



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:22 AM GMT

PDB ID : 3G3A  
Title : Structure of a lamprey variable lymphocyte receptor in complex with a protein antigen  
Authors : Deng, L.; Velikovsky, C.A.; Mariuzza, R.A.  
Deposited on : 2009-02-02  
Resolution : 2.20 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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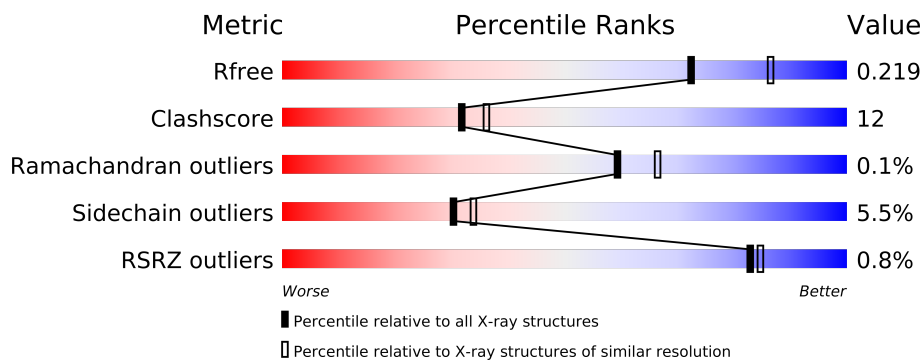
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	178	
1	C	178	
1	E	178	
1	G	178	
2	B	129	
2	D	129	
2	F	129	
2	H	129	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9537 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Variable lymphocyte receptor VLRB.2D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	0	0
			1274	797	217	252	8			
1	C	167	Total	C	N	O	S	0	0	0
			1274	797	217	252	8			
1	E	167	Total	C	N	O	S	0	0	0
			1274	797	217	252	8			
1	G	165	Total	C	N	O	S	0	0	0
			1259	789	214	248	8			

- Molecule 2 is a protein called Lysozyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			973	597	186	180	10			
2	D	126	Total	C	N	O	S	0	0	0
			973	597	186	180	10			
2	F	126	Total	C	N	O	S	0	0	0
			971	596	186	179	10			
2	H	124	Total	C	N	O	S	0	0	0
			961	591	184	176	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	93	Total	O	0	0
			93	93		
3	B	78	Total	O	0	0
			78	78		
3	C	81	Total	O	0	0
			81	81		
3	D	71	Total	O	0	0
			71	71		

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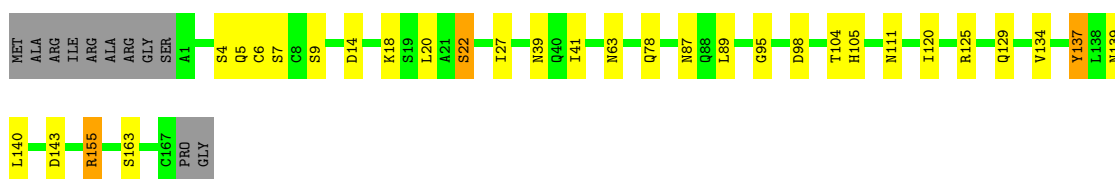
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	62	Total 62	O 62	0	0
3	F	59	Total 59	O 59	0	0
3	G	67	Total 67	O 67	0	0
3	H	67	Total 67	O 67	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

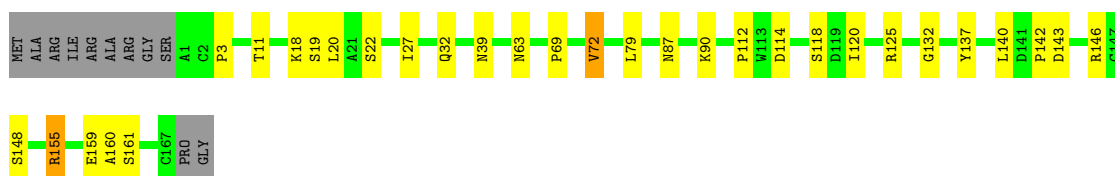
- Molecule 1: Variable lymphocyte receptor VLRB.2D

Chain A:



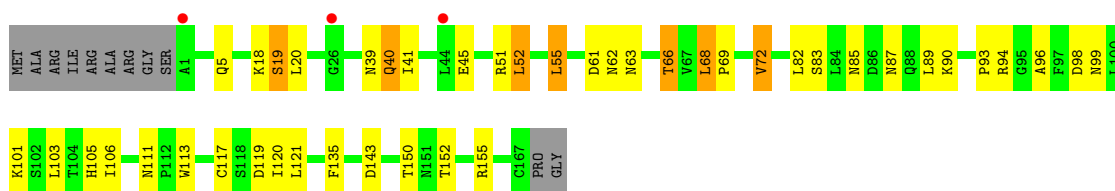
- Molecule 1: Variable lymphocyte receptor VLRB.2D

Chain C:



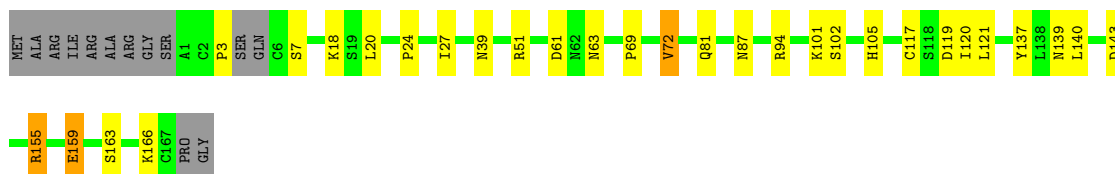
- Molecule 1: Variable lymphocyte receptor VLRB.2D

Chain E:



- Molecule 1: Variable lymphocyte receptor VLRB.2D

Chain G:



- Molecule 2: Lysozyme C

Chain B: 



• Molecule 2: Lysozyme C

Chain D: 



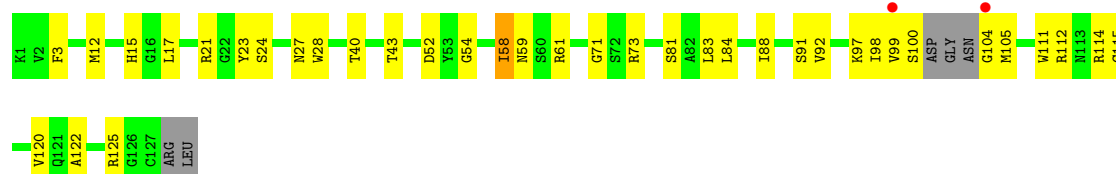
• Molecule 2: Lysozyme C

Chain F: 



• Molecule 2: Lysozyme C

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.30Å 133.65Å 90.44Å 90.00° 114.69° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 30.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-2.20) 98.5 (30.95-2.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.220 , 0.271 0.225 , 0.219	Depositor DCC
$R_{free}$ test set	4437 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 27.6	EDS
Estimated twinning fraction	0.094 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 88602 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9537	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.87	0/1300	0.85	1/1779 (0.1%)
1	C	0.83	0/1300	0.87	0/1779
1	E	0.83	0/1300	0.88	1/1779 (0.1%)
1	G	0.79	0/1284	0.83	0/1756
2	B	1.00	0/992	0.89	1/1340 (0.1%)
2	D	0.95	0/992	0.86	2/1340 (0.1%)
2	F	0.91	0/990	0.87	0/1337
2	H	0.95	0/980	0.87	1/1324 (0.1%)
All	All	0.89	0/9138	0.86	6/12434 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ASP	CB-CG-OD1	5.76	123.48	118.30
2	B	45	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	55	LEU	CA-CB-CG	5.66	128.33	115.30
2	D	45	ARG	NE-CZ-NH1	5.47	123.03	120.30
2	H	114	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	D	52	ASP	CB-CG-OD1	5.34	123.11	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1274	0	1259	26	0
1	C	1274	0	1257	25	0
1	E	1274	0	1257	34	0
1	G	1259	0	1243	18	0
2	B	973	0	930	26	0
2	D	973	0	930	24	0
2	F	971	0	926	25	0
2	H	961	0	921	31	0
3	A	93	0	0	5	0
3	B	78	0	0	6	0
3	C	81	0	0	5	0
3	D	71	0	0	6	0
3	E	62	0	0	8	0
3	F	59	0	0	4	0
3	G	67	0	0	1	0
3	H	67	0	0	2	0
All	All	9537	0	8723	203	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (203) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:51:ARG:HG2	3:G:401:HOH:O	1.51	1.10
2:F:27:ASN:HB3	2:F:105:MET:HE1	1.34	1.09
2:H:27:ASN:HB3	2:H:105:MET:HE1	1.45	0.97
2:F:27:ASN:HB3	2:F:105:MET:CE	1.96	0.95
1:G:69:PRO:HG2	1:G:72:VAL:HG13	1.51	0.91
2:D:59:ASN:OD1	2:D:61:ARG:HB3	1.71	0.90
1:A:39:ASN:HB2	1:A:63:ASN:HD21	1.35	0.90
1:E:51:ARG:HG2	3:E:182:HOH:O	1.74	0.87
1:G:143:ASP:OD1	1:G:155:ARG:HD3	1.77	0.84
1:E:41:ILE:H	1:E:63:ASN:HD22	1.26	0.81
2:B:21:ARG:CZ	2:B:100:SER:HA	2.10	0.80
2:H:27:ASN:HB3	2:H:105:MET:CE	2.14	0.78
1:E:143:ASP:OD1	1:E:155:ARG:HD3	1.85	0.77
2:B:28:TRP:HH2	2:B:99:VAL:HG21	1.50	0.77
1:A:22:SER:HB3	3:A:372:HOH:O	1.84	0.76
1:C:3:PRO:HG2	1:C:27:ILE:HD13	1.67	0.76
2:D:5:ARG:HD2	2:D:123:TRP:O	1.87	0.75
2:F:111:TRP:CD1	2:F:115:CYS:HB2	2.24	0.73
2:B:61:ARG:HD3	3:B:133:HOH:O	1.88	0.73
1:A:27:ILE:HG12	3:A:417:HOH:O	1.88	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:41:ILE:H	1:A:63:ASN:HD22	1.36	0.71
2:H:23:TYR:CD1	2:H:105:MET:HE3	2.25	0.71
1:E:39:ASN:HB2	1:E:63:ASN:HD21	1.57	0.70
2:B:59:ASN:OD1	2:B:61:ARG:HB3	1.92	0.70
1:C:18:LYS:H	1:C:39:ASN:HD21	1.40	0.70
2:H:59:ASN:OD1	2:H:61:ARG:HB3	1.92	0.69
1:C:125:ARG:NH1	3:C:526:HOH:O	2.25	0.69
1:A:78:GLN:NE2	3:A:378:HOH:O	2.25	0.69
1:A:125:ARG:HE	1:A:129:GLN:HE22	1.41	0.68
2:F:102:GLY:HA3	3:F:341:HOH:O	1.93	0.68
2:H:27:ASN:HD22	2:H:111:TRP:HE1	1.40	0.67
2:B:28:TRP:CH2	2:B:99:VAL:HG21	2.28	0.67
1:G:63:ASN:HB2	1:G:87:ASN:HD21	1.59	0.67
1:A:63:ASN:HB2	1:A:87:ASN:HD21	1.60	0.67
1:E:20:LEU:H	1:E:39:ASN:ND2	1.94	0.66
2:F:88:ILE:HG23	2:F:92:VAL:HG23	1.77	0.65
2:F:88:ILE:HG23	2:F:92:VAL:CG2	2.26	0.65
2:D:28:TRP:HH2	2:D:99:VAL:HG21	1.61	0.65
2:H:28:TRP:CH2	2:H:99:VAL:HG21	2.32	0.64
1:E:41:ILE:H	1:E:63:ASN:ND2	1.93	0.64
2:D:28:TRP:CH2	2:D:99:VAL:HG21	2.33	0.64
2:B:14:ARG:HD2	3:B:149:HOH:O	1.97	0.64
1:C:3:PRO:CG	1:C:27:ILE:HD13	2.28	0.64
1:A:87:ASN:HB2	1:A:111:ASN:HD21	1.63	0.64
1:E:68:LEU:HD13	1:E:89:LEU:HD21	1.78	0.64
2:B:21:ARG:HD2	2:B:99:VAL:HG12	1.78	0.63
1:A:139:ASN:HB2	3:A:182:HOH:O	1.97	0.63
2:D:125:ARG:O	2:D:125:ARG:HG3	1.99	0.63
1:A:89:LEU:H	1:A:111:ASN:HD22	1.45	0.62
3:A:394:HOH:O	2:B:71:GLY:HA2	2.00	0.61
1:C:63:ASN:HB2	1:C:87:ASN:HD21	1.65	0.61
2:B:61:ARG:NE	3:B:505:HOH:O	2.27	0.61
2:B:78:ILE:HD12	2:B:83:LEU:HD13	1.81	0.61
1:E:87:ASN:HB2	1:E:111:ASN:HD21	1.63	0.61
2:B:78:ILE:HD12	2:B:83:LEU:CD1	2.31	0.61
1:G:69:PRO:O	1:G:72:VAL:HG22	2.01	0.61
2:B:125:ARG:O	2:B:125:ARG:HG3	2.02	0.60
2:H:71:GLY:O	2:H:73:ARG:NH1	2.35	0.60
1:E:117:CYS:SG	1:E:119:ASP:HB2	2.42	0.59
2:H:23:TYR:CD1	2:H:105:MET:CE	2.85	0.59
1:E:66:THR:CG2	3:E:410:HOH:O	2.51	0.59
1:G:18:LYS:H	1:G:39:ASN:HD21	1.50	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:122:ALA:O	2:D:125:ARG:HG2	2.02	0.58
2:B:21:ARG:HG2	3:B:191:HOH:O	2.04	0.58
2:H:12:MET:HG2	2:H:17:LEU:HD12	1.85	0.58
1:A:20:LEU:H	1:A:39:ASN:ND2	2.01	0.57
2:B:78:ILE:HG21	3:B:255:HOH:O	2.05	0.56
2:H:88:ILE:HG22	2:H:92:VAL:HG23	1.86	0.56
1:C:69:PRO:HG2	1:C:72:VAL:HG13	1.87	0.56
1:E:66:THR:HG23	3:E:410:HOH:O	2.05	0.56
1:A:143:ASP:OD1	1:A:155:ARG:HD3	2.06	0.56
2:B:43:THR:HG21	3:D:141:HOH:O	2.04	0.56
1:G:20:LEU:H	1:G:39:ASN:ND2	2.04	0.56
1:A:39:ASN:HB2	1:A:63:ASN:ND2	2.14	0.56
2:F:27:ASN:CB	2:F:105:MET:CE	2.78	0.55
2:H:111:TRP:CD1	2:H:115:CYS:HB2	2.40	0.55
1:E:52:LEU:HB3	1:E:55:LEU:HD22	1.88	0.55
1:A:6:CYS:HA	1:A:18:LYS:HE3	1.88	0.55
1:E:61:ASP:OD2	1:E:62:ASN:OD1	2.24	0.55
1:G:20:LEU:HD13	1:G:24:PRO:HG3	1.89	0.54
2:D:83:LEU:HD22	2:D:91:SER:HA	1.89	0.54
1:E:68:LEU:HD13	1:E:89:LEU:CD2	2.38	0.54
1:A:20:LEU:H	1:A:39:ASN:HD22	1.55	0.54
2:H:28:TRP:HH2	2:H:99:VAL:HG21	1.71	0.53
2:F:32:ALA:HB1	2:F:55:ILE:HG23	1.89	0.53
2:D:121:GLN:NE2	3:D:145:HOH:O	2.39	0.53
1:A:39:ASN:CB	1:A:63:ASN:HD21	2.16	0.52
1:A:125:ARG:HE	1:A:129:GLN:NE2	2.05	0.52
2:F:15:HIS:HB3	2:F:92:VAL:HG11	1.91	0.52
1:E:150:THR:HB	1:E:152:THR:HG23	1.91	0.52
1:E:82:LEU:HD23	1:E:106:ILE:CD1	2.40	0.51
1:C:18:LYS:H	1:C:39:ASN:ND2	2.06	0.51
2:H:40:THR:O	2:H:54:GLY:HA2	2.10	0.51
2:H:112:ARG:HD2	3:H:215:HOH:O	2.09	0.51
2:F:6:CYS:HG	2:F:127:CYS:HG	0.62	0.51
2:B:122:ALA:O	2:B:125:ARG:HG2	2.11	0.51
1:G:18:LYS:H	1:G:39:ASN:ND2	2.09	0.51
1:E:101:LYS:HD2	3:E:265:HOH:O	2.09	0.51
1:C:3:PRO:HG2	1:C:27:ILE:CD1	2.36	0.51
1:E:82:LEU:HD23	1:E:106:ILE:HD12	1.93	0.51
1:E:18:LYS:H	1:E:39:ASN:HD21	1.58	0.50
2:H:58:ILE:HD13	2:H:98:ILE:CD1	2.41	0.50
2:D:111:TRP:CD1	2:D:115:CYS:HB2	2.46	0.50
1:E:61:ASP:HB2	1:E:85:ASN:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:69:PRO:HG2	1:G:72:VAL:CG1	2.34	0.50
1:E:39:ASN:CB	1:E:63:ASN:HD21	2.23	0.49
1:A:95:GLY:HA2	1:A:98:ASP:OD2	2.13	0.49
1:A:104:THR:OG1	1:A:105:HIS:HD2	1.96	0.49
1:G:121:LEU:HD21	1:G:159:GLU:HA	1.94	0.49
2:F:57:GLN:O	3:F:552:HOH:O	2.20	0.49
2:F:40:THR:O	2:F:54:GLY:HA2	2.13	0.49
1:C:143:ASP:OD1	1:C:155:ARG:HD3	2.13	0.48
2:B:81:SER:HB2	2:D:81:SER:O	2.13	0.48
1:A:134:VAL:O	1:A:140:LEU:HD12	2.13	0.48
1:E:143:ASP:OD1	1:E:155:ARG:CD	2.57	0.48
2:D:119:ASP:HB3	3:E:192:HOH:O	2.13	0.48
1:G:81:GLN:HG2	1:G:105:HIS:HB2	1.96	0.47
1:C:90:LYS:HD2	1:C:114:ASP:HB2	1.97	0.47
2:B:15:HIS:HB3	2:B:92:VAL:HG11	1.95	0.47
2:D:15:HIS:HB3	2:D:92:VAL:HG11	1.97	0.47
2:H:43:THR:HA	2:H:52:ASP:O	2.15	0.47
1:A:5:GLN:O	1:A:18:LYS:HD3	2.15	0.46
2:D:60:SER:O	3:D:130:HOH:O	2.21	0.46
1:G:117:CYS:SG	1:G:119:ASP:HB2	2.55	0.46
2:H:58:ILE:HB	2:H:83:LEU:HD13	1.98	0.46
2:F:1:LYS:HE2	2:F:3:PHE:CZ	2.51	0.46
2:F:44:ASN:ND2	3:F:295:HOH:O	2.47	0.46
1:G:61:ASP:OD1	2:H:73:ARG:NH2	2.49	0.46
1:E:19:SER:O	1:E:40:GLN:HG3	2.14	0.46
2:D:109:VAL:HG11	2:F:114:ARG:CZ	2.46	0.46
2:H:58:ILE:HD13	2:H:98:ILE:HD12	1.98	0.46
1:C:142:PRO:HD2	3:C:204:HOH:O	2.15	0.45
1:A:105:HIS:CE1	2:B:48:ASP:HB3	2.51	0.45
2:B:111:TRP:CD1	2:B:115:CYS:HB2	2.52	0.45
1:C:159:GLU:O	1:C:161:SER:N	2.50	0.45
1:E:90:LYS:HE2	3:E:540:HOH:O	2.17	0.45
1:C:132:GLY:HA2	1:C:140:LEU:HD21	1.99	0.45
2:D:62:TRP:HB2	2:D:63:TRP:CD1	2.52	0.45
1:A:41:ILE:H	1:A:63:ASN:ND2	2.09	0.45
2:D:3:PHE:CD1	2:D:7:GLU:HG2	2.52	0.45
2:B:21:ARG:NH2	2:B:100:SER:HA	2.32	0.44
2:D:3:PHE:HD1	2:D:7:GLU:HG2	1.82	0.44
2:H:27:ASN:ND2	2:H:111:TRP:HE1	2.13	0.44
2:H:88:ILE:HG22	2:H:88:ILE:O	2.17	0.44
1:C:112:PRO:HA	1:C:148:SER:HB3	2.00	0.44
1:E:113:TRP:HB3	1:E:120:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:90:LYS:HE2	3:C:195:HOH:O	2.18	0.44
2:H:122:ALA:HA	2:H:125:ARG:HG3	1.99	0.44
2:F:60:SER:O	3:F:130:HOH:O	2.21	0.44
1:A:125:ARG:NE	1:A:129:GLN:HE22	2.10	0.44
2:F:27:ASN:CB	2:F:105:MET:HE2	2.45	0.43
1:C:20:LEU:H	1:C:39:ASN:ND2	2.16	0.43
1:E:20:LEU:H	1:E:39:ASN:HD22	1.62	0.43
1:E:52:LEU:O	1:E:55:LEU:HB2	2.17	0.43
2:B:21:ARG:NH1	3:B:146:HOH:O	2.40	0.43
1:G:3:PRO:HG2	1:G:27:ILE:HD13	2.00	0.43
2:H:27:ASN:CB	2:H:105:MET:CE	2.93	0.43
1:E:105:HIS:CD2	1:E:135:PHE:CE2	3.07	0.43
1:C:18:LYS:HB2	1:C:20:LEU:HG	2.01	0.43
1:E:93:PRO:HG2	1:E:96:ALA:HB2	1.99	0.43
2:H:27:ASN:ND2	2:H:120:VAL:HG11	2.34	0.43
1:E:63:ASN:HB2	1:E:87:ASN:HD21	1.84	0.42
2:H:3:PHE:CE1	2:H:88:ILE:HD11	2.54	0.42
1:E:99:ASN:HB2	3:E:181:HOH:O	2.19	0.42
2:D:61:ARG:HD3	3:D:149:HOH:O	2.19	0.42
2:H:59:ASN:OD1	2:H:61:ARG:CB	2.65	0.42
1:C:155:ARG:O	3:C:524:HOH:O	2.22	0.42
1:A:137:TYR:HA	1:A:137:TYR:HD1	1.76	0.42
1:E:63:ASN:H	1:E:87:ASN:HD21	1.67	0.42
2:D:15:HIS:CE1	2:D:89:THR:OG1	2.72	0.42
2:H:61:ARG:HD3	3:H:143:HOH:O	2.20	0.42
2:D:3:PHE:HB3	2:D:8:LEU:HB2	2.01	0.42
2:F:111:TRP:CD1	2:F:115:CYS:CB	2.98	0.42
1:G:18:LYS:HA	1:G:18:LYS:HD3	1.87	0.42
2:F:97:LYS:NZ	2:F:101:ASP:OD2	2.52	0.42
1:C:143:ASP:O	1:C:146:ARG:NE	2.53	0.42
2:B:81:SER:O	2:D:81:SER:HB2	2.20	0.42
2:F:52:ASP:OD1	2:F:59:ASN:HB2	2.20	0.42
1:C:79:LEU:HD23	1:C:79:LEU:C	2.40	0.42
2:F:23:TYR:CD1	2:F:105:MET:CE	3.03	0.41
2:H:15:HIS:HB3	2:H:92:VAL:HG11	2.01	0.41
1:C:11:THR:OG1	1:C:32:GLN:OE1	2.38	0.41
1:A:120:ILE:O	1:A:120:ILE:HG13	2.21	0.41
2:B:60:SER:O	2:B:72:SER:HB2	2.20	0.41
2:D:24:SER:HB3	3:D:135:HOH:O	2.20	0.41
1:E:98:ASP:OD1	3:E:321:HOH:O	2.22	0.41
2:F:81:SER:O	2:H:81:SER:HB2	2.20	0.41
2:F:11:ALA:O	2:F:15:HIS:HD2	2.04	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:20:LEU:H	1:G:39:ASN:HD22	1.67	0.41
2:B:9:ALA:HB1	2:B:124:ILE:CD1	2.50	0.41
2:H:21:ARG:CZ	2:H:100:SER:HB2	2.51	0.41
1:C:120:ILE:HG13	1:C:120:ILE:O	2.21	0.41
2:D:54:GLY:HA3	3:D:140:HOH:O	2.21	0.41
1:E:69:PRO:O	1:E:72:VAL:HG22	2.20	0.41
1:C:22:SER:HB2	3:C:181:HOH:O	2.21	0.41
1:C:63:ASN:CB	1:C:87:ASN:HD21	2.30	0.41
2:D:58:ILE:HD12	2:D:98:ILE:CD1	2.50	0.41
2:F:88:ILE:HG23	2:F:92:VAL:HG21	1.99	0.40
1:C:63:ASN:C	1:C:87:ASN:ND2	2.75	0.40
2:B:78:ILE:CD1	2:B:83:LEU:HD11	2.51	0.40
2:F:55:ILE:HD12	2:F:88:ILE:HD11	2.03	0.40
1:G:163:SER:HB3	1:G:166:LYS:HG3	2.03	0.40
2:H:99:VAL:O	2:H:104:GLY:HA2	2.21	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	A	165/178 (93%)	152 (92%)	13 (8%)	0	100	100
1	C	165/178 (93%)	150 (91%)	14 (8%)	1 (1%)	33	32
1	E	165/178 (93%)	147 (89%)	18 (11%)	0	100	100
1	G	161/178 (90%)	151 (94%)	10 (6%)	0	100	100
2	B	122/129 (95%)	117 (96%)	5 (4%)	0	100	100
2	D	122/129 (95%)	119 (98%)	3 (2%)	0	100	100
2	F	122/129 (95%)	119 (98%)	3 (2%)	0	100	100
2	H	120/129 (93%)	114 (95%)	6 (5%)	0	100	100
All	All	1142/1228 (93%)	1069 (94%)	72 (6%)	1 (0%)	59	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	160	ALA

### 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	150/157 (96%)	143 (95%)	7 (5%)	36	42
1	C	150/157 (96%)	145 (97%)	5 (3%)	50	60
1	E	150/157 (96%)	138 (92%)	12 (8%)	17	16
1	G	148/157 (94%)	137 (93%)	11 (7%)	20	19
2	B	102/105 (97%)	97 (95%)	5 (5%)	35	40
2	D	102/105 (97%)	98 (96%)	4 (4%)	43	52
2	F	101/105 (96%)	95 (94%)	6 (6%)	28	30
2	H	101/105 (96%)	96 (95%)	5 (5%)	34	39
All	All	1004/1048 (96%)	949 (94%)	55 (6%)	30	34

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	7	SER
1	A	9	SER
1	A	22	SER
1	A	137	TYR
1	A	155	ARG
1	A	163	SER
2	B	14	ARG
2	B	37	ASN
2	B	58	ILE
2	B	83	LEU
2	B	114	ARG
1	C	19	SER
1	C	72	VAL
1	C	118	SER
1	C	137	TYR
1	C	155	ARG

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Mol	Chain	Res	Type
2	D	21	ARG
2	D	43	THR
2	D	75	LEU
2	D	91	SER
1	E	5	GLN
1	E	19	SER
1	E	40	GLN
1	E	45	GLU
1	E	52	LEU
1	E	66	THR
1	E	68	LEU
1	E	72	VAL
1	E	83	SER
1	E	94	ARG
1	E	103	LEU
1	E	121	LEU
2	F	55	ILE
2	F	59	ASN
2	F	79	PRO
2	F	88	ILE
2	F	114	ARG
2	F	125	ARG
1	G	7	SER
1	G	72	VAL
1	G	94	ARG
1	G	101	LYS
1	G	102	SER
1	G	120	ILE
1	G	137	TYR
1	G	139	ASN
1	G	140	LEU
1	G	155	ARG
1	G	159	GLU
2	H	24	SER
2	H	58	ILE
2	H	84	LEU
2	H	91	SER
2	H	97	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	39	ASN
1	A	54	GLN
1	A	63	ASN
1	A	78	GLN
1	A	87	ASN
1	A	105	HIS
1	A	111	ASN
1	A	129	GLN
2	B	15	HIS
2	B	57	GLN
2	B	106	ASN
2	B	113	ASN
1	C	39	ASN
1	C	54	GLN
1	C	87	ASN
1	C	99	ASN
1	C	110	ASN
2	D	15	HIS
2	D	93	ASN
2	D	106	ASN
2	D	113	ASN
1	E	39	ASN
1	E	54	GLN
1	E	62	ASN
1	E	63	ASN
1	E	78	GLN
1	E	87	ASN
1	E	111	ASN
2	F	15	HIS
2	F	44	ASN
2	F	46	ASN
1	G	39	ASN
1	G	62	ASN
1	G	87	ASN
2	H	15	HIS
2	H	19	ASN
2	H	27	ASN
2	H	46	ASN
2	H	93	ASN
2	H	113	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 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, 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	167/178 (93%)	-0.09	0 100 100	12, 24, 38, 52	0
1	C	167/178 (93%)	0.05	0 100 100	13, 27, 44, 54	0
1	E	167/178 (93%)	0.28	3 (1%) 65 66	18, 32, 49, 57	1 (0%)
1	G	165/178 (92%)	-0.10	0 100 100	14, 25, 37, 46	1 (0%)
2	B	126/129 (97%)	-0.04	2 (1%) 68 69	10, 20, 35, 43	4 (3%)
2	D	126/129 (97%)	0.01	2 (1%) 68 69	12, 23, 36, 42	3 (2%)
2	F	126/129 (97%)	0.02	0 100 100	14, 24, 40, 49	0
2	H	124/129 (96%)	-0.01	2 (1%) 68 69	13, 22, 34, 41	2 (1%)
All	All	1168/1228 (95%)	0.02	9 (0%) 83 85	10, 25, 40, 57	11 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	104	GLY	5.1
2	H	99	VAL	4.3
2	B	104	GLY	4.3
2	B	99	VAL	3.5
1	E	1	ALA	3.5
2	H	104	GLY	3.4
2	D	100	SER	3.3
1	E	44	LEU	2.4
1	E	26	GLY	2.4

### 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 carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.