



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 05:31 PM BST

PDB ID : 6OC3
Title : Crystal structure of FluA-20 Fab in complex with the head domain of H1
(A/Solomon Islands/3/2006)
Authors : Wilson, I.A.; Lang, S.
Deposited on : 2019-03-21
Resolution : 2.85 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 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 : 2.13.1
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) : 2.13.1

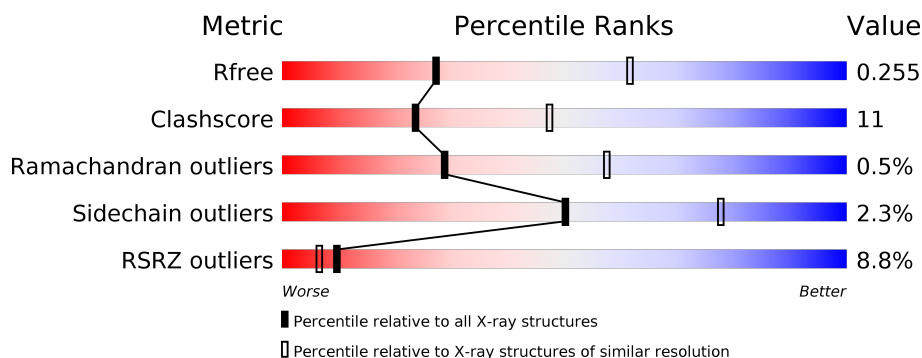
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 on 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	A	235	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	C	235	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• 6%</div> </div> </div>
2	B	214	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>•</div> </div> </div>
2	D	214	<div> <div>14%</div> <div> <div></div> <div>78%</div> <div>21%</div> <div>•</div> </div> </div>
3	E	227	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>• 7%</div> </div> </div>
3	F	227	<div> <div>16%</div> <div> <div></div> <div>68%</div> <div>23%</div> <div>• 7%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10038 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 Heavy chain of FluA-20 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1674	1056	275	336	7			
1	C	221	Total	C	N	O	S	0	0	0
			1656	1047	272	330	7			

- Molecule 2 is a protein called Light chain of FluA-20 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1646	1031	281	329	5			
2	D	213	Total	C	N	O	S	0	0	0
			1646	1031	281	329	5			

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	212	Total	C	N	O	S	0	0	0
			1701	1084	293	320	4			
3	F	212	Total	C	N	O	S	0	0	0
			1701	1084	293	320	4			

There are 30 discrepancies between the modelled and reference sequences:

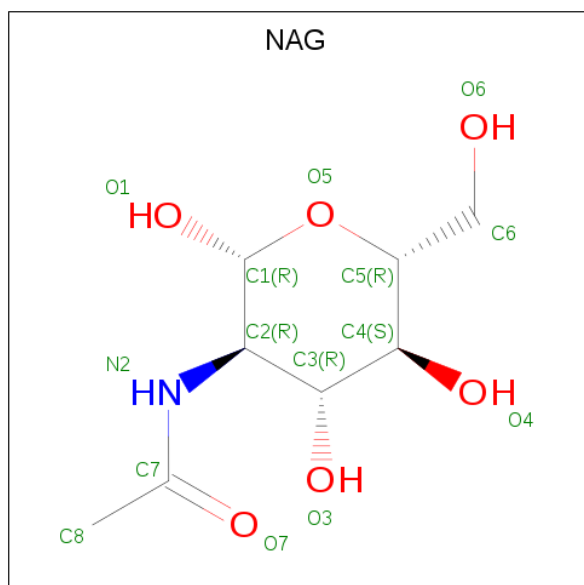
Chain	Residue	Modelled	Actual	Comment	Reference
E	264	SER	-	expression tag	UNP A7Y8I1
E	265	GLY	-	expression tag	UNP A7Y8I1
E	266	LEU	-	expression tag	UNP A7Y8I1
E	267	VAL	-	expression tag	UNP A7Y8I1
E	268	PRO	-	expression tag	UNP A7Y8I1
E	269	ARG	-	expression tag	UNP A7Y8I1
E	270	GLY	-	expression tag	UNP A7Y8I1
E	271	SER	-	expression tag	UNP A7Y8I1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	272	GLY	-	expression tag	UNP A7Y8I1
E	273	HIS	-	expression tag	UNP A7Y8I1
E	274	HIS	-	expression tag	UNP A7Y8I1
E	275	HIS	-	expression tag	UNP A7Y8I1
E	276	HIS	-	expression tag	UNP A7Y8I1
E	277	HIS	-	expression tag	UNP A7Y8I1
E	278	HIS	-	expression tag	UNP A7Y8I1
F	264	SER	-	expression tag	UNP A7Y8I1
F	265	GLY	-	expression tag	UNP A7Y8I1
F	266	LEU	-	expression tag	UNP A7Y8I1
F	267	VAL	-	expression tag	UNP A7Y8I1
F	268	PRO	-	expression tag	UNP A7Y8I1
F	269	ARG	-	expression tag	UNP A7Y8I1
F	270	GLY	-	expression tag	UNP A7Y8I1
F	271	SER	-	expression tag	UNP A7Y8I1
F	272	GLY	-	expression tag	UNP A7Y8I1
F	273	HIS	-	expression tag	UNP A7Y8I1
F	274	HIS	-	expression tag	UNP A7Y8I1
F	275	HIS	-	expression tag	UNP A7Y8I1
F	276	HIS	-	expression tag	UNP A7Y8I1
F	277	HIS	-	expression tag	UNP A7Y8I1
F	278	HIS	-	expression tag	UNP A7Y8I1

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

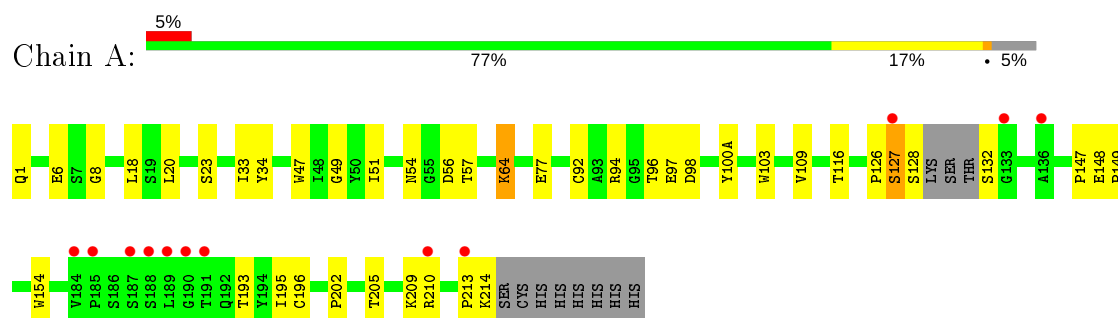


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	14	0
			14	8	1	5		

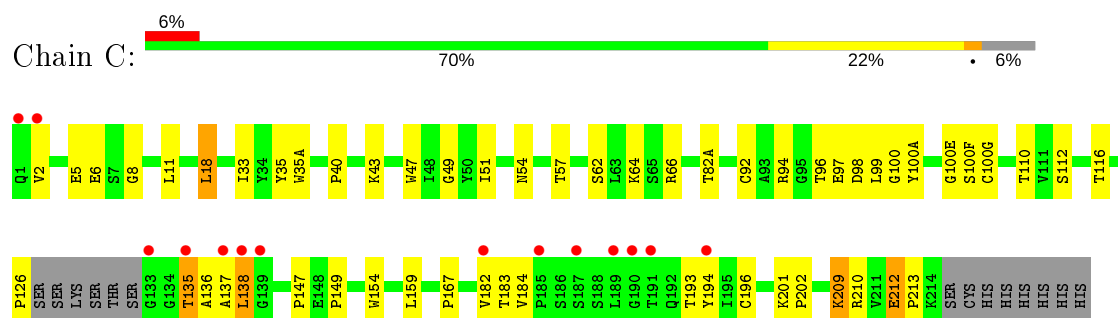
3 Residue-property plots [i](#)

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.

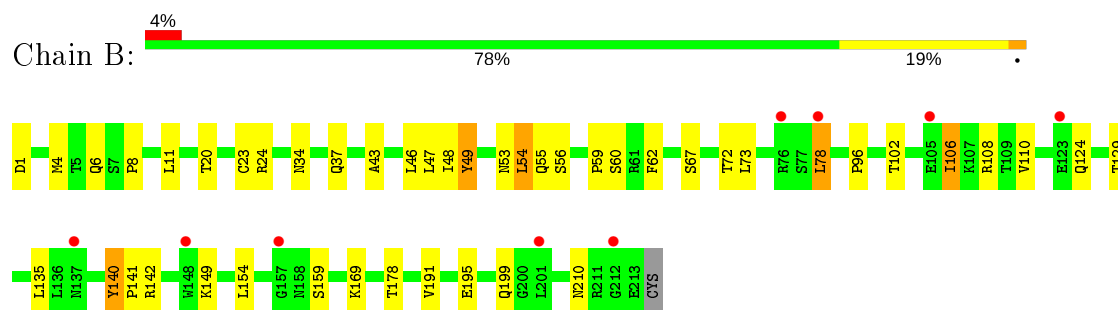
- Molecule 1: Heavy chain of FluA-20 Fab



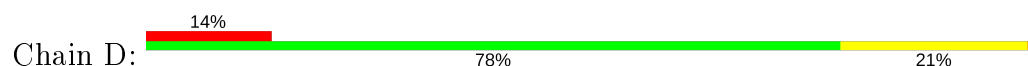
- Molecule 1: Heavy chain of FluA-20 Fab

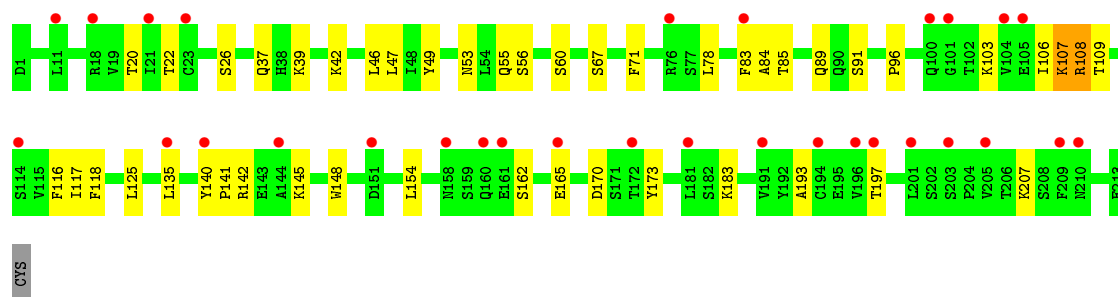


- Molecule 2: Light chain of FluA-20 Fab

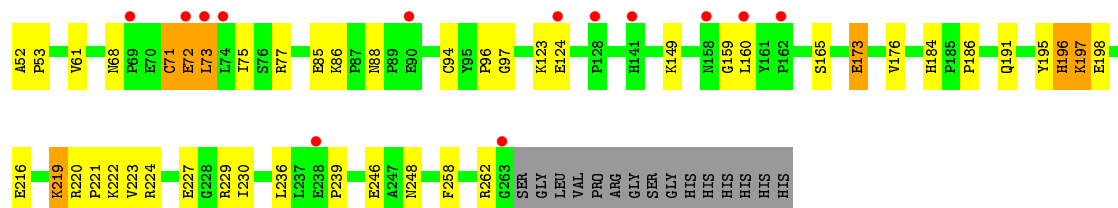
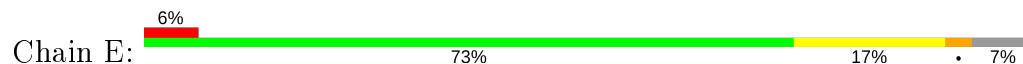


- Molecule 2: Light chain of FluA-20 Fab

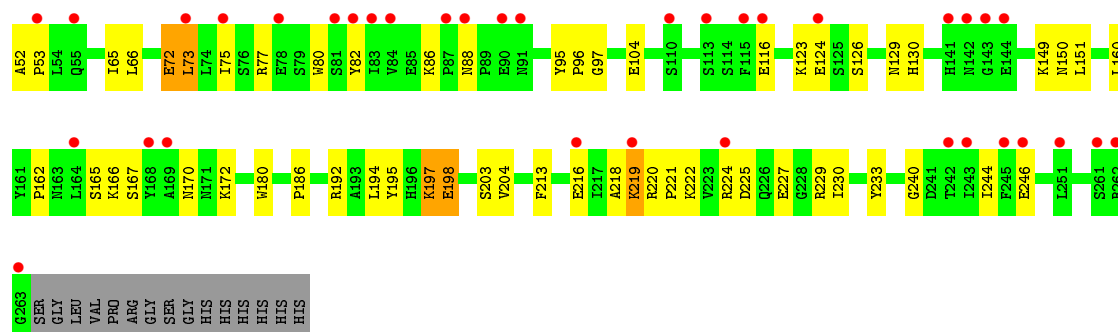




• Molecule 3: Hemagglutinin



• Molecule 3: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.47Å 109.78Å 146.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.85 48.17 – 2.85	Depositor EDS
% Data completeness (in resolution range)	95.5 (48.17-2.85) 95.7 (48.17-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.237 , 0.257 0.240 , 0.255	Depositor DCC
R_{free} test set	1791 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.949	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.9	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	0.92	EDS
Total number of atoms	10038	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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 [i](#)

5.1 Standard geometry [i](#)

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	A	0.71	0/1716	0.92	2/2346 (0.1%)
1	C	0.72	1/1698 (0.1%)	0.95	8/2322 (0.3%)
2	B	0.74	1/1683 (0.1%)	0.90	4/2285 (0.2%)
2	D	0.49	0/1683	0.71	0/2285
3	E	0.53	0/1753	0.81	2/2385 (0.1%)
3	F	0.52	0/1753	0.79	1/2385 (0.0%)
All	All	0.63	2/10286 (0.0%)	0.85	17/14008 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	B	0	1
2	D	0	1
3	E	0	2
3	F	0	2
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	100	GLY	C-N	8.12	1.52	1.34
2	B	140	TYR	CE1-CZ	-5.53	1.31	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	GLY	O-C-N	11.16	140.56	122.70
1	C	100	GLY	CA-C-N	-10.65	93.78	117.20
1	A	195	ILE	CG1-CB-CG2	-7.30	95.33	111.40
2	B	54	LEU	CA-CB-CG	7.09	131.61	115.30
1	C	99	LEU	C-N-CA	-7.04	107.52	122.30
1	C	100	GLY	C-N-CA	-6.53	105.38	121.70
1	C	212	GLU	C-N-CD	-6.46	106.39	120.60
1	C	99	LEU	O-C-N	-6.34	112.43	123.20
1	A	64	LYS	CA-CB-CG	6.21	127.06	113.40
1	C	18	LEU	CA-CB-CG	5.86	128.77	115.30
2	B	154	LEU	CA-CB-CG	5.63	128.26	115.30
3	E	71	CYS	CA-CB-SG	5.58	124.04	114.00
2	B	11	LEU	CB-CG-CD2	-5.46	101.71	111.00
3	E	173	GLU	CA-CB-CG	-5.40	101.52	113.40
1	C	99	LEU	CA-C-N	5.38	126.96	116.20
3	F	194	LEU	CB-CG-CD2	-5.09	102.34	111.00
2	B	49	TYR	CA-CB-CG	5.06	123.02	113.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	106	ILE	Mainchain
1	C	2	VAL	Peptide
2	D	106	ILE	Mainchain
3	E	72	GLU	Peptide
3	E	73	LEU	Peptide
3	F	72	GLU	Peptide
3	F	73	LEU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1674	0	1628	41	1
1	C	1656	0	1613	63	1
2	B	1646	0	1608	28	1
2	D	1646	0	1608	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1701	0	1621	46	0
3	F	1701	0	1622	58	1
4	E	14	0	13	0	0
All	All	10038	0	9713	220	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 11.

All (220) 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:E:159:GLY:O	3:E:196:HIS:CD2	1.82	1.31
3:F:192:ARG:NE	3:F:198:GLU:OE2	1.74	1.19
3:E:197:LYS:HD2	3:E:248:ASN:O	1.51	1.09
1:A:33:ILE:HD13	3:F:216:GLU:OE1	1.54	1.05
1:C:137:ALA:HB1	1:C:182:VAL:O	1.61	1.00
1:C:138:LEU:HD11	1:C:182:VAL:CG1	1.94	0.98
3:E:72:GLU:HB2	3:E:149:LYS:HZ1	1.30	0.95
2:D:55:GLN:HE22	3:E:221:PRO:HA	1.32	0.95
1:C:135:THR:OG1	2:D:117:ILE:O	1.84	0.94
3:E:159:GLY:O	3:E:196:HIS:HD2	1.37	0.94
2:B:67:SER:OG	3:F:88:ASN:ND2	2.02	0.92
2:B:149:LYS:NZ	2:B:195:GLU:OE1	2.03	0.90
2:D:53:ASN:ND2	3:E:224:ARG:H	1.70	0.89
3:E:159:GLY:C	3:E:196:HIS:CD2	2.47	0.88
1:C:138:LEU:CD1	1:C:182:VAL:HG12	2.03	0.88
1:C:135:THR:HG21	2:D:118:PHE:CE1	2.10	0.86
3:E:195:TYR:O	3:E:197:LYS:HG2	1.76	0.85
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.59	0.85
2:D:145:LYS:HB3	2:D:197:THR:HB	1.60	0.82
2:D:67:SER:OG	3:E:88:ASN:ND2	2.12	0.82
1:A:126:PRO:HG2	1:A:213:PRO:HA	1.60	0.81
3:E:197:LYS:CD	3:E:248:ASN:O	2.30	0.79
1:C:138:LEU:HD11	1:C:182:VAL:HG12	1.61	0.78
1:A:193:THR:HG21	1:A:210:ARG:HH21	1.50	0.76
3:F:186:PRO:HB3	3:F:227:GLU:HG2	1.67	0.76
1:A:128:SER:C	1:A:132:SER:HB3	2.06	0.75
1:A:33:ILE:CD1	3:F:216:GLU:OE1	2.34	0.75
3:E:159:GLY:C	3:E:196:HIS:NE2	2.39	0.75
2:B:56:SER:N	3:F:222:LYS:HD3	2.03	0.72
2:B:56:SER:H	3:F:222:LYS:HD3	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LEU:CD1	1:C:182:VAL:CG1	2.65	0.72
3:E:159:GLY:O	3:E:196:HIS:NE2	2.23	0.71
1:C:137:ALA:HB2	1:C:183:THR:HG22	1.72	0.71
3:E:94:CYS:HA	3:E:224:ARG:HH11	1.55	0.71
1:A:94:ARG:HH12	3:F:219:LYS:HD2	1.58	0.69
1:C:135:THR:CG2	2:D:118:PHE:CE1	2.76	0.69
2:B:46:LEU:HD21	2:B:49:TYR:HB2	1.75	0.69
2:D:56:SER:HB2	3:E:222:LYS:HD3	1.76	0.68
3:E:94:CYS:HA	3:E:224:ARG:NH1	2.09	0.68
3:E:52:ALA:HB3	3:E:77:ARG:HH22	1.59	0.67
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.77	0.67
3:E:72:GLU:HB2	3:E:149:LYS:NZ	2.06	0.66
2:D:46:LEU:HD21	2:D:49:TYR:HB2	1.78	0.66
3:E:236:LEU:HD13	3:E:262:ARG:HH21	1.61	0.65
1:C:51:ILE:HG13	1:C:57:THR:HG22	1.79	0.63
1:A:51:ILE:HG13	1:A:57:THR:HG22	1.82	0.62
3:F:204:VAL:HG23	3:F:213:PHE:HE1	1.65	0.62
1:A:96:THR:HG21	3:F:220:ARG:HG2	1.83	0.61
1:C:167:PRO:HD2	2:D:162:SER:OG	2.00	0.61
1:A:128:SER:O	1:A:132:SER:HB3	2.00	0.61
1:C:135:THR:HG22	1:C:135:THR:O	2.00	0.60
1:C:138:LEU:HD11	1:C:182:VAL:HG13	1.81	0.60
1:A:33:ILE:O	1:A:33:ILE:HG13	2.02	0.60
3:F:72:GLU:HB2	3:F:149:LYS:HZ3	1.66	0.59
1:A:47:TRP:CD2	2:B:96:PRO:HD2	2.38	0.59
1:A:64:LYS:HE2	1:C:54:ASN:HD21	1.69	0.58
1:A:64:LYS:HE2	1:C:54:ASN:ND2	2.19	0.58
2:D:56:SER:HB2	3:E:222:LYS:CD	2.33	0.58
1:C:193:THR:HG23	1:C:210:ARG:HD2	1.86	0.57
1:C:137:ALA:CB	1:C:183:THR:HA	2.34	0.57
1:A:47:TRP:CH2	1:A:49:GLY:HA2	2.39	0.56
1:A:97:GLU:O	3:F:220:ARG:NH1	2.38	0.56
1:A:94:ARG:HH22	3:F:219:LYS:HD2	1.69	0.56
2:D:108:ARG:HG3	2:D:109:THR:O	2.05	0.56
2:D:39:LYS:HD2	2:D:42:LYS:HE2	1.87	0.56
1:C:97:GLU:O	3:E:220:ARG:NH1	2.39	0.55
2:D:108:ARG:NH1	2:D:170:ASP:O	2.38	0.55
3:E:53:PRO:O	3:E:77:ARG:NH1	2.39	0.55
1:C:138:LEU:C	1:C:138:LEU:HD12	2.27	0.55
3:E:173:GLU:HA	3:E:239:PRO:HB3	1.87	0.54
1:A:147:PRO:HD2	1:A:202:PRO:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLN:HE22	3:F:219:LYS:HZ2	1.53	0.54
1:A:56:ASP:OD2	1:C:64:LYS:HE2	2.08	0.54
1:A:127:SER:HB3	1:A:214:LYS:HG3	1.90	0.54
2:B:55:GLN:HE22	3:F:221:PRO:HA	1.72	0.54
2:D:26:SER:HB2	3:F:104:GLU:OE2	2.08	0.54
1:C:137:ALA:HB2	1:C:183:THR:HA	1.90	0.54
3:E:160:LEU:HA	3:E:196:HIS:HD2	1.73	0.53
3:F:129:ASN:HB3	3:F:162:PRO:HG2	1.91	0.53
1:C:159:LEU:HD21	1:C:182:VAL:HG21	1.91	0.53
3:F:66:LEU:HD22	3:F:151:LEU:HD11	1.91	0.53
2:D:125:LEU:O	2:D:183:LYS:HD2	2.08	0.52
1:A:193:THR:CG2	1:A:210:ARG:HH21	2.21	0.52
1:C:116:THR:HG21	1:C:202:PRO:O	2.09	0.52
1:C:137:ALA:HB1	1:C:182:VAL:C	2.29	0.52
1:C:100(F):SER:HB3	2:D:96:PRO:HG3	1.92	0.52
1:C:137:ALA:CB	1:C:183:THR:HG22	2.40	0.52
1:C:137:ALA:O	2:D:118:PHE:HZ	1.93	0.52
1:A:100(A):TYR:HE2	3:F:97:GLY:N	2.07	0.52
1:C:40:PRO:HB2	1:C:43:LYS:HG3	1.92	0.51
3:E:165:SER:HB3	3:E:246:GLU:HG2	1.92	0.51
3:F:116:GLU:OE2	3:F:172:LYS:NZ	2.43	0.51
2:B:54:LEU:HD21	2:B:60:SER:HA	1.93	0.51
1:A:116:THR:HG21	1:A:202:PRO:O	2.11	0.51
2:D:108:ARG:HG3	2:D:109:THR:N	2.26	0.51
2:D:140:TYR:CG	2:D:141:PRO:HA	2.46	0.51
1:A:100(A):TYR:HE2	3:F:97:GLY:H	1.59	0.51
1:C:135:THR:HG23	2:D:118:PHE:CZ	2.46	0.50
1:A:1:GLN:HE22	3:F:219:LYS:NZ	2.09	0.50
3:F:195:TYR:O	3:F:197:LYS:HG2	2.12	0.50
2:B:108:ARG:HG3	2:B:140:TYR:CD2	2.47	0.50
3:F:165:SER:HB3	3:F:246:GLU:HG2	1.92	0.50
2:D:55:GLN:HE22	3:E:221:PRO:CA	2.14	0.50
2:B:78:LEU:HD13	2:B:106:ILE:HG13	1.93	0.50
3:F:124:GLU:N	3:F:124:GLU:OE1	2.45	0.50
1:A:154:TRP:CH2	1:A:196:CYS:HB3	2.47	0.50
1:A:1:GLN:NE2	3:F:219:LYS:NZ	2.60	0.50
1:A:6:GLU:HG2	1:A:92:CYS:SG	2.52	0.49
2:B:6:GLN:NE2	2:B:102:THR:OG1	2.46	0.49
1:C:126:PRO:HG2	1:C:213:PRO:HA	1.93	0.49
3:F:52:ALA:O	3:F:80:TRP:HA	2.12	0.49
1:C:47:TRP:CD2	2:D:96:PRO:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:52:ALA:HB3	3:F:77:ARG:HH22	1.78	0.49
1:C:137:ALA:O	2:D:118:PHE:CZ	2.66	0.49
1:C:35(A):TRP:CZ3	1:C:94:ARG:HG3	2.48	0.49
1:C:8:GLY:O	1:C:201:LYS:NZ	2.32	0.48
1:C:47:TRP:CH2	1:C:49:GLY:HA2	2.49	0.48
1:C:11:LEU:HD11	1:C:112:SER:HB3	1.96	0.48
1:C:154:TRP:CH2	1:C:196:CYS:HB3	2.49	0.48
1:C:100(G):CYS:SG	2:D:91:SER:OG	2.64	0.48
2:B:59:PRO:HG2	2:B:62:PHE:CE2	2.48	0.48
3:F:53:PRO:HB3	3:F:82:TYR:CZ	2.49	0.48
1:C:147:PRO:HD2	1:C:202:PRO:HB2	1.96	0.47
3:E:61:VAL:HG23	3:E:85:GLU:OE1	2.14	0.47
2:B:191:VAL:HG22	2:B:210:ASN:OD1	2.13	0.47
3:E:124:GLU:N	3:E:124:GLU:OE1	2.47	0.47
1:A:94:ARG:NH1	3:F:219:LYS:HD2	2.28	0.47
1:C:94:ARG:HH22	3:E:219:LYS:HD2	1.78	0.47
2:D:85:THR:OG1	2:D:103:LYS:HD2	2.14	0.47
1:A:34:TYR:OH	3:F:218:ALA:HB1	2.14	0.47
1:C:94:ARG:HH12	3:E:219:LYS:HD2	1.80	0.47
1:C:135:THR:CG2	2:D:118:PHE:CZ	2.98	0.46
1:A:18:LEU:CD1	1:A:109:VAL:HG11	2.45	0.46
2:B:53:ASN:ND2	3:F:224:ARG:H	2.13	0.46
2:B:140:TYR:CD1	2:B:141:PRO:HA	2.50	0.46
1:C:100(A):TYR:OH	3:E:96:PRO:HA	2.16	0.46
1:C:138:LEU:HD12	1:C:182:VAL:HG12	1.92	0.46
2:D:142:ARG:HB2	2:D:173:TYR:CE2	2.50	0.46
1:C:126:PRO:HD2	1:C:213:PRO:HA	1.98	0.46
2:B:4:MET:HE3	2:B:23:CYS:SG	2.56	0.46
1:C:98:ASP:OD2	3:E:229:ARG:NH2	2.44	0.46
2:D:83:PHE:CE2	2:D:165:GLU:HB3	2.51	0.46
1:C:135:THR:HG21	2:D:118:PHE:CD1	2.50	0.45
1:A:54:ASN:ND2	1:C:64:LYS:HG2	2.32	0.45
2:B:20:THR:HG23	2:B:72:THR:HG23	1.97	0.45
2:B:8:PRO:O	2:B:102:THR:HG23	2.17	0.45
3:E:186:PRO:HB3	3:E:227:GLU:HG2	1.99	0.45
3:F:130:HIS:CE1	3:F:162:PRO:HD2	2.52	0.45
3:F:126:SER:HB3	3:F:166:LYS:HE2	1.99	0.45
2:B:159:SER:HA	2:B:178:THR:O	2.16	0.45
3:E:97:GLY:HA3	3:E:230:ILE:O	2.16	0.45
3:F:167:SER:OG	3:F:244:ILE:HG13	2.16	0.45
1:C:147:PRO:HD2	1:C:202:PRO:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:SER:OG	3:F:222:LYS:HD2	2.16	0.45
2:B:48:ILE:HD12	2:B:73:LEU:CD1	2.46	0.45
1:C:35:TYR:CD2	1:C:100(E):GLY:HA2	2.51	0.45
3:F:186:PRO:CB	3:F:227:GLU:HG2	2.42	0.45
1:C:138:LEU:HD12	1:C:138:LEU:O	2.17	0.44
3:F:123:LYS:HB3	3:F:124:GLU:OE1	2.17	0.44
3:F:170:ASN:HB3	3:F:240:GLY:H	1.82	0.44
3:F:97:GLY:HA3	3:F:230:ILE:O	2.17	0.44
1:C:138:LEU:CD1	1:C:138:LEU:C	2.86	0.44
3:F:95:TYR:CD1	3:F:96:PRO:HD2	2.53	0.44
1:A:8:GLY:HA3	1:A:20:LEU:HD23	1.98	0.44
3:E:176:VAL:HA	3:E:258:PHE:O	2.18	0.44
1:A:128:SER:O	1:A:132:SER:CB	2.66	0.44
1:C:11:LEU:HD12	1:C:110:THR:O	2.18	0.44
3:F:222:LYS:HE3	3:F:225:ASP:HA	1.98	0.44
3:F:72:GLU:HB2	3:F:149:LYS:NZ	2.31	0.44
2:D:89:GLN:HE21	2:D:96:PRO:HB3	1.82	0.44
1:A:18:LEU:HD12	1:A:109:VAL:HG11	2.00	0.44
3:F:65:ILE:HD12	3:F:65:ILE:HA	1.80	0.44
1:A:23:SER:HA	1:A:77:GLU:HG2	1.98	0.43
1:A:98:ASP:OD2	3:F:229:ARG:NH2	2.45	0.43
3:E:220:ARG:HD2	3:E:229:ARG:HG2	1.99	0.43
3:E:68:ASN:HB3	3:E:71:CYS:SG	2.58	0.43
2:D:107:LYS:HA	2:D:140:TYR:OH	2.18	0.43
3:F:160:LEU:HA	3:F:160:LEU:HD23	1.70	0.43
3:F:216:GLU:HG3	3:F:220:ARG:NH2	2.33	0.43
3:F:97:GLY:HA2	3:F:229:ARG:HD2	2.00	0.43
3:F:130:HIS:NE2	3:F:162:PRO:HD2	2.34	0.43
1:C:136:ALA:H	2:D:116:PHE:HD2	1.64	0.43
1:C:97:GLU:OE1	1:C:97:GLU:HA	2.18	0.43
2:D:39:LYS:HG2	2:D:84:ALA:HB2	2.00	0.43
1:C:6:GLU:HG3	1:C:92:CYS:SG	2.58	0.43
3:E:186:PRO:CB	3:E:227:GLU:HG2	2.48	0.43
1:A:100(A):TYR:OH	3:F:96:PRO:HA	2.18	0.43
3:E:160:LEU:HA	3:E:196:HIS:CD2	2.53	0.43
3:E:191:GLN:HG3	3:E:197:LYS:O	2.19	0.43
1:C:212:GLU:HA	1:C:213:PRO:HD3	1.42	0.42
3:F:180:TRP:CE2	3:F:233:TYR:HB2	2.54	0.42
2:D:140:TYR:CD1	2:D:141:PRO:HA	2.54	0.42
3:F:180:TRP:CE2	3:F:204:VAL:HG21	2.54	0.42
2:D:53:ASN:OD1	3:E:223:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:GLN:NE2	3:E:221:PRO:HA	2.16	0.42
3:F:66:LEU:O	3:F:150:ASN:HB2	2.20	0.42
2:D:148:TRP:O	2:D:154:LEU:HD12	2.19	0.42
2:B:169:LYS:HB3	2:B:169:LYS:HE2	1.70	0.41
1:C:212:GLU:CB	1:C:213:PRO:HD2	2.48	0.41
1:C:66:ARG:HD2	1:C:82(A):THR:O	2.20	0.41
2:D:22:THR:HA	2:D:71:PHE:O	2.20	0.41
2:B:34:ASN:HB3	2:B:46:LEU:HD11	2.02	0.41
3:E:184:HIS:CE1	3:E:216:GLU:HG2	2.56	0.41
1:A:94:ARG:NH2	3:F:219:LYS:HD2	2.35	0.41
1:C:35:TYR:CE2	1:C:100(E):GLY:HA2	2.55	0.41
2:B:124:GLN:HG2	2:B:129:THR:O	2.20	0.41
3:E:123:LYS:HB3	3:E:124:GLU:OE1	2.20	0.41
1:A:103:TRP:O	2:B:43:ALA:HB1	2.21	0.41
1:C:96:THR:HG21	3:E:219:LYS:O	2.20	0.41
2:B:110:VAL:HG21	2:B:199:GLN:NE2	2.36	0.41
3:F:220:ARG:H	3:F:227:GLU:HG3	1.86	0.41
3:F:72:GLU:HG3	3:F:149:LYS:HE2	2.03	0.40
2:B:142:ARG:O	2:B:142:ARG:HG2	2.20	0.40
2:D:193:ALA:HA	2:D:207:LYS:O	2.22	0.40
1:C:184:VAL:HG11	1:C:194:TYR:CZ	2.56	0.40
1:C:33:ILE:HD13	3:E:216:GLU:OE1	2.22	0.40
3:F:86:LYS:HE2	3:F:86:LYS:HB3	1.96	0.40
1:A:33:ILE:HD13	3:F:216:GLU:CD	2.35	0.40
3:E:86:LYS:HE2	3:E:86:LYS:HB3	1.77	0.40
2:D:39:LYS:HD2	2:D:42:LYS:CE	2.49	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:A:205:THR:OG1	1:C:209:LYS:NZ[2_445]	1.45	0.75
2:B:24:ARG:NH2	3:F:198:GLU:OE1[4_545]	2.02	0.18

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	A	220/235 (94%)	214 (97%)	4 (2%)	2 (1%)	17	43
1	C	217/235 (92%)	208 (96%)	7 (3%)	2 (1%)	17	43
2	B	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
2	D	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
3	E	210/227 (92%)	200 (95%)	9 (4%)	1 (0%)	29	57
3	F	210/227 (92%)	198 (94%)	11 (5%)	1 (0%)	29	57
All	All	1279/1352 (95%)	1230 (96%)	43 (3%)	6 (0%)	29	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	73	LEU
3	F	73	LEU
1	A	127	SER
1	C	135	THR
1	A	149	PRO
1	C	149	PRO

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	A	194/205 (95%)	192 (99%)	2 (1%)	76	91
1	C	191/205 (93%)	186 (97%)	5 (3%)	46	75
2	B	189/190 (100%)	186 (98%)	3 (2%)	62	84
2	D	189/190 (100%)	183 (97%)	6 (3%)	39	69
3	E	185/197 (94%)	180 (97%)	5 (3%)	44	74
3	F	185/197 (94%)	180 (97%)	5 (3%)	44	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1133/1184 (96%)	1107 (98%)	26 (2%)	50 78

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

Mol	Chain	Res	Type
1	A	148	GLU
1	A	209	LYS
2	B	1	ASP
2	B	78	LEU
2	B	135	LEU
1	C	5	GLU
1	C	18	LEU
1	C	62	SER
1	C	138	LEU
1	C	209	LYS
2	D	20	THR
2	D	60	SER
2	D	78	LEU
2	D	107	LYS
2	D	108	ARG
2	D	135	LEU
3	E	75	ILE
3	E	196	HIS
3	E	197	LYS
3	E	198	GLU
3	E	219	LYS
3	F	75	ILE
3	F	197	LYS
3	F	198	GLU
3	F	203	SER
3	F	219	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
2	B	53	ASN
2	D	53	ASN
3	E	88	ASN
3	E	196	HIS
3	F	88	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 ⓘ

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	$\# Z > 2$
4	NAG	E	301	3	14,14,15	0.29	0	17,19,21	0.62	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	301	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	301	NAG	O5-C5-C6-O6
4	E	301	NAG	C4-C5-C6-O6

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, 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	A	224/235 (95%)	0.44	12 (5%)	25 21	30, 61, 84, 100	0
1	C	221/235 (94%)	0.44	14 (6%)	20 15	42, 66, 93, 114	0
2	B	213/214 (99%)	0.52	9 (4%)	36 31	43, 65, 93, 113	0
2	D	213/214 (99%)	0.77	30 (14%)	2 2	45, 78, 114, 123	0
3	E	212/227 (93%)	0.60	13 (6%)	21 17	50, 76, 105, 117	0
3	F	212/227 (93%)	0.91	36 (16%)	1 1	46, 83, 132, 144	0
All	All	1295/1352 (95%)	0.61	114 (8%)	10 6	30, 71, 110, 144	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	263	GLY	6.9
3	E	263	GLY	6.8
3	F	90	GLU	5.7
3	F	82	TYR	5.2
2	D	205	VAL	4.9
3	E	90	GLU	4.6
3	F	142	ASN	4.6
1	C	1	GLN	4.6
3	F	88	ASN	4.1
3	F	143	GLY	4.0
2	D	76	ARG	3.9
1	C	133	GLY	3.9
3	F	75	ILE	3.9
1	C	138	LEU	3.8
3	F	261	SER	3.8
3	E	141	HIS	3.7
2	D	144	ALA	3.7
3	F	141	HIS	3.7
3	F	83	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	201	LEU	3.6
1	C	182	VAL	3.6
3	F	164	LEU	3.5
2	D	196	VAL	3.5
2	D	101	GLY	3.5
1	A	187	SER	3.3
1	A	190	GLY	3.3
3	F	73	LEU	3.2
1	A	213	PRO	3.1
1	A	184	VAL	3.1
3	E	124	GLU	3.0
2	D	151	ASP	3.0
2	D	165	GLU	3.0
2	D	181	LEU	3.0
3	F	242	THR	2.9
1	A	136	ALA	2.9
3	F	110	SER	2.9
3	F	115	PHE	2.9
2	D	197	THR	2.8
3	E	128	PRO	2.8
1	A	133	GLY	2.8
3	F	53	PRO	2.7
1	C	194	TYR	2.7
2	D	210	ASN	2.7
2	D	161	GLU	2.6
1	C	189	LEU	2.6
3	F	55	GLN	2.6
2	D	23	CYS	2.6
2	B	212	GLY	2.5
1	C	187	SER	2.5
1	C	190	GLY	2.5
2	D	100	GLN	2.5
2	D	194	CYS	2.5
2	D	11	LEU	2.5
2	B	201	LEU	2.5
3	F	81	SER	2.5
2	B	137	ASN	2.5
3	F	78	GLU	2.5
1	C	139	GLY	2.4
1	A	185	PRO	2.4
3	E	162	PRO	2.4
3	F	116	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	262	ARG	2.3
1	A	189	LEU	2.3
1	C	137	ALA	2.3
2	D	191	VAL	2.3
2	D	140	TYR	2.3
2	D	135	LEU	2.3
2	B	78	LEU	2.3
1	C	135	THR	2.3
2	B	148	TRP	2.3
3	F	169	ALA	2.3
2	B	105	GLU	2.3
3	E	158	ASN	2.2
1	A	127	SER	2.2
1	C	191	THR	2.2
2	D	203	SER	2.2
3	F	113	SER	2.2
2	D	209	PHE	2.2
2	D	160	GLN	2.2
2	D	158	ASN	2.2
3	F	91	ASN	2.2
1	A	191	THR	2.2
3	F	251	LEU	2.2
3	F	243	ILE	2.2
2	D	21	ILE	2.2
3	E	238	GLU	2.2
3	F	246	GLU	2.2
2	D	83	PHE	2.2
3	F	124	GLU	2.2
3	F	224	ARG	2.2
1	A	188	SER	2.1
2	B	157	GLY	2.1
3	F	144	GLU	2.1
3	E	74	LEU	2.1
1	A	210	ARG	2.1
2	B	76	ARG	2.1
3	E	72	GLU	2.1
3	E	69	PRO	2.1
3	E	73	LEU	2.1
3	F	245	PHE	2.1
2	D	114	SER	2.1
3	E	160	LEU	2.1
2	D	104	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	219	LYS	2.1
2	D	172	THR	2.1
3	F	168	TYR	2.1
3	F	216	GLU	2.1
1	C	2	VAL	2.0
2	D	18	ARG	2.0
2	D	105	GLU	2.0
1	C	185	PRO	2.0
2	B	123	GLU	2.0
3	F	84	VAL	2.0
3	F	87	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 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(\AA^2)	Q<0.9
4	NAG	E	301	14/15	-	-	83,90,93,93	14

6.5 Other polymers [i](#)

There are no such residues in this entry.