



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 09:27 pm BST

PDB ID : 6EWB  
Title : Crystal structure of GII.4 UNSW 2012 P domain in complex with Fab 10E9  
Authors : Koromyslova, A.D.; Hansman, G.S.  
Deposited on : 2017-11-03  
Resolution : 2.78 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](mailto: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.

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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 : 2.11  
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) : 2.11

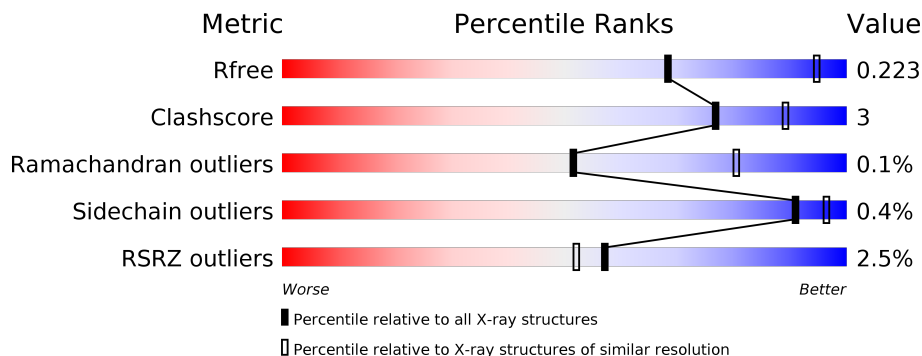
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 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.



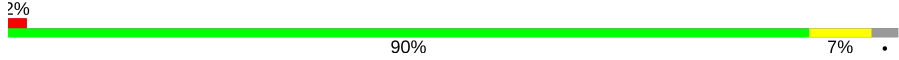
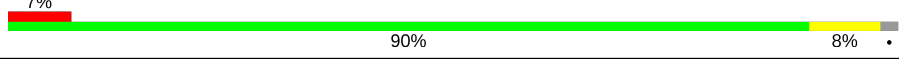
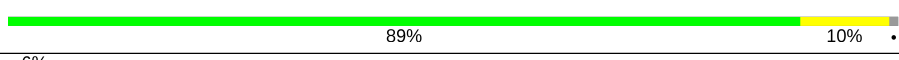
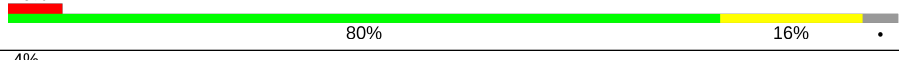
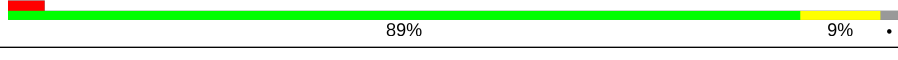
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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  $\geq 3$ , 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	310	94% (green), 5% (yellow), 5% (red)
1	B	310	89% (green), 9% (yellow), 2% (red)
1	C	310	94% (green), 6% (yellow)
1	D	310	94% (green), 6% (yellow)
2	E	216	5% (red), 86% (green), 5% (yellow), 10% (grey)
2	G	216	90% (green), 8% (yellow), 2% (red)

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Mol	Chain	Length	Quality of chain
2	H	216	 <p>2% 90% 7%</p>
2	J	216	 <p>7% 90% 6%</p>
3	F	214	 <p>7% 90% 8%</p>
3	I	214	 <p>89% 10%</p>
3	K	214	 <p>6% 80% 16%</p>
3	L	214	 <p>4% 89% 9%</p>

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 21709 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	307	2376	1511	400	455	10	0	0	0
1	B	306	2384	1512	405	457	10	0	0	0
1	C	310	2388	1517	402	459	10	0	0	0
1	D	309	2400	1522	409	459	10	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	GLY	-	expression tag	UNP K4LM89
A	222	PRO	-	expression tag	UNP K4LM89
A	223	GLY	-	expression tag	UNP K4LM89
A	224	SER	-	expression tag	UNP K4LM89
B	221	GLY	-	expression tag	UNP K4LM89
B	222	PRO	-	expression tag	UNP K4LM89
B	223	GLY	-	expression tag	UNP K4LM89
B	224	SER	-	expression tag	UNP K4LM89
C	221	GLY	-	expression tag	UNP K4LM89
C	222	PRO	-	expression tag	UNP K4LM89
C	223	GLY	-	expression tag	UNP K4LM89
C	224	SER	-	expression tag	UNP K4LM89
D	221	GLY	-	expression tag	UNP K4LM89
D	222	PRO	-	expression tag	UNP K4LM89
D	223	GLY	-	expression tag	UNP K4LM89
D	224	SER	-	expression tag	UNP K4LM89

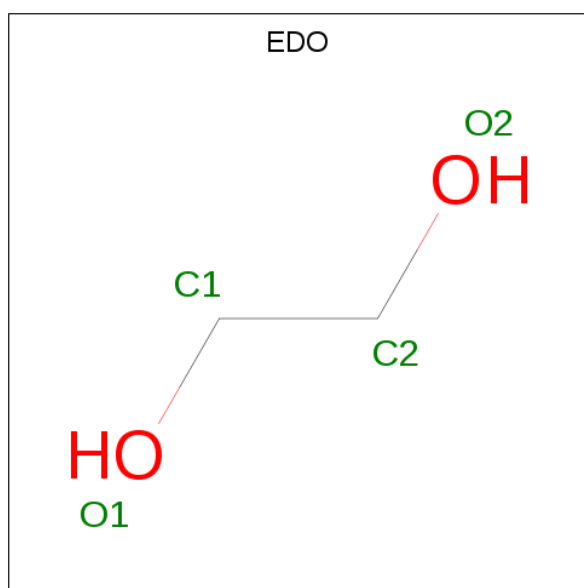
- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	195	Total	C	N	O	S	0	0	0
			1366	871	222	267	6			
2	G	211	Total	C	N	O	S	0	0	0
			1566	995	257	307	7			
2	H	210	Total	C	N	O	S	0	0	0
			1558	987	255	310	6			
2	J	207	Total	C	N	O	S	0	0	0
			1483	946	242	289	6			

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	209	Total	C	N	O	S	0	0	0
			1517	951	252	305	9			
3	I	211	Total	C	N	O	S	0	0	0
			1589	992	261	327	9			
3	K	205	Total	C	N	O	S	0	0	0
			1513	952	248	304	9			
3	L	210	Total	C	N	O	S	0	0	0
			1561	976	258	318	9			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



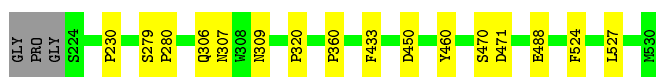
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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.

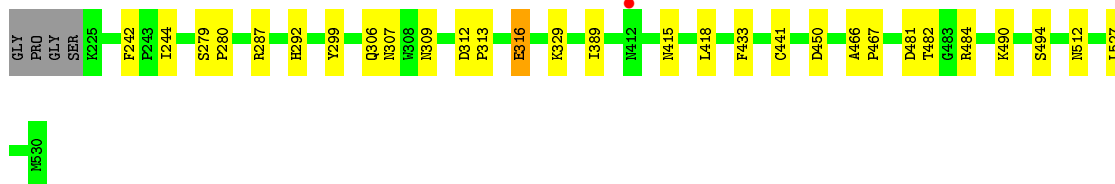
- Molecule 1: VP1

Chain A: 



- Molecule 1: VP1

Chain B: 



- Molecule 1: VP1

Chain C: 




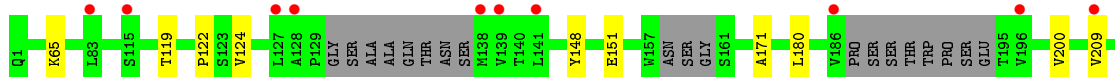
- Molecule 1: VP1

Chain D: 




- Molecule 2: Fab heavy chain

Chain E: 



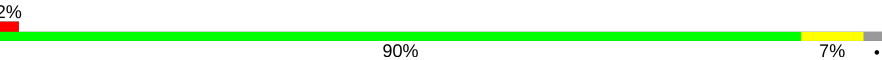
V214  
PRO  
ARG

- Molecule 2: Fab heavy chain

Chain G:  90% 8%


Q1 R40 A92 H103 P122 G130 SER ALA ALA GLN THR S137 S137 L141 Y148 E151 P152 V153 V154 L162 A171 W191 P192 S193 E194 H199 V200 A201 D210 R216

- Molecule 2: Fab heavy chain

Chain H:  90% 7%


Q1 V2 R40 K67 S84 A92 R98 P126 L127 G130 SER ALA ALA GLN THR S137 S137 C143 L144 E151 P152 V153 S175 P181 W191 P192 M199 D210 R216

- Molecule 2: Fab heavy chain

Chain J:  90% 6%

Q1 P122 Y125 A128 P129 SER ALA ALA GLN THR ASN S137 C143 L144 Y148 P149 P150 P150 E151 P152 V153 V154 T156 W157 H158 S159 G160 S161 L162 S163 S168 SER T190 W191 P192 S193 C196 M199 V200 A201 E202 P203 T207 V209 P215 ARG


- Molecule 3: Fab light chain

Chain F:  90% 8%

GLY Q1 P8 M11 Y35 R45 V57 P58 N75 N76 A79 K102 L105 P106 R107 A108 A111 P112 I116 L124 T125 S126 G127 G128 Y139 G151 S152 Q155 L160 Y185 T196 H197 K198 T199 S200 K208 T201 S202 P203 L204 V205 N209


ARG  
ASN  
GLU  
CYS

- Molecule 3: Fab light chain

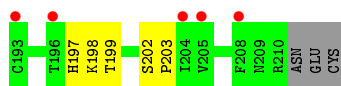
Chain I:  89% 10%

G0 S12 V57 P58 A58 R60 N75 S76 E80 Q89 S92 K106 R107 A108 P118 T125 T181 K182 D183 E184 R187 E194 V205 F208 N209 R210 ASN GLU CYS

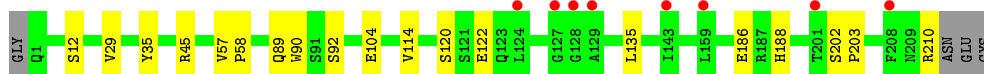
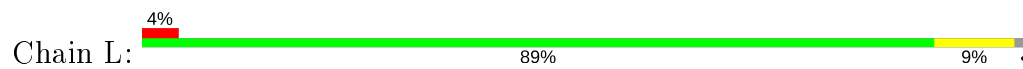
- Molecule 3: Fab light chain

Chain K:  80% 16%

G0 M11 S12 M21 W34 Y35 R45 W46 I47 V57 P58 A79 Q89 R90 S91 S92 L105 K106 R107 A108 D109 V114 P118 S126 G127 F134 L135 D142 W147 K148 L149 D150 G151 SER GLU ARG ARG GLN N156 G157 T181 K182 ASP GLU Y185



- Molecule 3: Fab light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.84Å 111.63Å 288.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 2.78 48.76 – 2.78	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.76-2.78) 98.8 (48.76-2.78)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.186 , 0.222 0.188 , 0.223	Depositor DCC
$R_{free}$ test set	4336 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.9	Xtrriage
Anisotropy	0.388	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 33.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.023 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21709	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO

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	0.32	0/2446	0.50	0/3349
1	B	0.31	0/2453	0.49	0/3357
1	C	0.30	0/2459	0.47	0/3368
1	D	0.32	0/2470	0.51	0/3380
2	E	0.28	0/1397	0.49	0/1923
2	G	0.32	0/1608	0.51	0/2204
2	H	0.34	0/1600	0.53	0/2196
2	J	0.29	0/1523	0.50	0/2096
3	F	0.27	0/1555	0.48	0/2128
3	I	0.30	0/1628	0.49	0/2219
3	K	0.30	0/1550	0.50	0/2113
3	L	0.31	0/1600	0.51	0/2185
All	All	0.31	0/22289	0.50	0/30518

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 [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	2376	0	2258	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2384	0	2276	15	0
1	C	2388	0	2263	10	0
1	D	2400	0	2284	10	0
2	E	1366	0	1211	5	0
2	G	1566	0	1506	9	0
2	H	1558	0	1486	9	0
2	J	1483	0	1344	9	0
3	F	1517	0	1354	9	0
3	I	1589	0	1480	12	0
3	K	1513	0	1389	19	0
3	L	1561	0	1428	12	0
4	B	4	0	6	0	0
4	L	4	0	6	0	0
All	All	21709	0	20291	125	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 3.

All (125) 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:K:89:GLN:HE21	3:K:92:SER:H	1.25	0.83
3:I:89:GLN:HE21	3:I:92:SER:H	1.27	0.80
1:C:329:LYS:HE3	1:C:352:TYR:HB2	1.68	0.74
3:I:89:GLN:NE2	3:I:92:SER:H	1.85	0.74
2:G:154:THR:HB	2:G:201:ALA:HB3	1.72	0.72
3:K:89:GLN:NE2	3:K:92:SER:H	1.89	0.70
3:K:107:ARG:NH1	3:K:108:ALA:O	2.25	0.69
1:B:433:PHE:HB3	1:B:450:ASP:HB3	1.77	0.67
3:I:194:GLU:HG2	3:I:205:VAL:HG22	1.78	0.66
3:F:124:LEU:O	3:F:126:SER:HA	1.98	0.64
3:F:79:ALA:HA	3:F:105:LEU:HD21	1.82	0.61
2:E:124:VAL:HG21	2:E:209:VAL:HG21	1.83	0.61
1:A:524:PHE:HB3	2:G:194:GLU:HG3	1.83	0.60
1:A:307:ASN:ND2	1:A:309:ASN:OD1	2.35	0.59
2:H:130:GLY:HA2	2:H:216:ARG:HD2	1.85	0.59
1:B:329:LYS:HD2	1:B:389:ILE:HD11	1.85	0.58
1:D:389:ILE:HG22	1:D:441:CYS:HB2	1.86	0.58
3:K:114:VAL:HG22	3:K:135:LEU:HD22	1.87	0.56
2:H:40:ARG:HG3	2:H:92:ALA:HB2	1.89	0.55
2:H:151:GLU:OE1	2:H:152:PRO:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:67:LYS:NZ	2:H:84:SER:O	2.40	0.55
3:L:89:GLN:HE21	3:L:92:SER:H	1.55	0.54
1:C:490:LYS:HG3	1:C:527:LEU:HD11	1.89	0.54
1:C:433:PHE:HB3	1:C:450:ASP:HB3	1.90	0.54
2:G:199:ASN:ND2	2:G:210:ASP:OD1	2.38	0.54
3:L:89:GLN:NE2	3:L:92:SER:H	2.06	0.53
1:A:433:PHE:HB3	1:A:450:ASP:HB3	1.91	0.53
2:H:175:SER:O	2:H:175:SER:OG	2.26	0.52
3:K:181:THR:O	3:K:185:TYR:N	2.43	0.52
3:L:35:TYR:OH	3:L:45:ARG:NH1	2.43	0.52
2:G:151:GLU:OE1	2:G:171:ALA:HB3	2.10	0.51
3:I:107:ARG:NH1	3:I:108:ALA:O	2.44	0.51
1:C:320:PRO:HD2	1:C:360:PRO:HB2	1.93	0.51
3:K:79:ALA:HA	3:K:105:LEU:HD21	1.92	0.51
1:B:415:ASN:HB2	1:B:418:LEU:HD11	1.92	0.51
3:F:124:LEU:C	3:F:126:SER:HA	2.30	0.50
3:L:120:SER:OG	3:L:122:GLU:OE1	2.29	0.50
2:G:122:PRO:HB3	2:G:148:TYR:HB3	1.92	0.50
1:B:490:LYS:HG3	1:B:527:LEU:HD11	1.94	0.50
3:K:109:ASP:OD2	3:K:198:LYS:HE2	2.12	0.49
1:D:433:PHE:HB3	1:D:450:ASP:HB3	1.94	0.49
1:D:230:PRO:HG3	1:D:460:TYR:CG	2.47	0.49
2:E:171:ALA:HB2	2:E:180:LEU:HB2	1.93	0.49
3:I:12:SER:HB2	3:I:106:LYS:HG2	1.94	0.49
3:K:11:MET:HE2	3:K:21:MET:HB3	1.94	0.48
2:J:143:CYS:HB2	2:J:157:TRP:CH2	2.49	0.48
2:J:191:TRP:CE2	2:J:192:PRO:HB3	2.48	0.48
1:D:287:ARG:HD2	1:D:306:GLN:HA	1.95	0.48
3:K:197:HIS:HB3	3:K:199:THR:HG22	1.95	0.48
1:B:482:THR:OG1	1:B:484:ARG:HG2	2.13	0.48
2:H:191:TRP:CD1	2:H:192:PRO:HA	2.49	0.48
1:C:328:GLY:HA3	1:C:400:PRO:HB3	1.96	0.48
3:L:114:VAL:HG22	3:L:135:LEU:HD22	1.97	0.47
3:K:12:SER:O	3:K:106:LYS:HE3	2.15	0.47
1:D:284:CYS:HA	1:D:324:PRO:HD3	1.97	0.47
3:I:60:ARG:NH2	3:I:80:GLU:OE2	2.36	0.47
3:F:35:TYR:OH	3:F:45:ARG:NH1	2.48	0.46
3:K:156:ASN:HA	3:K:157:GLY:HA3	1.58	0.46
1:A:470:SER:OG	1:A:471:ASP:N	2.48	0.46
2:J:150:PRO:O	2:J:202:HIS:NE2	2.41	0.46
1:A:488:GLU:HG3	1:A:527:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:SER:OG	1:C:471:ASP:N	2.48	0.46
1:B:316:GLU:H	1:B:316:GLU:HG2	1.55	0.46
1:A:279:SER:HA	1:A:280:PRO:HD3	1.78	0.46
2:G:40:ARG:HG3	2:G:92:ALA:HB2	1.98	0.46
1:C:292:HIS:HB2	1:C:299:TYR:CE1	2.51	0.45
2:J:191:TRP:CG	2:J:192:PRO:HA	2.52	0.45
2:H:199:ASN:ND2	2:H:210:ASP:OD2	2.42	0.45
3:F:107:ARG:HG2	3:F:108:ALA:N	2.31	0.45
1:B:279:SER:HA	1:B:280:PRO:HD3	1.84	0.44
2:J:151:GLU:HB2	2:J:152:PRO:HA	1.99	0.44
1:B:389:ILE:HG22	1:B:441:CYS:HB2	1.99	0.44
1:C:311:TYR:CE1	1:C:320:PRO:HG3	2.52	0.44
2:E:151:GLU:OE2	2:E:171:ALA:HB3	2.17	0.44
3:K:89:GLN:HG2	3:K:91:SER:H	1.81	0.44
3:L:57:VAL:HA	3:L:58:PRO:HD3	1.83	0.44
1:D:488:GLU:HG3	1:D:527:LEU:HD22	1.99	0.44
2:J:149:PHE:HA	2:J:150:PRO:HA	1.71	0.44
2:J:122:PRO:HB3	2:J:148:TYR:HB3	2.00	0.44
3:K:35:TYR:OH	3:K:45:ARG:NH1	2.50	0.43
1:B:242:PHE:O	1:B:244:ILE:N	2.49	0.43
2:J:159:SER:OG	2:J:159:SER:O	2.32	0.43
2:H:2:VAL:HG21	2:H:98:ARG:NH1	2.32	0.43
3:I:75:ASN:OD1	3:I:76:SER:N	2.51	0.43
3:F:8:PRO:HG2	3:F:11:MET:HB3	2.00	0.43
3:L:12:SER:HA	3:L:104:GLU:O	2.19	0.43
1:B:307:ASN:ND2	1:B:309:ASN:HD22	2.16	0.43
3:K:89:GLN:HG2	3:K:90:TRP:N	2.33	0.43
3:L:89:GLN:HG2	3:L:90:TRP:N	2.33	0.43
1:A:320:PRO:HD2	1:A:360:PRO:HB2	2.01	0.43
1:B:466:ALA:HA	1:B:467:PRO:HD3	1.92	0.43
1:D:279:SER:OG	1:D:281:VAL:HG22	2.19	0.43
1:B:481:ASP:OD1	1:B:512:ASN:ND2	2.48	0.42
1:A:230:PRO:HD3	1:A:460:TYR:CD2	2.54	0.42
1:D:340:THR:O	2:G:103:ASN:HB2	2.20	0.42
2:J:191:TRP:CD2	2:J:192:PRO:HB3	2.54	0.42
1:C:476:ARG:NH1	1:C:488:GLU:OE1	2.53	0.42
1:D:469:GLN:HB2	1:D:520:TRP:CD1	2.54	0.42
2:G:141:LEU:HD11	2:G:191:TRP:CG	2.55	0.42
3:L:188:HIS:O	3:L:210:ARG:NH2	2.52	0.42
3:F:106:LYS:HA	3:F:139:TYR:OH	2.19	0.42
2:H:191:TRP:CG	2:H:192:PRO:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:202:SER:HA	3:K:203:PRO:HD3	1.91	0.42
3:F:57:VAL:HA	3:F:58:PRO:HD3	1.87	0.42
1:B:292:HIS:HB2	1:B:299:TYR:CE1	2.55	0.42
1:D:225:LYS:HA	1:D:226:PRO:HD3	1.83	0.42
3:K:11:MET:CE	3:K:21:MET:HB3	2.49	0.41
1:B:312:ASP:HA	1:B:313:PRO:HD3	1.90	0.41
3:K:57:VAL:HA	3:K:58:PRO:HD3	1.87	0.41
3:K:34:TRP:HB2	3:K:47:ILE:HB	2.02	0.41
2:E:122:PRO:HB3	2:E:148:TYR:HB3	2.03	0.41
2:E:200:VAL:HB	2:E:209:VAL:CG2	2.51	0.41
2:G:148:TYR:CE1	2:G:153:VAL:HG13	2.56	0.41
3:I:181:THR:OG1	3:I:184:GLU:HG3	2.20	0.41
3:I:107:ARG:HG2	3:I:108:ALA:N	2.36	0.41
3:I:57:VAL:HA	3:I:58:PRO:HD3	1.94	0.41
3:F:111:ALA:HA	3:F:112:PRO:HD3	1.95	0.41
3:K:182:LYS:HA	3:K:185:TYR:HB3	2.02	0.41
3:L:202:SER:HA	3:L:203:PRO:HD3	1.91	0.41
1:C:466:ALA:HA	1:C:467:PRO:HD3	1.92	0.40
3:I:118:PRO:HB3	3:I:208:PHE:CE1	2.55	0.40
3:L:186:GLU:HA	3:L:210:ARG:HH12	1.85	0.40
1:B:287:ARG:HD2	1:B:306:GLN:HA	2.03	0.40
3:L:29:VAL:HG11	3:L:89:GLN:HG3	2.03	0.40
3:I:183:ASP:O	3:I:187:ARG:HG3	2.22	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	A	305/310 (98%)	294 (96%)	11 (4%)	0	100 100
1	B	304/310 (98%)	293 (96%)	11 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	308/310 (99%)	296 (96%)	12 (4%)	0	100	100
1	D	307/310 (99%)	296 (96%)	11 (4%)	0	100	100
2	E	187/216 (87%)	182 (97%)	4 (2%)	1 (0%)	29	58
2	G	207/216 (96%)	202 (98%)	5 (2%)	0	100	100
2	H	206/216 (95%)	202 (98%)	4 (2%)	0	100	100
2	J	201/216 (93%)	199 (99%)	2 (1%)	0	100	100
3	F	207/214 (97%)	199 (96%)	8 (4%)	0	100	100
3	I	209/214 (98%)	201 (96%)	8 (4%)	0	100	100
3	K	199/214 (93%)	191 (96%)	5 (2%)	3 (2%)	10	30
3	L	208/214 (97%)	201 (97%)	7 (3%)	0	100	100
All	All	2848/2960 (96%)	2756 (97%)	88 (3%)	4 (0%)	51	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	150	ASP
2	E	65	LYS
3	K	127	GLY
3	K	126	SER

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/268 (97%)	260 (100%)	1 (0%)	91	96
1	B	264/268 (98%)	262 (99%)	2 (1%)	81	93
1	C	262/268 (98%)	262 (100%)	0	100	100
1	D	264/268 (98%)	264 (100%)	0	100	100
2	E	129/184 (70%)	128 (99%)	1 (1%)	81	93
2	G	172/184 (94%)	170 (99%)	2 (1%)	71	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	172/184 (94%)	171 (99%)	1 (1%)	86	95
2	J	148/184 (80%)	148 (100%)	0	100	100
3	F	153/188 (81%)	152 (99%)	1 (1%)	84	94
3	I	175/188 (93%)	174 (99%)	1 (1%)	86	95
3	K	159/188 (85%)	159 (100%)	0	100	100
3	L	166/188 (88%)	166 (100%)	0	100	100
All	All	2325/2560 (91%)	2316 (100%)	9 (0%)	91	96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	GLN
1	B	316	GLU
1	B	494	SER
2	E	119	THR
3	F	76	SER
2	G	137	SER
2	G	193	SER
2	H	143	CYS
3	I	125	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	B	309	ASN
3	K	89	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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
4	EDO	B	601	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	L	301	-	3,3,3	0.49	0	2,2,2	0.26	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	EDO	B	601	-	-	0/1/1/1	-
4	EDO	L	301	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	307/310 (99%)	-0.11	0 <span style="border: 1px solid blue; padding: 1px;">100</span> <span style="border: 1px solid blue; padding: 1px;">100</span>	30, 45, 63, 80	0
1	B	306/310 (98%)	-0.15	1 (0%) <span style="border: 1px solid blue; padding: 1px;">94</span> <span style="border: 1px solid blue; padding: 1px;">94</span>	33, 49, 78, 100	0
1	C	310/310 (100%)	-0.17	1 (0%) <span style="border: 1px solid blue; padding: 1px;">94</span> <span style="border: 1px solid blue; padding: 1px;">94</span>	30, 49, 77, 101	0
1	D	309/310 (99%)	-0.11	0 <span style="border: 1px solid blue; padding: 1px;">100</span> <span style="border: 1px solid blue; padding: 1px;">100</span>	30, 41, 65, 101	0
2	E	195/216 (90%)	0.41	10 (5%) <span style="border: 1px solid red; padding: 1px;">28</span> <span style="border: 1px solid red; padding: 1px;">22</span>	50, 86, 117, 134	0
2	G	211/216 (97%)	-0.08	1 (0%) <span style="border: 1px solid blue; padding: 1px;">91</span> <span style="border: 1px solid blue; padding: 1px;">90</span>	31, 51, 74, 87	0
2	H	210/216 (97%)	0.16	5 (2%) <span style="border: 1px solid gray; padding: 1px;">59</span> <span style="border: 1px solid gray; padding: 1px;">54</span>	30, 50, 85, 105	0
2	J	207/216 (95%)	0.39	16 (7%) <span style="border: 1px solid red; padding: 1px;">13</span> <span style="border: 1px solid red; padding: 1px;">9</span>	40, 71, 117, 147	0
3	F	209/214 (97%)	0.66	16 (7%) <span style="border: 1px solid red; padding: 1px;">13</span> <span style="border: 1px solid red; padding: 1px;">9</span>	49, 84, 115, 124	0
3	I	211/214 (98%)	0.17	1 (0%) <span style="border: 1px solid blue; padding: 1px;">91</span> <span style="border: 1px solid blue; padding: 1px;">90</span>	41, 67, 89, 118	0
3	K	205/214 (95%)	0.24	12 (5%) <span style="border: 1px solid red; padding: 1px;">22</span> <span style="border: 1px solid red; padding: 1px;">17</span>	37, 61, 116, 138	0
3	L	210/214 (98%)	0.04	8 (3%) <span style="border: 1px solid red; padding: 1px;">40</span> <span style="border: 1px solid red; padding: 1px;">35</span>	30, 56, 99, 124	0
All	All	2890/2960 (97%)	0.08	71 (2%) <span style="border: 1px solid gray; padding: 1px;">57</span> <span style="border: 1px solid gray; padding: 1px;">52</span>	30, 55, 104, 147	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	139	VAL	4.5
2	J	209	VAL	4.0
3	K	205	VAL	3.8
3	K	147	TRP	3.8
3	F	196	THR	3.7
3	F	199	THR	3.6
3	F	185	TYR	3.6
3	F	116	ILE	3.3
2	J	198	CYS	3.2
3	L	128	GLY	3.2
2	J	207	THR	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	F	204	ILE	3.1
3	K	0	GLY	3.0
3	F	205	VAL	2.9
2	H	127	LEU	2.9
2	J	125	TYR	2.9
2	J	201	ALA	2.9
2	E	127	LEU	2.8
2	H	126	PRO	2.8
3	F	202	SER	2.8
3	K	193	CYS	2.8
2	J	162	LEU	2.7
3	F	201	THR	2.7
3	F	128	GLY	2.7
1	B	412	ASN	2.7
3	K	118	PRO	2.6
2	H	181	SER	2.6
2	J	155	VAL	2.6
2	E	115	SER	2.6
3	F	197	HIS	2.5
2	J	144	LEU	2.5
2	J	193	SER	2.5
2	J	200	VAL	2.5
3	K	142	ASP	2.4
3	F	102	LYS	2.4
2	H	153	VAL	2.4
2	E	128	ALA	2.4
3	K	196	THR	2.4
3	K	208	PHE	2.4
3	L	208	PHE	2.4
2	H	144	LEU	2.3
1	C	221	GLY	2.3
3	L	127	GLY	2.3
3	K	134	PHE	2.3
2	G	162	LEU	2.3
3	L	159	LEU	2.3
3	F	155	GLN	2.3
2	E	141	LEU	2.3
3	L	129	ALA	2.3
3	K	114	VAL	2.3
2	J	161	SER	2.3
2	E	186	VAL	2.3
3	K	149	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	152	SER	2.2
3	I	0	GLY	2.2
3	L	143	ILE	2.2
3	L	124	LEU	2.2
2	E	83	LEU	2.2
2	E	196	VAL	2.2
2	E	138	MET	2.1
2	J	163	SER	2.1
2	J	160	GLY	2.1
2	J	203	PRO	2.1
3	F	151	GLY	2.1
3	F	75	ASN	2.1
2	E	209	VAL	2.1
2	J	154	THR	2.1
3	K	204	ILE	2.1
3	F	180	LEU	2.0
2	J	128	ALA	2.0
3	L	201	THR	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	EDO	L	301	4/4	0.89	0.24	60,61,61,61	0
4	EDO	B	601	4/4	0.92	0.28	68,69,69,70	0

## 6.5 Other polymers

There are no such residues in this entry.