:39:GLN:HB2	3:H:91:TYR:HE1	1.86	0.40
3:H:100(A):PHE:CE2	4:L:91:TRP:HH2	2.39	0.40
2:F:166:SER:O	2:F:170:ARG:HB3	2.22	0.40
3:H:47:TRP:CZ3	3:H:60:ALA:HA	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	323/325 (99%)	310 (96%)	13 (4%)	0	100	100
2	F	170/220 (77%)	166 (98%)	4 (2%)	0	100	100
3	H	219/235 (93%)	192 (88%)	27 (12%)	0	100	100
4	L	211/213 (99%)	184 (87%)	26 (12%)	1 (0%)	29	68
All	All	923/993 (93%)	852 (92%)	70 (8%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	159	VAL

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	285/285 (100%)	280 (98%)	5 (2%)	59	81
2	F	146/185 (79%)	142 (97%)	4 (3%)	44	73
3	H	188/198 (95%)	180 (96%)	8 (4%)	29	62
4	L	147/177 (83%)	139 (95%)	8 (5%)	22	55
All	All	766/845 (91%)	741 (97%)	25 (3%)	38	68

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	81	ASP
1	E	277	CYS
1	E	278	ASP
1	E	281	CYS
1	E	315	ARG
2	F	19	ASP
2	F	24	TYR
2	F	75	ARG
2	F	148	CYS
3	H	19	ARG

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Mol	Chain	Res	Type
3	H	22	CYS
3	H	27	PHE
3	H	38	ARG
3	H	82(A)	GLU
3	H	100	TYR
3	H	100(E)	PHE
3	H	102	PHE
4	L	54	ARG
4	L	66	LYS
4	L	78	LEU
4	L	93	ASN
4	L	104	LEU
4	L	109	PRO
4	L	159	VAL
4	L	188	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	226	GLN

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 ⓘ

1 ligand is 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	NAG	E	401	1	14,14,15	0.31	0	17,19,21	0.59	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	NAG	E	401	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	401	NAG	O5-C5-C6-O6
5	E	401	NAG	C4-C5-C6-O6
5	E	401	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	325/325 (100%)	0.45	19 (5%)	23	20	37, 81, 120, 172	0
2	F	172/220 (78%)	0.58	14 (8%)	12	12	38, 94, 141, 166	0
3	H	223/235 (94%)	1.70	78 (34%)	0	0	85, 158, 204, 234	0
4	L	213/213 (100%)	1.15	52 (24%)	0	0	70, 127, 189, 218	0
All	All	933/993 (93%)	0.94	163 (17%)	1	1	37, 109, 187, 234	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	112	SER	14.2
4	L	180	LEU	8.2
3	H	119	PRO	7.5
3	H	117	LYS	7.4
3	H	120	SER	6.8
1	E	9	PRO	6.8
3	H	113	SER	6.8
1	E	10	GLY	6.6
3	H	196	CYS	6.2
3	H	69	ILE	6.2
3	H	118	GLY	5.9
1	E	287	VAL	5.8
1	E	52	CYS	5.7
1	E	12	LYS	5.5
3	H	115	SER	5.5
4	L	195	VAL	5.4
4	L	187	SER	5.4
4	L	130	ALA	5.1
3	H	110	THR	5.0
3	H	111	VAL	4.9
4	L	152	SER	4.8

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Mol	Chain	Res	Type	RSRZ
3	H	145	TYR	4.8
3	H	144	ASP	4.8
3	H	82	MET	4.6
1	E	160	THR	4.5
3	H	11	VAL	4.5
3	H	204	ASN	4.5
3	H	124	LEU	4.5
3	H	17	SER	4.5
3	H	84	PRO	4.5
4	L	111	ALA	4.4
3	H	28	THR	4.4
4	L	65	SER	4.3
4	L	24	SER	4.3
3	H	126	PRO	4.1
4	L	117	LEU	4.1
4	L	205	THR	4.0
3	H	80	LEU	4.0
3	H	91	TYR	4.0
3	H	109	VAL	4.0
3	H	154	TRP	3.9
4	L	19	VAL	3.8
3	H	198	VAL	3.8
2	F	29	SER	3.8
4	L	23	CYS	3.8
3	H	152	VAL	3.7
4	L	151	ASP	3.7
4	L	177	TYR	3.7
4	L	76	SER	3.6
3	H	159	LEU	3.6
2	F	27	GLU	3.6
4	L	113	PRO	3.5
4	L	179	SER	3.5
4	L	192	SER	3.5
3	H	59	TYR	3.5
3	H	22	CYS	3.5
3	H	151	THR	3.5
3	H	199	ASN	3.5
3	H	187	SER	3.4
2	F	26	HIS	3.4
4	L	22	SER	3.4
4	L	178	LEU	3.3
4	L	193	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
3	H	146	PHE	3.3
4	L	150	ALA	3.3
3	H	174	GLY	3.2
4	L	75	ILE	3.2
3	H	121	VAL	3.2
4	L	120	PRO	3.2
3	H	181	VAL	3.2
3	H	116	THR	3.1
1	E	302	ILE	3.1
2	F	33	GLY	3.1
4	L	131	THR	3.1
1	E	282	GLN	3.1
3	H	87	THR	3.1
3	H	185	PRO	3.1
3	H	82(A)	GLU	3.1
3	H	68	THR	3.1
3	H	107	ILE	3.0
3	H	12	VAL	3.0
4	L	133	VAL	3.0
4	L	128	ASN	3.0
4	L	149	LYS	3.0
4	L	112	ALA	3.0
3	H	191	THR	2.9
3	H	184	VAL	2.9
3	H	212	GLU	2.9
3	H	170	LEU	2.9
3	H	123	PRO	2.9
3	H	90	TYR	2.9
3	H	149	PRO	2.9
1	E	81	ASP	2.8
3	H	189	LEU	2.8
3	H	140	CYS	2.8
4	L	81	GLU	2.8
4	L	28	ILE	2.8
3	H	18	LEU	2.8
4	L	72	SER	2.7
1	E	86	TYR	2.7
4	L	115	VAL	2.7
4	L	119	PRO	2.7
1	E	15	ILE	2.7
4	L	37	GLN	2.6
3	H	114	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
4	L	18	ARG	2.6
1	E	129	GLY	2.6
3	H	10	GLY	2.6
2	F	65	ALA	2.6
3	H	108	LEU	2.6
2	F	28	ASN	2.6
4	L	183	GLU	2.6
4	L	162	THR	2.5
3	H	29	PHE	2.5
4	L	153	SER	2.5
4	L	7	PRO	2.5
3	H	142	VAL	2.5
1	E	325	GLN	2.5
4	L	106	VAL	2.5
2	F	142	HIS	2.5
4	L	190	SER	2.5
2	F	140	PHE	2.4
3	H	188	SER	2.4
4	L	163	THR	2.4
3	H	73	ASN	2.4
3	H	147	PRO	2.4
1	E	16	GLY	2.4
2	F	16	GLY	2.4
2	F	13	GLY	2.4
4	L	78	LEU	2.4
3	H	213	PRO	2.3
1	E	276	ASN	2.3
2	F	154	ASN	2.3
3	H	81	GLN	2.3
3	H	211	VAL	2.3
3	H	150	VAL	2.3
4	L	90	ALA	2.3
1	E	266	ALA	2.3
3	H	66	ARG	2.3
4	L	45	LYS	2.3
4	L	129	LYS	2.3
3	H	88	ALA	2.2
4	L	182	PRO	2.2
3	H	86	ASP	2.2
1	E	267	VAL	2.2
1	E	268	PHE	2.2
3	H	82(B)	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	34	TYR	2.2
3	H	207	VAL	2.2
3	H	36	TRP	2.2
3	H	20	LEU	2.2
4	L	147	ALA	2.1
3	H	175	LEU	2.1
2	F	63	PHE	2.1
4	L	134	CYS	2.1
1	E	288	LEU	2.1
3	H	13	GLN	2.1
3	H	67	SER	2.1
3	H	190	GLY	2.0
4	L	188	HIS	2.0
2	F	64	GLU	2.0
4	L	118	PHE	2.0
3	H	178	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
5	NAG	E	401	14/15	0.83	0.27	89,108,117,118	0

6.5 Other polymers ⓘ

There are no such residues in this entry.