



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:20 PM GMT

PDB ID : 4R96  
Title : Structure of a Llama Glama Fab 48A2 against human cMet  
Authors : Klarenbeek, A.; El Mazouari, K.; Desmyter, A.; Blanchetot, C.; Hultberg, A.; Roovers, R.C.; Cambillau, C.; Spinelli, S.; Del-Favero, J.; Verrips, T.; de Haard, H.; Achour, I.  
Deposited on : 2014-09-03  
Resolution : 3.31 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  
<http://wwpdb.org/validation/2016/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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

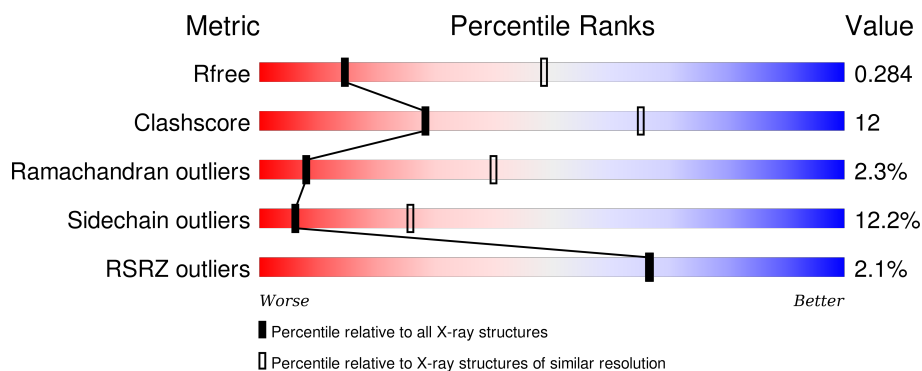
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.31 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))
$R_{free}$	91344	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)

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. 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	221	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>..</div> </div> </div>
1	C	221	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
1	E	221	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>.</div> </div> </div>
1	L	221	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>
2	B	219	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>26%</div> <div>6%</div> <div>..</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	219	<div><div></div><div>2%</div><div>61%</div><div>26%</div><div>8%</div><div></div><div></div></div>
2	F	219	<div><div></div><div>4%</div><div>70%</div><div>19%</div><div>6%</div><div></div><div></div></div>
2	H	219	<div><div></div><div>%</div><div>64%</div><div>27%</div><div>8%</div><div></div><div></div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13536 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 Llama glama Fab 48A2 against human cMet L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1703	1068	288	342	5			
1	C	219	Total	C	N	O	S	0	0	0
			1703	1068	288	342	5			
1	E	221	Total	C	N	O	S	0	0	0
			1714	1074	290	344	6			
1	L	221	Total	C	N	O	S	0	0	0
			1718	1076	290	346	6			

- Molecule 2 is a protein called Llama glama Fab 48A2 against human cMet H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1606	1015	263	322	6			
2	D	213	Total	C	N	O	S	0	0	0
			1612	1018	266	322	6			
2	F	213	Total	C	N	O	S	0	0	0
			1612	1018	266	322	6			
2	H	217	Total	C	N	O	S	0	0	0
			1634	1030	270	328	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	C	16	Total	O	0	0
			16	16		
3	E	28	Total	O	0	0
			28	28		
3	L	29	Total	O	0	0
			29	29		

*Continued on next page...*

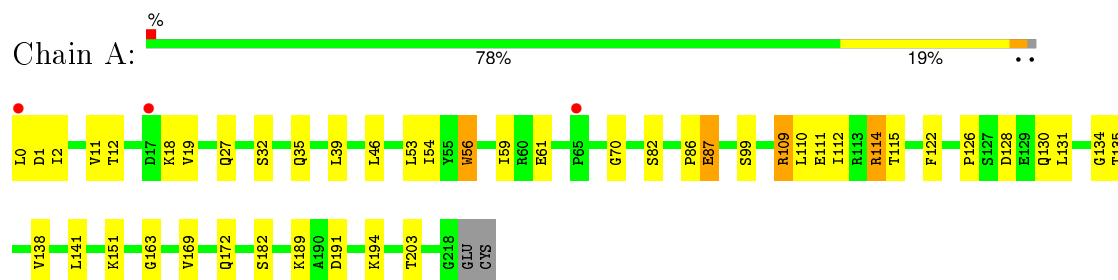
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	40	Total 40	O 40	0	0
3	D	25	Total 25	O 25	0	0
3	F	35	Total 35	O 35	0	0
3	H	22	Total 22	O 22	0	0

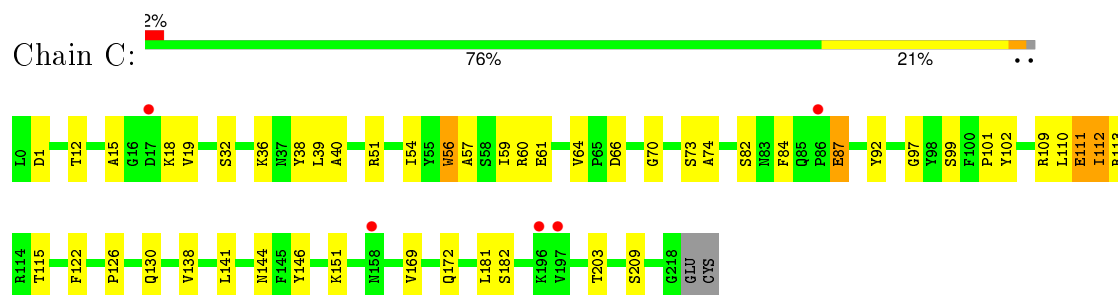
### 3 Residue-property plots [i](#)

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

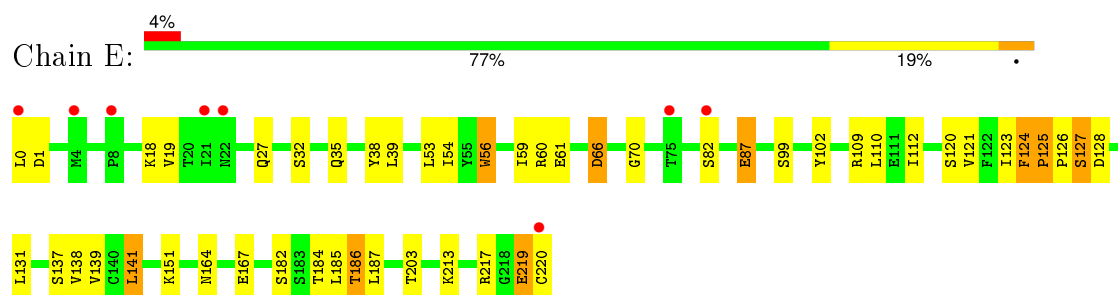
- Molecule 1: Llama glama Fab 48A2 against human cMet L chain



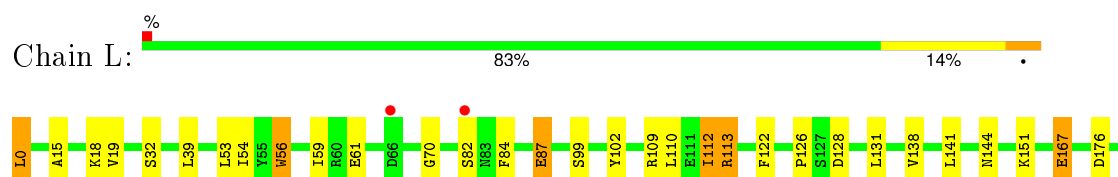
- Molecule 1: Llama glama Fab 48A2 against human cMet L chain



- Molecule 1: Llama glama Fab 48A2 against human cMet L chain

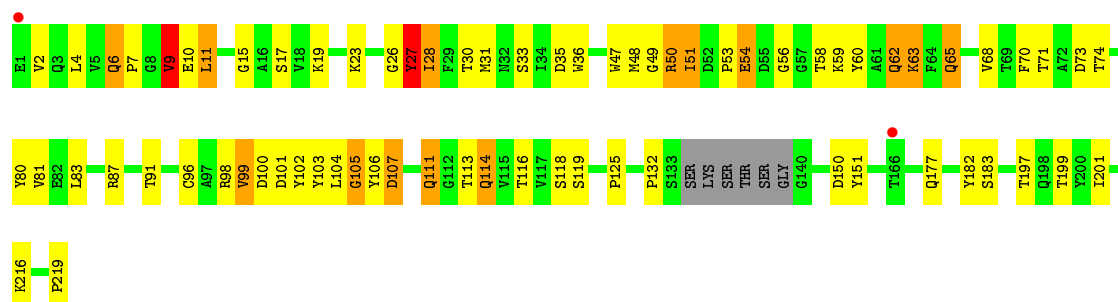


- Molecule 1: Llama glama Fab 48A2 against human cMet L chain

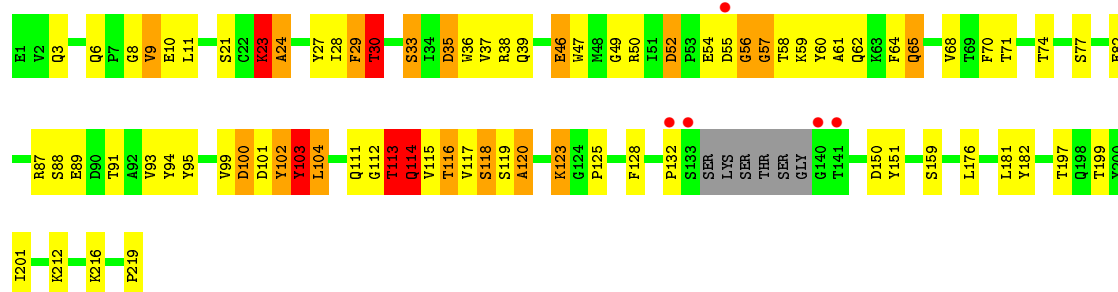




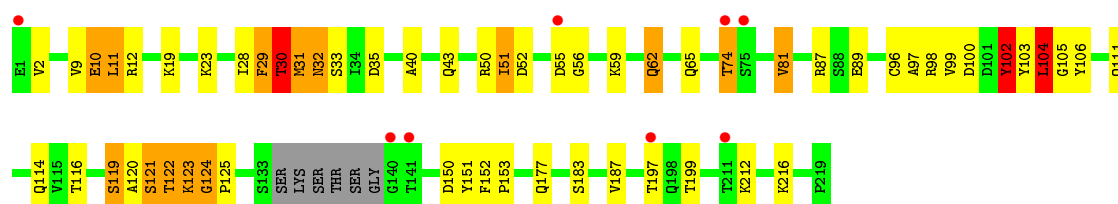
- Molecule 2: Llama glama Fab 48A2 against human cMet H chain



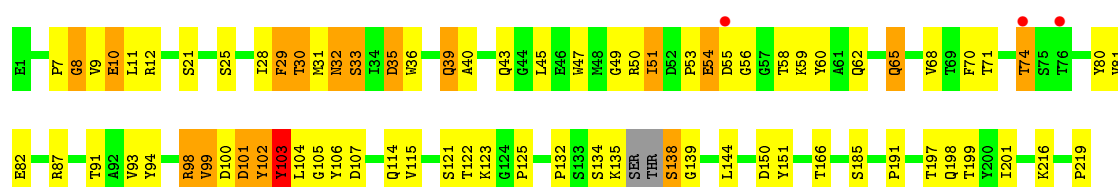
- Molecule 2: Llama glama Fab 48A2 against human cMet H chain



- Molecule 2: Llama glama Fab 48A2 against human cMet H chain



- Molecule 2: Llama glama Fab 48A2 against human cMet H chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.02Å 121.54Å 185.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.39 – 3.31 43.39 – 3.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.39-3.31) 97.6 (43.39-3.31)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, $R_{free}$	0.217 , 0.261 0.239 , 0.284	Depositor DCC
$R_{free}$ test set	3578 reflections (9.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.2	Xtriage
Anisotropy	0.891	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 64.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	3 of 35872 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	13536	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 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	0.46	0/1741	0.68	0/2365
1	C	0.45	0/1741	0.68	0/2365
1	E	0.54	1/1752 (0.1%)	0.74	2/2380 (0.1%)
1	L	0.44	0/1756	0.69	0/2385
2	B	0.57	0/1645	0.85	1/2247 (0.0%)
2	D	0.50	0/1651	0.89	2/2254 (0.1%)
2	F	0.51	0/1651	0.84	2/2254 (0.1%)
2	H	0.50	0/1673	0.82	3/2283 (0.1%)
All	All	0.50	1/13610 (0.0%)	0.77	10/18533 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	125	PRO	N-CD	5.81	1.55	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	30	THR	C-N-CA	7.14	139.55	121.70
2	D	23	LYS	C-N-CA	7.10	139.45	121.70
1	E	125	PRO	C-N-CD	6.26	141.56	128.40
2	F	124	GLY	C-N-CD	6.24	141.50	128.40
2	H	103	TYR	CA-CB-CG	6.16	125.10	113.40
2	B	105	GLY	C-N-CA	5.98	136.65	121.70
2	H	103	TYR	C-N-CA	5.73	136.02	121.70
1	E	124	PHE	C-N-CD	5.64	140.25	128.40
2	D	103	TYR	CA-CB-CG	5.58	124.00	113.40
2	H	134	SER	N-CA-C	-5.15	97.11	111.00

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	A	1703	0	1645	33	0
1	C	1703	0	1645	34	0
1	E	1714	0	1652	31	0
1	L	1718	0	1656	19	0
2	B	1606	0	1548	53	0
2	D	1612	0	1559	65	0
2	F	1612	0	1559	46	0
2	H	1634	0	1576	46	0
3	A	39	0	0	1	0
3	B	40	0	0	0	0
3	C	16	0	0	0	0
3	D	25	0	0	1	0
3	E	28	0	0	2	0
3	F	35	0	0	0	0
3	H	22	0	0	0	0
3	L	29	0	0	1	0
All	All	13536	0	12840	303	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 12.

All (303) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:THR:CB	2:F:31:MET:HB2	1.72	1.18
2:F:123:LYS:NZ	2:F:150:ASP:O	1.78	1.16
2:B:50:ARG:HG2	2:B:50:ARG:HH11	1.14	1.12
2:F:30:THR:HB	2:F:31:MET:CB	1.84	1.06
2:F:100:ASP:HB3	2:F:102:TYR:CE2	1.93	1.02
2:D:103:TYR:HB2	2:D:104:LEU:HA	1.42	1.00
1:C:15:ALA:O	2:B:15:GLY:HA3	1.63	0.98
2:B:9:VAL:CG2	2:B:114:GLN:HB3	1.96	0.95
1:C:12:THR:HG22	1:C:111:GLU:OE1	1.67	0.94
2:F:125:PRO:HB3	2:F:151:TYR:HB3	1.46	0.94
2:H:51:ILE:HD12	2:H:58:THR:HG22	1.49	0.94

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:VAL:HG11	1:L:110:LEU:HD21	1.51	0.93
2:F:100:ASP:HB3	2:F:102:TYR:HE2	1.33	0.92
1:E:137:SER:HA	1:E:185:LEU:O	1.68	0.92
1:C:12:THR:CG2	1:C:111:GLU:OE1	2.19	0.91
1:A:19:VAL:HG11	1:A:110:LEU:HD21	1.49	0.91
2:B:9:VAL:HG23	2:B:114:GLN:HB3	1.55	0.87
2:B:30:THR:HG22	2:B:31:MET:H	1.38	0.87
1:E:123:ILE:HG13	1:E:124:PHE:H	1.37	0.87
1:E:123:ILE:HG13	1:E:124:PHE:N	1.90	0.86
2:F:30:THR:HB	2:F:31:MET:HB2	0.87	0.85
1:A:12:THR:HG22	1:A:111:GLU:HB3	1.58	0.84
2:F:10:GLU:OE2	2:F:12:ARG:HG2	1.78	0.84
2:F:33:SER:HB2	2:F:99:VAL:HG13	1.60	0.84
2:F:123:LYS:NZ	2:F:150:ASP:C	2.31	0.82
2:D:117:VAL:HG12	2:D:120:ALA:CB	2.12	0.80
2:F:11:LEU:HD11	2:F:152:PHE:HZ	1.47	0.79
2:B:70:PHE:HD1	2:B:81:VAL:HG22	1.47	0.79
2:D:125:PRO:HB3	2:D:151:TYR:HB3	1.65	0.79
1:A:130:GLN:NE2	1:A:135:THR:HG22	1.98	0.78
2:D:8:GLY:CA	2:D:113:THR:HG23	2.14	0.78
2:F:11:LEU:HD11	2:F:152:PHE:CZ	2.20	0.77
1:E:141:LEU:HD13	2:F:187:VAL:HG21	1.66	0.77
2:D:100:ASP:O	2:D:104:LEU:HB3	1.84	0.77
2:H:102:TYR:O	2:H:104:LEU:HA	1.87	0.74
2:F:33:SER:HB2	2:F:99:VAL:CG1	2.19	0.73
2:D:33:SER:O	2:D:99:VAL:HG12	1.88	0.73
2:B:70:PHE:CD1	2:B:81:VAL:HG22	2.24	0.72
1:E:126:PRO:HG2	3:E:306:HOH:O	1.89	0.72
2:H:60:TYR:HB2	2:H:65:GLN:HG3	1.72	0.71
2:H:93:VAL:HG22	2:H:114:GLN:HG2	1.72	0.71
2:H:123:LYS:HE3	2:H:150:ASP:HB3	1.72	0.71
2:D:103:TYR:CB	2:D:104:LEU:HA	2.20	0.70
2:B:6:GLN:O	2:B:111:GLN:OE1	2.10	0.70
2:D:29:PHE:CE2	2:D:77:SER:HA	2.27	0.70
2:D:91:THR:HG23	2:D:115:VAL:HA	1.72	0.69
2:B:50:ARG:CG	2:B:50:ARG:HH11	2.01	0.69
2:D:117:VAL:HG12	2:D:120:ALA:HB3	1.73	0.69
1:C:36:LYS:HB3	1:C:56:TRP:CZ3	2.28	0.69
1:A:12:THR:HG22	1:A:111:GLU:CB	2.23	0.69
1:C:112:ILE:HG22	1:C:172:GLN:HE22	1.58	0.68
2:D:8:GLY:HA2	2:D:113:THR:HG23	1.75	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLN:HE21	1:A:135:THR:HG22	1.58	0.67
2:F:2:VAL:HG11	2:F:98:ARG:HH21	1.59	0.67
1:E:127:SER:O	1:E:131:LEU:HD11	1.95	0.67
2:D:212:LYS:HB3	2:F:212:LYS:HE3	1.76	0.66
1:A:0:LEU:HB3	1:A:27:GLN:HE22	1.60	0.66
1:C:19:VAL:HG11	1:C:110:LEU:CD2	2.26	0.66
2:D:104:LEU:H	2:D:104:LEU:HD22	1.60	0.66
1:C:60:ARG:HD3	1:C:64:VAL:O	1.95	0.66
2:D:56:GLY:O	2:D:58:THR:HG23	1.96	0.65
1:A:134:GLY:HA2	1:A:189:LYS:HB2	1.79	0.65
2:D:117:VAL:HG12	2:D:120:ALA:HB2	1.78	0.65
1:L:176:ASP:HB3	3:L:306:HOH:O	1.96	0.64
2:B:9:VAL:HG22	2:B:114:GLN:O	1.97	0.64
2:D:8:GLY:HA3	2:D:113:THR:CG2	2.28	0.63
2:D:103:TYR:HB2	2:D:104:LEU:CA	2.25	0.63
1:C:115:THR:HG21	2:B:119:SER:HB3	1.80	0.63
1:A:128:ASP:HA	1:A:131:LEU:HD12	1.79	0.63
2:B:2:VAL:HG22	2:B:27:TYR:HB3	1.80	0.63
2:D:24:ALA:HB3	2:D:77:SER:O	1.98	0.63
2:B:50:ARG:HG2	2:B:50:ARG:NH1	1.94	0.62
1:E:126:PRO:HD3	1:E:138:VAL:HG22	1.82	0.62
1:A:86:PRO:HA	1:A:112:ILE:HD12	1.81	0.62
2:H:93:VAL:HG22	2:H:114:GLN:CG	2.29	0.61
2:B:51:ILE:HG12	2:B:58:THR:HG22	1.82	0.61
2:B:182:TYR:HE1	2:H:191:PRO:HB3	1.64	0.61
2:H:103:TYR:HB2	2:H:105:GLY:H	1.66	0.61
2:H:132:PRO:HG3	2:H:144:LEU:HB3	1.81	0.61
1:C:113:ARG:HA	1:C:146:TYR:OH	2.02	0.60
2:D:8:GLY:HA3	2:D:113:THR:HG23	1.84	0.60
1:A:112:ILE:HG22	1:A:172:GLN:OE1	2.02	0.60
2:F:11:LEU:HD12	2:F:116:THR:HB	1.84	0.59
2:B:60:TYR:HB2	2:B:65:GLN:HG3	1.82	0.59
2:F:32:ASN:HD21	2:F:100:ASP:CG	2.06	0.59
2:D:9:VAL:HB	2:D:113:THR:OG1	2.01	0.59
2:F:122:THR:HG22	2:F:122:THR:O	2.02	0.59
1:E:127:SER:O	1:E:131:LEU:CD1	2.51	0.58
2:F:123:LYS:HG2	2:F:124:GLY:N	2.18	0.58
2:D:30:THR:O	2:D:54:GLU:HB2	2.03	0.58
2:H:199:THR:HG23	2:H:216:LYS:HE2	1.85	0.58
2:F:9:VAL:HG12	2:F:114:GLN:O	2.04	0.58
2:B:35:ASP:HB3	2:B:50:ARG:HA	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:123:LYS:HZ2	2:F:150:ASP:C	2.06	0.58
1:E:164:ASN:O	1:E:186:THR:OG1	2.22	0.57
2:H:28:ILE:HG22	2:H:30:THR:HG22	1.86	0.57
2:D:46:GLU:OE1	2:D:64:PHE:HZ	1.88	0.57
2:H:29:PHE:O	2:H:30:THR:HB	2.05	0.57
2:H:10:GLU:OE1	2:H:12:ARG:NH2	2.37	0.57
1:L:167:GLU:HA	1:L:182:SER:O	2.04	0.56
2:D:37:VAL:HG22	2:D:47:TRP:HA	1.86	0.56
2:H:135:LYS:O	2:H:138:SER:N	2.38	0.56
1:A:126:PRO:HD3	1:A:138:VAL:HG22	1.88	0.56
2:B:35:ASP:OD2	2:B:99:VAL:HG22	2.05	0.56
1:C:12:THR:HG21	1:C:111:GLU:OE1	2.01	0.56
1:A:11:VAL:O	1:A:111:GLU:HB2	2.06	0.56
2:D:112:GLY:CA	2:D:113:THR:HG22	2.35	0.56
2:D:23:LYS:HA	2:D:24:ALA:HB3	1.88	0.56
2:B:27:TYR:CG	2:B:28:ILE:N	2.74	0.56
2:H:103:TYR:CB	2:H:105:GLY:H	2.19	0.55
2:D:46:GLU:OE1	2:D:64:PHE:CZ	2.59	0.55
2:H:99:VAL:HG23	2:H:106:TYR:CE1	2.41	0.55
1:C:56:TRP:CZ3	2:D:103:TYR:O	2.59	0.55
1:E:66:ASP:HB3	2:B:201:ILE:HD13	1.87	0.55
2:H:40:ALA:HB3	2:H:43:GLN:HB2	1.88	0.55
1:A:122:PHE:HB2	1:A:141:LEU:HB3	1.89	0.55
1:A:163:GLY:HA2	2:H:166:THR:HG21	1.89	0.55
1:E:139:VAL:HG22	1:E:184:THR:HG23	1.89	0.55
2:F:40:ALA:HB3	2:F:43:GLN:HB2	1.89	0.55
2:D:114:GLN:HE21	2:D:115:VAL:N	2.05	0.55
1:C:122:PHE:HB2	1:C:141:LEU:HB3	1.89	0.54
1:E:102:TYR:OH	2:F:50:ARG:NH2	2.40	0.54
1:L:126:PRO:HD3	1:L:138:VAL:HG22	1.90	0.54
2:D:100:ASP:HB3	2:D:102:TYR:O	2.07	0.54
2:D:102:TYR:O	2:D:103:TYR:CD2	2.61	0.54
1:A:109:ARG:CG	1:A:109:ARG:HH11	2.20	0.54
2:B:11:LEU:HD11	2:B:118:SER:HB3	1.89	0.54
2:H:51:ILE:HD12	2:H:58:THR:CG2	2.32	0.54
2:D:23:LYS:HA	2:D:24:ALA:CB	2.37	0.54
2:H:132:PRO:HD2	2:H:219:PRO:HA	1.90	0.54
2:H:9:VAL:HG22	2:H:114:GLN:HB2	1.89	0.54
2:D:94:TYR:CE1	2:D:114:GLN:HG2	2.42	0.54
1:C:126:PRO:HD3	1:C:138:VAL:HG22	1.89	0.54
2:H:30:THR:HA	2:H:53:PRO:HB2	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:ARG:NH1	2:B:199:THR:HG21	2.23	0.53
2:F:121:SER:O	2:F:123:LYS:N	2.42	0.53
2:F:29:PHE:HD2	2:F:29:PHE:O	1.92	0.53
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.91	0.53
2:B:47:TRP:HZ2	2:B:50:ARG:HD3	1.73	0.53
2:H:30:THR:HG23	2:H:31:MET:HG2	1.91	0.53
1:A:18:LYS:HG3	1:A:82:SER:HA	1.90	0.53
2:H:8:GLY:O	2:H:9:VAL:HG23	2.09	0.52
1:L:122:PHE:HB2	1:L:141:LEU:HB3	1.90	0.52
2:B:26:GLY:HA3	2:B:27:TYR:C	2.31	0.52
1:C:54:ILE:HG21	1:C:70:GLY:HA3	1.92	0.52
2:B:30:THR:HG22	2:B:31:MET:N	2.18	0.52
2:B:60:TYR:HD2	2:B:65:GLN:HG3	1.73	0.52
1:E:18:LYS:HG3	1:E:82:SER:HA	1.91	0.52
2:B:35:ASP:OD2	2:B:50:ARG:HD2	2.10	0.52
2:D:117:VAL:O	2:D:118:SER:O	2.28	0.51
1:C:18:LYS:HG3	1:C:82:SER:HA	1.91	0.51
2:B:199:THR:HG23	2:B:216:LYS:HE2	1.91	0.51
1:L:18:LYS:HG3	1:L:82:SER:HA	1.92	0.51
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.75	0.51
1:L:167:GLU:HB2	1:L:181:LEU:HD21	1.93	0.51
2:D:103:TYR:CB	2:D:104:LEU:CA	2.87	0.51
2:D:199:THR:HG23	2:D:216:LYS:HE2	1.93	0.51
1:A:109:ARG:CG	1:A:109:ARG:NH1	2.73	0.51
2:B:2:VAL:HG13	2:B:27:TYR:CD1	2.46	0.50
2:B:17:SER:OG	2:B:83:LEU:O	2.24	0.50
2:B:35:ASP:HB2	2:B:49:GLY:O	2.11	0.50
2:H:29:PHE:HE2	2:H:74:THR:HA	1.76	0.50
2:H:36:TRP:CE2	2:H:81:VAL:HG23	2.47	0.50
2:F:104:LEU:HD22	2:F:104:LEU:N	2.27	0.50
1:A:114:ARG:HG2	1:A:115:THR:N	2.26	0.50
1:C:151:LYS:HB3	1:C:203:THR:HB	1.94	0.50
2:F:125:PRO:HB3	2:F:151:TYR:CB	2.32	0.50
1:L:84:PHE:CE2	1:L:112:ILE:HG13	2.46	0.50
1:A:46:LEU:HD11	3:A:307:HOH:O	2.12	0.49
1:E:124:PHE:HB2	1:E:139:VAL:O	2.12	0.49
2:B:60:TYR:CD2	2:B:65:GLN:HG3	2.47	0.49
2:B:30:THR:HG21	2:B:54:GLU:N	2.27	0.49
2:H:9:VAL:HG13	2:H:114:GLN:O	2.11	0.49
1:A:2:ILE:HG12	1:A:27:GLN:HB2	1.93	0.49
2:B:36:TRP:CZ3	2:B:96:CYS:HB2	2.47	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:102:TYR:O	2:H:103:TYR:HB2	2.13	0.49
2:D:33:SER:HA	2:D:52:ASP:HA	1.95	0.49
1:L:128:ASP:HA	1:L:131:LEU:HD12	1.94	0.49
2:H:51:ILE:CD1	2:H:58:THR:HG22	2.34	0.49
1:E:124:PHE:O	1:E:138:VAL:HG13	2.13	0.49
1:L:151:LYS:HB3	1:L:203:THR:HB	1.94	0.49
1:C:112:ILE:HG22	1:C:172:GLN:NE2	2.25	0.49
1:E:38:TYR:CD2	2:F:104:LEU:HD23	2.48	0.49
1:E:151:LYS:HB3	1:E:203:THR:HB	1.95	0.48
1:C:19:VAL:HG11	1:C:110:LEU:HD23	1.95	0.48
2:B:177:GLN:NE2	2:B:183:SER:HB2	2.28	0.48
2:B:125:PRO:HB3	2:B:151:TYR:HB3	1.95	0.48
2:D:212:LYS:HB3	2:F:212:LYS:CE	2.42	0.48
2:H:70:PHE:CD1	2:H:81:VAL:HG22	2.48	0.48
2:B:35:ASP:OD2	2:B:99:VAL:CG2	2.61	0.48
2:D:117:VAL:CG1	2:D:120:ALA:HB2	2.44	0.48
1:A:151:LYS:HB3	1:A:203:THR:HB	1.94	0.48
2:F:122:THR:HG23	2:F:153:PRO:HD3	1.96	0.47
2:F:11:LEU:CD1	2:F:152:PHE:CZ	2.95	0.47
2:D:8:GLY:HA3	2:D:113:THR:HG21	1.96	0.47
2:H:33:SER:HA	2:H:53:PRO:HD3	1.96	0.47
1:A:56:TRP:HB2	1:A:59:ILE:HG12	1.96	0.47
2:H:32:ASN:HD22	2:H:98:ARG:NH2	2.12	0.47
2:D:117:VAL:CG1	2:D:120:ALA:CB	2.88	0.47
2:B:7:PRO:O	2:B:113:THR:OG1	2.28	0.47
1:C:1:ASP:OD1	1:C:101:PRO:HD2	2.15	0.47
2:D:114:GLN:NE2	2:D:116:THR:HG22	2.30	0.46
1:C:92:TYR:CD2	1:C:110:LEU:HD13	2.51	0.46
1:A:114:ARG:HG3	1:A:114:ARG:HH11	1.80	0.46
2:B:36:TRP:O	2:B:48:MET:HB2	2.15	0.46
2:D:8:GLY:CA	2:D:113:THR:CG2	2.87	0.46
2:H:39:GLN:HG3	2:H:45:LEU:HG	1.96	0.46
1:A:12:THR:CG2	1:A:111:GLU:CB	2.93	0.46
2:B:33:SER:HA	2:B:53:PRO:HD3	1.98	0.46
1:E:213:LYS:HD3	3:E:310:HOH:O	2.16	0.46
2:D:100:ASP:O	2:D:104:LEU:CB	2.60	0.46
1:C:102:TYR:OH	2:D:50:ARG:NH2	2.49	0.46
2:D:6:GLN:CG	2:D:111:GLN:H	2.29	0.46
2:D:60:TYR:CE1	2:D:70:PHE:CD2	3.04	0.46
2:H:9:VAL:CG2	2:H:114:GLN:HB2	2.46	0.46
2:F:177:GLN:NE2	2:F:183:SER:HB2	2.31	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:TYR:HB2	2:D:65:GLN:HE21	1.81	0.45
1:C:130:GLN:HG3	2:D:128:PHE:CE2	2.51	0.45
2:H:9:VAL:HG22	2:H:114:GLN:H	1.81	0.45
1:C:19:VAL:HG11	1:C:110:LEU:HD21	1.98	0.45
1:C:102:TYR:OH	2:D:104:LEU:HD23	2.17	0.45
2:D:29:PHE:O	2:D:29:PHE:CD2	2.70	0.45
2:H:35:ASP:OD1	2:H:35:ASP:N	2.49	0.45
2:H:28:ILE:HG22	2:H:30:THR:CG2	2.47	0.45
2:D:35:ASP:CB	2:D:49:GLY:O	2.65	0.45
2:B:91:THR:HG23	2:B:116:THR:HA	1.98	0.45
1:C:40:ALA:HA	1:C:54:ILE:O	2.17	0.45
1:L:19:VAL:HG11	1:L:110:LEU:CD2	2.34	0.44
2:D:61:ALA:HB3	2:D:64:PHE:HD1	1.82	0.44
1:C:38:TYR:N	1:C:38:TYR:CD1	2.85	0.44
2:F:97:ALA:HB1	2:F:106:TYR:HB3	1.99	0.44
1:A:130:GLN:HE21	1:A:135:THR:CG2	2.30	0.44
1:A:54:ILE:HG21	1:A:70:GLY:HA3	1.99	0.44
2:B:30:THR:HG21	2:B:54:GLU:CA	2.47	0.44
1:E:123:ILE:O	1:E:124:PHE:CG	2.70	0.44
1:A:111:GLU:OE2	1:A:111:GLU:HA	2.17	0.44
1:C:209:SER:HB3	1:L:113:ARG:CD	2.47	0.44
2:F:103:TYR:CD1	2:F:103:TYR:O	2.70	0.44
1:L:56:TRP:CZ2	2:H:102:TYR:HB3	2.52	0.44
1:E:0:LEU:HD13	1:E:27:GLN:NE2	2.32	0.44
2:F:29:PHE:HE2	2:F:74:THR:HA	1.83	0.44
1:E:56:TRP:HB2	1:E:59:ILE:HG12	1.99	0.44
1:L:54:ILE:HG21	1:L:70:GLY:HA3	2.00	0.44
1:E:87:GLU:H	1:E:87:GLU:HG2	1.46	0.44
2:F:50:ARG:HG2	2:F:51:ILE:N	2.32	0.44
1:E:54:ILE:HG21	1:E:70:GLY:HA3	2.00	0.44
1:A:169:VAL:HG23	2:H:198:GLN:HE22	1.83	0.43
2:F:199:THR:HG23	2:F:216:LYS:HE2	1.99	0.43
2:D:123:LYS:HE3	2:D:181:LEU:HD22	2.00	0.43
1:C:97:GLY:O	2:D:104:LEU:CD2	2.66	0.43
2:B:2:VAL:CG2	2:B:27:TYR:HB3	2.48	0.43
2:H:29:PHE:CD2	2:H:29:PHE:O	2.71	0.43
2:B:36:TRP:CH2	2:B:96:CYS:HB2	2.53	0.43
2:D:36:TRP:HD1	2:D:70:PHE:HE1	1.66	0.43
1:E:121:VAL:HG12	1:E:213:LYS:HG3	1.99	0.43
1:A:87:GLU:H	1:A:87:GLU:HG2	1.47	0.43
2:D:29:PHE:O	2:D:30:THR:HG23	2.19	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:19:LYS:HA	2:F:81:VAL:O	2.19	0.43
1:L:56:TRP:HB2	1:L:59:ILE:HG12	2.00	0.43
1:A:0:LEU:HB3	1:A:27:GLN:NE2	2.31	0.43
2:F:30:THR:CB	2:F:31:MET:CB	2.67	0.43
2:F:50:ARG:HG2	2:F:51:ILE:H	1.83	0.43
2:D:112:GLY:HA3	2:D:113:THR:HG22	1.99	0.43
2:F:121:SER:O	2:F:123:LYS:HB3	2.19	0.42
1:C:56:TRP:HD1	1:C:59:ILE:HD12	1.84	0.42
2:B:30:THR:HG21	2:B:54:GLU:HA	2.00	0.42
2:B:63:LYS:HE3	2:B:63:LYS:HB2	1.73	0.42
2:H:71:THR:OG1	2:H:80:TYR:HB2	2.20	0.42
1:E:185:LEU:HG	1:E:186:THR:N	2.34	0.42
2:B:4:LEU:HD11	2:B:98:ARG:HB2	2.02	0.42
2:D:10:GLU:HG2	3:D:313:HOH:O	2.19	0.42
1:C:84:PHE:CE2	1:C:112:ILE:HG13	2.55	0.42
2:F:119:SER:C	2:F:120:ALA:O	2.53	0.42
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.55	0.42
2:B:19:LYS:HD2	2:B:80:TYR:CD2	2.55	0.42
2:B:35:ASP:OD1	2:B:106:TYR:OH	2.20	0.42
1:E:141:LEU:HD22	2:F:187:VAL:HG11	2.02	0.42
1:C:169:VAL:HG22	1:C:181:LEU:HD12	2.01	0.42
2:D:176:LEU:HD13	2:D:182:TYR:CZ	2.55	0.42
1:L:191:ASP:HA	1:L:194:LYS:HD2	2.02	0.42
1:L:102:TYR:HB2	2:H:47:TRP:CG	2.54	0.41
2:D:55:ASP:O	2:D:57:GLY:N	2.52	0.41
2:H:7:PRO:HD2	2:H:21:SER:O	2.20	0.41
1:L:0:LEU:N	1:L:0:LEU:CD2	2.83	0.41
2:D:33:SER:O	2:D:99:VAL:CG1	2.64	0.41
1:E:124:PHE:HE2	1:E:141:LEU:HD23	1.85	0.41
1:E:38:TYR:CE2	2:F:104:LEU:HD23	2.56	0.41
2:D:36:TRP:HA	2:D:95:TYR:O	2.21	0.41
1:C:102:TYR:HB2	2:D:47:TRP:CG	2.55	0.41
1:A:191:ASP:HA	1:A:194:LYS:HD2	2.03	0.41
1:A:0:LEU:HD13	1:A:27:GLN:HE22	1.86	0.41
1:C:15:ALA:O	2:B:15:GLY:CA	2.51	0.41
2:F:103:TYR:O	2:F:105:GLY:N	2.53	0.41
2:D:132:PRO:HD2	2:D:219:PRO:HA	2.03	0.41
1:C:87:GLU:H	1:C:87:GLU:HG2	1.47	0.41
2:D:35:ASP:HB2	2:D:49:GLY:O	2.21	0.40
2:B:100:ASP:HB2	2:B:107:ASP:OD1	2.20	0.40
2:B:105:GLY:HA3	2:B:106:TYR:CD1	2.57	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:PRO:HD2	2:B:219:PRO:HA	2.03	0.40
1:E:128:ASP:HA	1:E:131:LEU:CD1	2.51	0.40
1:E:19:VAL:HG11	1:E:110:LEU:HD11	2.03	0.40
1:L:87:GLU:HG2	1:L:87:GLU:H	1.46	0.40
2:H:94:TYR:CD1	2:H:115:VAL:HG23	2.56	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	217/221 (98%)	201 (93%)	15 (7%)	1 (0%)	34	72
1	C	217/221 (98%)	205 (94%)	9 (4%)	3 (1%)	14	50
1	E	219/221 (99%)	203 (93%)	15 (7%)	1 (0%)	34	72
1	L	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	14	50
2	B	209/219 (95%)	190 (91%)	14 (7%)	5 (2%)	7	38
2	D	209/219 (95%)	177 (85%)	20 (10%)	12 (6%)	2	16
2	F	209/219 (95%)	186 (89%)	18 (9%)	5 (2%)	7	38
2	H	213/219 (97%)	185 (87%)	18 (8%)	10 (5%)	3	21
All	All	1712/1760 (97%)	1551 (91%)	121 (7%)	40 (2%)	8	40

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	E	219	GLU
1	L	219	GLU
2	D	24	ALA
2	D	56	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	103	TYR
2	D	114	GLN
2	D	118	SER
2	F	56	GLY
2	F	122	THR
2	H	30	THR
2	H	56	GLY
2	H	98	ARG
2	H	99	VAL
2	B	56	GLY
2	D	57	GLY
2	H	8	GLY
2	H	54	GLU
2	H	139	GLY
1	L	144	ASN
2	B	62	GLN
2	D	27	TYR
2	D	30	THR
2	D	120	ALA
2	D	150	ASP
1	C	144	ASN
2	B	27	TYR
2	F	102	TYR
2	H	103	TYR
1	C	74	ALA
1	L	15	ALA
2	B	9	VAL
2	B	150	ASP
2	F	104	LEU
2	H	91	THR
1	C	57	ALA
2	D	28	ILE
2	D	113	THR
2	F	62	GLN
2	H	101	ASP

### 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	193/195 (99%)	182 (94%)	11 (6%)	25	64
1	C	193/195 (99%)	180 (93%)	13 (7%)	20	58
1	E	194/195 (100%)	171 (88%)	23 (12%)	6	27
1	L	195/195 (100%)	180 (92%)	15 (8%)	16	51
2	B	179/185 (97%)	151 (84%)	28 (16%)	3	15
2	D	180/185 (97%)	144 (80%)	36 (20%)	1	6
2	F	180/185 (97%)	153 (85%)	27 (15%)	3	17
2	H	182/185 (98%)	153 (84%)	29 (16%)	3	14
All	All	1496/1520 (98%)	1314 (88%)	182 (12%)	6	26

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	35	GLN
1	A	39	LEU
1	A	53	LEU
1	A	56	TRP
1	A	61	GLU
1	A	87	GLU
1	A	99	SER
1	A	109	ARG
1	A	114	ARG
1	A	182	SER
1	C	32	SER
1	C	39	LEU
1	C	51	ARG
1	C	56	TRP
1	C	61	GLU
1	C	66	ASP
1	C	73	SER
1	C	87	GLU
1	C	99	SER
1	C	109	ARG
1	C	111	GLU
1	C	112	ILE
1	C	182	SER
1	E	1	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	32	SER
1	E	35	GLN
1	E	39	LEU
1	E	53	LEU
1	E	56	TRP
1	E	61	GLU
1	E	66	ASP
1	E	87	GLU
1	E	99	SER
1	E	109	ARG
1	E	112	ILE
1	E	120	SER
1	E	125	PRO
1	E	127	SER
1	E	141	LEU
1	E	167	GLU
1	E	182	SER
1	E	186	THR
1	E	187	LEU
1	E	217	ARG
1	E	219	GLU
1	E	220	CYS
1	L	0	LEU
1	L	32	SER
1	L	39	LEU
1	L	53	LEU
1	L	56	TRP
1	L	61	GLU
1	L	87	GLU
1	L	99	SER
1	L	109	ARG
1	L	112	ILE
1	L	113	ARG
1	L	167	GLU
1	L	182	SER
1	L	185	LEU
1	L	219	GLU
2	B	6	GLN
2	B	9	VAL
2	B	10	GLU
2	B	11	LEU
2	B	23	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	27	TYR
2	B	28	ILE
2	B	50	ARG
2	B	51	ILE
2	B	54	GLU
2	B	59	LYS
2	B	62	GLN
2	B	63	LYS
2	B	65	GLN
2	B	68	VAL
2	B	71	THR
2	B	73	ASP
2	B	74	THR
2	B	87	ARG
2	B	99	VAL
2	B	101	ASP
2	B	102	TYR
2	B	103	TYR
2	B	104	LEU
2	B	107	ASP
2	B	111	GLN
2	B	114	GLN
2	B	197	THR
2	D	3	GLN
2	D	9	VAL
2	D	11	LEU
2	D	21	SER
2	D	23	LYS
2	D	29	PHE
2	D	30	THR
2	D	33	SER
2	D	35	ASP
2	D	38	ARG
2	D	39	GLN
2	D	46	GLU
2	D	52	ASP
2	D	59	LYS
2	D	62	GLN
2	D	65	GLN
2	D	68	VAL
2	D	71	THR
2	D	74	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	82	GLU
2	D	87	ARG
2	D	88	SER
2	D	89	GLU
2	D	93	VAL
2	D	100	ASP
2	D	101	ASP
2	D	102	TYR
2	D	104	LEU
2	D	113	THR
2	D	114	GLN
2	D	116	THR
2	D	119	SER
2	D	123	LYS
2	D	159	SER
2	D	197	THR
2	D	201	ILE
2	F	10	GLU
2	F	11	LEU
2	F	23	LYS
2	F	28	ILE
2	F	29	PHE
2	F	30	THR
2	F	31	MET
2	F	32	ASN
2	F	35	ASP
2	F	51	ILE
2	F	52	ASP
2	F	55	ASP
2	F	59	LYS
2	F	62	GLN
2	F	65	GLN
2	F	74	THR
2	F	81	VAL
2	F	87	ARG
2	F	89	GLU
2	F	96	CYS
2	F	102	TYR
2	F	104	LEU
2	F	111	GLN
2	F	119	SER
2	F	121	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	F	123	LYS
2	F	197	THR
2	H	10	GLU
2	H	11	LEU
2	H	25	SER
2	H	29	PHE
2	H	32	ASN
2	H	33	SER
2	H	35	ASP
2	H	39	GLN
2	H	50	ARG
2	H	51	ILE
2	H	54	GLU
2	H	55	ASP
2	H	59	LYS
2	H	62	GLN
2	H	65	GLN
2	H	68	VAL
2	H	74	THR
2	H	82	GLU
2	H	87	ARG
2	H	100	ASP
2	H	101	ASP
2	H	102	TYR
2	H	107	ASP
2	H	121	SER
2	H	122	THR
2	H	138	SER
2	H	185	SER
2	H	197	THR
2	H	201	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	83	ASN
1	A	130	GLN
1	A	143	ASN
1	C	83	ASN
1	C	172	GLN
1	E	27	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	83	ASN
1	L	83	ASN
1	L	143	ASN
2	B	32	ASN
2	B	65	GLN
2	B	111	GLN
2	D	65	GLN
2	D	114	GLN
2	F	32	ASN
2	F	65	GLN
2	F	111	GLN
2	F	114	GLN
2	H	65	GLN
2	H	170	HIS
2	H	198	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](#)

There are no ligands in this entry.

### 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, 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	219/221 (99%)	0.34	3 (1%) 78 78	22, 46, 67, 82	3 (1%)
1	C	219/221 (99%)	0.39	5 (2%) 64 63	21, 42, 69, 85	3 (1%)
1	E	221/221 (100%)	0.43	8 (3%) 46 45	19, 46, 73, 125	3 (1%)
1	L	221/221 (100%)	0.12	3 (1%) 78 78	15, 38, 59, 120	3 (1%)
2	B	213/219 (97%)	0.19	2 (0%) 85 86	21, 44, 65, 79	0
2	D	213/219 (97%)	0.33	5 (2%) 64 63	21, 45, 68, 85	0
2	F	213/219 (97%)	0.44	8 (3%) 44 42	23, 48, 70, 84	0
2	H	217/219 (99%)	0.10	3 (1%) 78 78	17, 42, 66, 75	0
All	All	1736/1760 (98%)	0.29	37 (2%) 67 66	15, 44, 67, 125	12 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	220	CYS	5.7
1	L	220	CYS	4.3
1	E	0	LEU	3.7
1	C	158	ASN	3.5
2	D	140	GLY	3.4
2	F	74	THR	3.0
1	A	0	LEU	2.7
2	D	133	SER	2.6
1	C	196	LYS	2.6
1	C	86	PRO	2.6
1	A	65	PRO	2.6
1	E	22	ASN	2.6
2	F	140	GLY	2.5
2	H	74	THR	2.5
1	L	66	ASP	2.5
1	E	82	SER	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	8	PRO	2.3
2	D	141	THR	2.3
1	C	197	VAL	2.3
1	A	17	ASP	2.2
1	E	4	MET	2.2
2	B	1	GLU	2.2
2	D	55	ASP	2.2
2	F	141	THR	2.2
1	L	82	SER	2.2
2	F	75	SER	2.2
1	E	75	THR	2.2
2	D	132	PRO	2.1
2	F	197	THR	2.1
2	H	55	ASP	2.1
2	H	76	THR	2.1
2	F	55	ASP	2.1
1	C	17	ASP	2.1
2	F	211	THR	2.1
2	B	166	THR	2.0
2	F	1	GLU	2.0
1	E	21	ILE	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.