



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2017 – 09:57 PM EST

PDB ID : 5TPN  
Title : Crystal structure of RSV F in complex with human antibody hRSV90  
Authors : Mousa, J.J.; Crowe, J.E.  
Deposited on : 2016-10-20  
Resolution : 3.14 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-20028442  
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-20028442

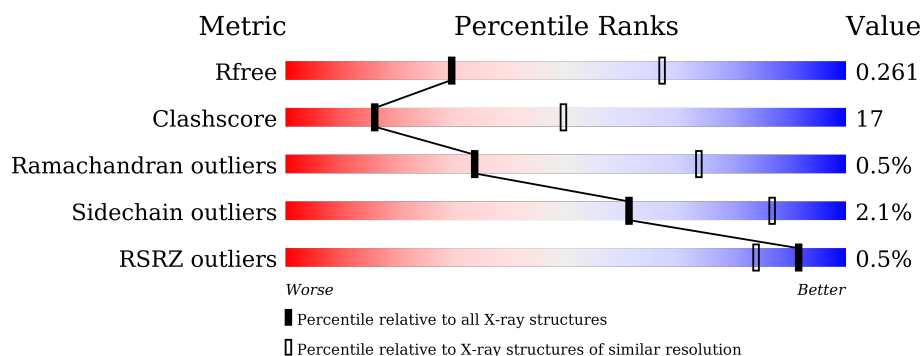
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.14 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	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)

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	510	<div> <div></div> <div>68%26% . .</div> </div>
2	H	225	<div> <div>57%36% . .</div> </div>
3	L	214	<div> <div>64%35% .</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7073 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 Fusion glycoprotein F0,Fibritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3783	2389	629	744	21			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	LYS	GLU	conflict	UNP P03420
A	67	ILE	ASN	engineered mutation	UNP P03420
A	76	ILE	VAL	conflict	UNP P03420
A	102	ALA	PRO	conflict	UNP P03420
A	128	GLN	ARG	conflict	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	GLU	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420
A	?	-	PRO	deletion	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	PHE	deletion	UNP P03420
A	?	-	MET	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	TYR	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	ALA	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	VAL	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420
A	?	-	SER	deletion	UNP P03420

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	GLY	LYS	linker	UNP P03420
A	132	SER	LYS	linker	UNP P03420
A	133	GLY	ARG	linker	UNP P03420
A	134	SER	LYS	linker	UNP P03420
A	135	GLY	ARG	linker	UNP P03420
A	137	SER	PHE	conflict	UNP P03420
A	215	PRO	SER	engineered mutation	UNP P03420
A	379	VAL	ILE	engineered mutation	UNP P03420
A	447	VAL	MET	engineered mutation	UNP P03420
A	487	GLN	GLU	conflict	UNP P03420
A	514	SER	-	linker	UNP P03420
A	515	ALA	-	linker	UNP P03420
A	516	ILE	-	linker	UNP P03420
A	517	GLY	-	linker	UNP P03420
A	545	GLY	-	expression tag	UNP Q38650
A	546	GLY	-	expression tag	UNP Q38650
A	547	LEU	-	expression tag	UNP Q38650
A	548	VAL	-	expression tag	UNP Q38650
A	549	PRO	-	expression tag	UNP Q38650
A	550	ARG	-	expression tag	UNP Q38650
A	551	GLY	-	expression tag	UNP Q38650
A	552	SER	-	expression tag	UNP Q38650
A	553	HIS	-	expression tag	UNP Q38650
A	554	HIS	-	expression tag	UNP Q38650
A	555	HIS	-	expression tag	UNP Q38650
A	556	HIS	-	expression tag	UNP Q38650
A	557	HIS	-	expression tag	UNP Q38650
A	558	HIS	-	expression tag	UNP Q38650

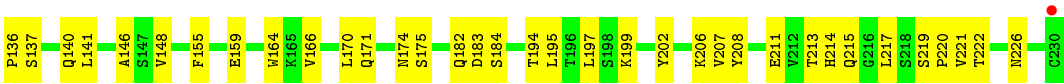
- Molecule 2 is a protein called hRSV90 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1655	1051	280	319	5			

- Molecule 3 is a protein called hRSV0 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1635	1022	278	329	6			





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.25Å 148.25Å 538.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.29 – 3.14 49.29 – 3.14	Depositor EDS
% Data completeness (in resolution range)	75.7 (49.29-3.14) 75.7 (49.29-3.14)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.224 , 0.262 0.222 , 0.261	Depositor DCC
$R_{free}$ test set	1540 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	79.5	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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](#)

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	0.55	0/3840	0.77	7/5205 (0.1%)
2	H	0.60	1/1697 (0.1%)	0.81	3/2315 (0.1%)
3	L	0.65	0/1670	0.71	0/2270
All	All	0.59	1/7207 (0.0%)	0.77	10/9790 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	211	CYS	CB-SG	-5.85	1.72	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	THR	C-N-CA	8.33	142.52	121.70
1	A	471	GLY	C-N-CA	-7.97	101.78	121.70
1	A	210	GLN	N-CA-C	-7.48	90.81	111.00
1	A	382	CYS	CA-CB-SG	-7.18	101.08	114.00
1	A	393	CYS	CA-CB-SG	-6.20	102.85	114.00
2	H	57	THR	N-CA-C	6.03	127.29	111.00
1	A	171	LEU	CA-CB-CG	-6.02	101.45	115.30
2	H	78	ILE	N-CA-C	5.75	126.52	111.00
1	A	46	SER	N-CA-C	5.21	125.07	111.00
2	H	94	LEU	CA-CB-CG	5.11	127.06	115.30

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	3783	0	3835	103	0
2	H	1655	0	1607	78	0
3	L	1635	0	1576	69	0
All	All	7073	0	7018	239	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 17.

All (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:SER:HB3	1:A:313:CYS:SG	1.70	1.29
2:H:76:PHE:CZ	2:H:91:MET:SD	2.37	1.18
3:L:29:VAL:HG11	3:L:106:GLN:HB2	1.21	1.10
1:A:178:VAL:CG2	3:L:36:ILE:HD11	1.91	1.01
3:L:29:VAL:HG11	3:L:106:GLN:CB	1.90	1.01
2:H:101:LEU:HG	2:H:122:THR:O	1.61	1.01
3:L:29:VAL:CG1	3:L:106:GLN:HB2	1.95	0.95
2:H:38:THR:CG2	2:H:57:THR:OG1	2.19	0.91
1:A:178:VAL:HG23	3:L:36:ILE:HD11	1.54	0.88
2:H:38:THR:HG21	2:H:57:THR:OG1	1.74	0.87
2:H:41:TRP:HD1	2:H:78:ILE:HD12	1.39	0.87
2:H:58:TRP:H	2:H:80:ARG:NH1	1.73	0.85
2:H:57:THR:O	2:H:58:TRP:HB3	1.74	0.84
1:A:210:GLN:O	1:A:211:SER:C	2.14	0.83
2:H:59:ASN:O	2:H:62:SER:C	2.15	0.82
1:A:178:VAL:HG21	3:L:36:ILE:HD11	1.59	0.82
1:A:174:THR:HG21	3:L:107:TYR:CD1	2.15	0.81
1:A:321:LEU:O	1:A:322:CYS:HB2	1.80	0.81
1:A:174:THR:HG21	3:L:107:TYR:HD1	1.46	0.81
3:L:13:VAL:HG23	3:L:94:LEU:HD12	1.64	0.77
2:H:201:SER:HA	2:H:204:LEU:HD13	1.67	0.75
2:H:76:PHE:CE1	2:H:91:MET:SD	2.80	0.75
2:H:168:SER:O	2:H:212:ASN:CB	2.35	0.74
1:A:174:THR:CG2	3:L:107:TYR:HD1	2.00	0.74
3:L:159:GLU:OE1	3:L:159:GLU:N	2.19	0.73
2:H:99:THR:HG22	2:H:126:VAL:H	1.53	0.73
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.69	0.72
2:H:59:ASN:O	2:H:63:GLY:N	2.21	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ILE:HG12	1:A:274:MET:HE3	1.72	0.71
3:L:214:HIS:CD2	3:L:215:GLN:H	2.11	0.68
2:H:168:SER:O	2:H:212:ASN:HB2	1.94	0.68
2:H:56:ILE:HD13	2:H:80:ARG:HD2	1.74	0.68
1:A:178:VAL:HG23	3:L:36:ILE:CD1	2.22	0.68
2:H:56:ILE:HG22	2:H:65:ILE:CG2	2.25	0.67
2:H:136:VAL:HG21	2:H:213:VAL:HG21	1.75	0.67
1:A:136:ARG:HH12	1:A:320:PRO:HG3	1.57	0.67
1:A:59:ILE:HG23	1:A:193:LEU:HB3	1.78	0.66
1:A:267:THR:HG22	1:A:269:ASP:H	1.61	0.65
2:H:183:ALA:HA	2:H:193:LEU:HB3	1.78	0.65
2:H:56:ILE:HG22	2:H:65:ILE:HG22	1.77	0.64
2:H:78:ILE:HG23	2:H:78:ILE:O	1.96	0.64
2:H:76:PHE:HA	2:H:90:GLN:O	1.98	0.64
3:L:213:THR:HG22	3:L:220:PRO:HB3	1.79	0.64
2:H:58:TRP:H	2:H:80:ARG:HH12	1.46	0.63
2:H:13:VAL:HG21	2:H:19:LEU:HD22	1.80	0.63
3:L:129:PRO:HD2	3:L:217:LEU:HD21	1.78	0.63
1:A:46:SER:CB	1:A:313:CYS:SG	2.66	0.62
1:A:425:SER:HB3	1:A:431:ILE:HA	1.80	0.61
1:A:211:SER:N	1:A:212:CYS:HB3	2.15	0.61
3:L:174:ASN:OD1	3:L:174:ASN:N	2.33	0.61
1:A:173:SER:HB2	3:L:110:TRP:HE1	1.66	0.61
1:A:267:THR:HB	1:A:270:GLN:H	1.66	0.61
1:A:200:ASP:HA	1:A:204:LEU:HG	1.84	0.60
1:A:336:ARG:HA	1:A:395:ILE:HG22	1.83	0.60
2:H:94:LEU:HG	2:H:126:VAL:HG21	1.83	0.60
2:H:168:SER:O	2:H:212:ASN:HB3	2.01	0.60
1:A:229:ARG:O	1:A:233:ILE:HG13	2.02	0.59
3:L:207:VAL:HG22	3:L:226:ASN:OD1	2.03	0.59
2:H:38:THR:HG22	2:H:57:THR:OG1	2.02	0.59
1:A:248:SER:HB2	1:A:251:MET:H	1.68	0.59
1:A:46:SER:HG	1:A:311:THR:HG1	1.45	0.59
1:A:321:LEU:O	1:A:322:CYS:CB	2.45	0.59
3:L:129:PRO:HD3	3:L:214:HIS:ND1	2.18	0.58
3:L:95:GLN:HG2	3:L:96:SER:H	1.67	0.58
2:H:99:THR:CG2	2:H:126:VAL:H	2.16	0.58
2:H:42:VAL:O	2:H:103:TYR:HB2	2.03	0.58
2:H:99:THR:HB	2:H:125:THR:HA	1.84	0.58
1:A:198:TYR:CE1	1:A:202:GLN:HG3	2.39	0.58
2:H:59:ASN:C	2:H:63:GLY:N	2.56	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:67:TYR:HE2	2:H:78:ILE:HG22	1.69	0.57
1:A:316:LEU:HD11	1:A:336:ARG:NH2	2.19	0.57
3:L:3:VAL:H	3:L:26:SER:HB3	1.70	0.57
1:A:380:ASN:ND2	1:A:380:ASN:O	2.26	0.56
2:H:41:TRP:CD1	2:H:78:ILE:HD12	2.30	0.56
1:A:173:SER:O	1:A:174:THR:HB	2.06	0.55
3:L:183:ASP:OD1	3:L:184:SER:N	2.39	0.55
2:H:23:CYS:HB3	2:H:87:LEU:HB3	1.88	0.55
2:H:41:TRP:HD1	2:H:78:ILE:CD1	2.16	0.55
1:A:167:ILE:HG23	1:A:189:THR:HG21	1.88	0.55
2:H:180:THR:HG22	2:H:195:SER:OG	2.06	0.55
2:H:156:LEU:HD22	2:H:158:LYS:HB2	1.88	0.55
1:A:385:ASP:HB2	1:A:388:ASN:HB2	1.88	0.55
1:A:198:TYR:O	1:A:202:GLN:HB2	2.06	0.55
1:A:320:PRO:HA	1:A:335:THR:OG1	2.06	0.54
2:H:106:ARG:NH1	2:H:116:ASP:OD2	2.40	0.54
2:H:75:ARG:NH1	2:H:98:ASP:OD2	2.41	0.54
2:H:67:TYR:OH	2:H:77:THR:HA	2.08	0.54
2:H:76:PHE:CE2	2:H:91:MET:SD	2.99	0.54
1:A:136:ARG:NH1	1:A:320:PRO:HG3	2.21	0.54
2:H:17:ARG:HG2	2:H:18:SER:H	1.72	0.54
3:L:57:ALA:HB1	3:L:79:SER:O	2.08	0.54
1:A:261:ILE:HG23	1:A:274:MET:HE2	1.89	0.53
3:L:29:VAL:CG1	3:L:106:GLN:CB	2.69	0.53
1:A:316:LEU:HD11	1:A:336:ARG:HH22	1.74	0.53
2:H:141:PRO:HD3	2:H:153:LEU:HB3	1.91	0.53
3:L:128:ALA:HB1	3:L:217:LEU:HD23	1.91	0.53
1:A:194:ASP:O	1:A:197:ASN:N	2.38	0.53
1:A:322:CYS:SG	1:A:401:ASP:HB3	2.48	0.53
2:H:35:ASP:O	2:H:58:TRP:HE3	1.91	0.53
1:A:257:LEU:HD22	1:A:278:VAL:HG13	1.90	0.53
3:L:10:THR:HG23	3:L:119:GLN:HB3	1.90	0.53
1:A:148:ILE:O	1:A:152:VAL:HG23	2.09	0.52
1:A:332:ILE:HB	1:A:483:PHE:CE2	2.45	0.52
1:A:448:ASP:O	1:A:459:VAL:HG22	2.09	0.52
1:A:163:GLU:OE2	1:A:182:SER:N	2.42	0.52
3:L:121:ASN:HB2	3:L:182:GLN:OE1	2.10	0.52
3:L:174:ASN:ND2	3:L:195:LEU:HD11	2.24	0.51
1:A:410:LEU:HD21	1:A:464:GLY:HA3	1.93	0.51
1:A:45:LEU:HD22	1:A:310:ASP:HA	1.92	0.51
2:H:163:GLU:HG2	2:H:164:PRO:HA	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:ILE:HG23	2:H:78:ILE:HG23	1.93	0.51
1:A:522:GLU:HG3	1:A:523:ALA:O	2.10	0.51
1:A:308:VAL:O	1:A:309:ILE:HD13	2.11	0.50
1:A:209:LYS:HE2	1:A:212:CYS:H	1.77	0.50
1:A:201:LYS:HG3	2:H:58:TRP:CH2	2.47	0.50
2:H:81:ASP:C	2:H:83:ALA:H	2.14	0.50
1:A:96:LEU:HD13	1:A:237:PHE:HB3	1.94	0.49
1:A:163:GLU:OE2	1:A:182:SER:OG	2.21	0.49
3:L:206:LYS:HE3	3:L:226:ASN:HD22	1.78	0.49
2:H:163:GLU:HB2	2:H:191:TYR:CE2	2.48	0.49
2:H:87:LEU:HD12	2:H:88:TYR:H	1.76	0.49
3:L:105:GLN:HG2	3:L:106:GLN:N	2.27	0.49
3:L:175:SER:HA	3:L:194:THR:O	2.13	0.49
1:A:306:TYR:HB3	1:A:309:ILE:HD11	1.95	0.49
2:H:101:LEU:HD21	2:H:121:GLY:HA3	1.95	0.49
2:H:71:VAL:HG11	2:H:76:PHE:CE2	2.48	0.49
3:L:2:ILE:HD11	3:L:106:GLN:HG3	1.95	0.49
2:H:163:GLU:HB2	2:H:191:TYR:HE2	1.77	0.49
3:L:105:GLN:HB2	3:L:114:PHE:CD1	2.48	0.48
1:A:173:SER:O	1:A:174:THR:CB	2.61	0.48
1:A:247:VAL:O	1:A:282:ARG:HD3	2.12	0.48
2:H:199:VAL:HG21	2:H:209:TYR:CZ	2.49	0.48
1:A:46:SER:HB3	1:A:343:CYS:SG	2.54	0.48
1:A:487:GLN:HB3	1:A:490:ALA:HB2	1.96	0.48
1:A:178:VAL:CG2	3:L:36:ILE:CD1	2.77	0.48
3:L:53:LEU:HA	3:L:71:ILE:HG12	1.96	0.47
3:L:174:ASN:CG	3:L:195:LEU:HD11	2.35	0.47
2:H:108:ALA:HB2	2:H:116:ASP:OD1	2.14	0.47
1:A:349:VAL:HG12	1:A:350:SER:O	2.14	0.47
3:L:3:VAL:H	3:L:26:SER:CB	2.27	0.47
3:L:36:ILE:HG22	3:L:37:SER:N	2.30	0.47
2:H:6:GLU:CD	2:H:121:GLY:HA2	2.35	0.47
2:H:109:TYR:HA	2:H:112:TYR:O	2.16	0.46
3:L:217:LEU:HD13	3:L:221:VAL:HG23	1.97	0.46
1:A:48:LEU:HB2	1:A:308:VAL:HB	1.98	0.46
2:H:110:VAL:HG11	2:H:111(B):SER:HB3	1.97	0.46
3:L:164:TRP:O	3:L:170:LEU:HD12	2.15	0.46
1:A:378:GLU:O	1:A:381:LEU:HG	2.15	0.46
1:A:482:VAL:O	1:A:499:ILE:HG12	2.16	0.46
3:L:129:PRO:HB3	3:L:155:PHE:HB3	1.97	0.46
3:L:13:VAL:CG2	3:L:94:LEU:HD12	2.40	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:TRP:NE1	1:A:342:TYR:HB2	2.31	0.46
3:L:106:GLN:HG2	3:L:108:ASN:H	1.81	0.46
1:A:76:ILE:HG13	1:A:215:PRO:HD2	1.97	0.46
1:A:83:LEU:HD21	1:A:203:LEU:HD23	1.98	0.45
3:L:11:LEU:O	3:L:120:VAL:HA	2.16	0.45
3:L:124:ARG:HG2	3:L:125:THR:N	2.30	0.45
1:A:174:THR:CG2	3:L:107:TYR:CD1	2.86	0.45
1:A:341:TRP:CZ3	1:A:365:VAL:HG21	2.52	0.45
2:H:161:PHE:O	2:H:215:HIS:HE1	1.99	0.45
3:L:29:VAL:HG13	3:L:106:GLN:HG3	1.98	0.45
3:L:141:LEU:O	3:L:199:LYS:HD2	2.17	0.45
2:H:13:VAL:CG2	2:H:19:LEU:HD22	2.47	0.45
3:L:202:TYR:CE1	3:L:208:TYR:CE1	3.05	0.45
3:L:211:GLU:HG3	3:L:222:THR:OG1	2.17	0.45
3:L:136:PRO:HG3	3:L:146:ALA:HB1	1.98	0.44
2:H:58:TRP:H	2:H:80:ARG:HH11	1.58	0.44
3:L:12:SER:HB3	3:L:121:ASN:OD1	2.17	0.44
1:A:405:SER:HB2	1:A:452:VAL:HG21	2.00	0.44
1:A:210:GLN:O	1:A:211:SER:O	2.33	0.44
1:A:260:LEU:HA	1:A:260:LEU:HD12	1.79	0.44
3:L:136:PRO:HD3	3:L:148:VAL:HG22	1.99	0.44
1:A:204:LEU:HA	1:A:204:LEU:HD23	1.46	0.44
2:H:188:SER:OG	2:H:190:LEU:HB2	2.18	0.44
2:H:95:ARG:HA	2:H:95:ARG:HD3	1.81	0.44
1:A:317:HIS:CE1	1:A:408:THR:HA	2.53	0.43
1:A:73:ASP:OD2	1:A:75:LYS:HG3	2.18	0.43
2:H:105:VAL:CG1	2:H:115:LEU:HB3	2.47	0.43
2:H:54:SER:HB3	2:H:67:TYR:CD2	2.53	0.43
3:L:6:SER:O	3:L:7:SER:HB3	2.18	0.43
1:A:394:LYS:HE3	1:A:394:LYS:HB3	1.55	0.43
2:H:110:VAL:HG11	2:H:111(B):SER:CB	2.48	0.43
2:H:91:MET:HB3	2:H:94:LEU:HD13	2.01	0.43
3:L:37:SER:HB3	3:L:83:SER:HB2	2.00	0.43
1:A:216:ASN:OD1	1:A:218:GLU:HB2	2.18	0.43
1:A:523:ALA:HB2	1:A:537:TRP:CE2	2.54	0.43
1:A:47:ALA:O	1:A:366:PHE:HA	2.18	0.43
3:L:27:GLN:HG3	3:L:28:SER:H	1.84	0.43
3:L:25:ALA:O	3:L:85:THR:HG23	2.18	0.43
3:L:197:LEU:HD23	3:L:197:LEU:HA	1.66	0.43
1:A:293:LYS:HE2	1:A:294:GLU:HG3	2.01	0.43
1:A:472:GLU:HG2	1:A:473:PRO:HD2	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:MET:HB2	1:A:488:PHE:O	2.19	0.43
3:L:195:LEU:HD12	3:L:195:LEU:HA	1.74	0.43
2:H:186:GLN:HE21	2:H:186:GLN:HB2	1.52	0.43
1:A:211:SER:CA	1:A:212:CYS:HB3	2.49	0.42
2:H:57:THR:HG23	2:H:57:THR:O	2.19	0.42
3:L:171:GLN:HE21	3:L:174:ASN:HD21	1.67	0.42
1:A:479:ASP:HB3	1:A:482:VAL:HG22	2.01	0.42
2:H:161:PHE:HB2	2:H:190:LEU:HD13	2.01	0.42
1:A:258:LEU:HD21	1:A:278:VAL:CG2	2.49	0.42
2:H:38:THR:HB	2:H:57:THR:CB	2.49	0.42
2:H:96:ALA:O	2:H:99:THR:HG23	2.19	0.42
1:A:37:CYS:HB2	1:A:321:LEU:HD13	2.01	0.42
1:A:88:ASN:O	1:A:92:GLU:HB2	2.19	0.42
3:L:214:HIS:CD2	3:L:215:GLN:N	2.85	0.42
1:A:267:THR:HB	1:A:270:GLN:HG3	2.01	0.42
1:A:284:GLN:HB2	1:A:304:PRO:HG3	2.01	0.42
2:H:178:VAL:HG22	2:H:197:VAL:HG23	2.00	0.42
3:L:128:ALA:HB1	3:L:217:LEU:CD2	2.50	0.42
1:A:98:GLN:HG3	1:A:99:SER:N	2.35	0.41
3:L:37:SER:O	3:L:39:LEU:N	2.53	0.41
3:L:94:LEU:HD22	3:L:98:ASP:HB2	2.02	0.41
1:A:103:THR:OG1	1:A:105:ASN:ND2	2.53	0.41
1:A:333:CYS:HB3	1:A:398:SER:O	2.20	0.41
1:A:83:LEU:HA	1:A:83:LEU:HD13	1.83	0.41
1:A:407:ILE:HD11	1:A:457:TYR:HB3	2.02	0.41
2:H:156:LEU:CD2	2:H:158:LYS:HB2	2.49	0.41
2:H:44:GLN:HG3	2:H:49:GLY:O	2.20	0.41
1:A:59:ILE:HD12	1:A:297:LEU:HD23	2.03	0.41
1:A:328:GLU:CD	1:A:328:GLU:H	2.21	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.89	0.41
3:L:52:LEU:O	3:L:71:ILE:HD11	2.21	0.41
1:A:313:CYS:HA	1:A:342:TYR:O	2.21	0.41
1:A:375:LEU:HA	1:A:376:PRO:HD3	1.92	0.41
1:A:442:VAL:CG2	1:A:447:VAL:HG21	2.50	0.41
1:A:394:LYS:HA	1:A:491:SER:HA	2.02	0.41
1:A:477:PHE:CD2	1:A:477:PHE:N	2.88	0.41
1:A:95:LEU:O	1:A:98:GLN:HG2	2.21	0.40
2:H:170:ASN:HB3	2:H:173:ALA:HB3	2.02	0.40
3:L:94:LEU:HD23	3:L:94:LEU:HA	1.54	0.40
1:A:33:TYR:CE2	1:A:383:ASN:HB3	2.55	0.40
2:H:81:ASP:O	2:H:82:ASN:HB2	2.22	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:166:VAL:HG22	3:L:171:GLN:OE1	2.20	0.40
3:L:95:GLN:HG2	3:L:96:SER:N	2.35	0.40
1:A:475:ILE:HD12	1:A:475:ILE:HA	1.88	0.40
2:H:45:ALA:HB3	2:H:48:LYS:HB2	2.03	0.40
2:H:99:THR:HA	2:H:124:VAL:O	2.22	0.40
3:L:137:SER:HB2	3:L:140:GLN:HB3	2.03	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	486/510 (95%)	462 (95%)	22 (4%)	2 (0%)	39	77
2	H	213/225 (95%)	198 (93%)	14 (7%)	1 (0%)	34	74
3	L	212/214 (99%)	195 (92%)	15 (7%)	2 (1%)	21	62
All	All	911/949 (96%)	855 (94%)	51 (6%)	5 (0%)	34	74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	THR
2	H	62	SER
3	L	36	ILE
3	L	38	ASN
1	A	211	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	442/456 (97%)	432 (98%)	10 (2%)	58	85
2	H	182/189 (96%)	177 (97%)	5 (3%)	52	83
3	L	184/186 (99%)	182 (99%)	2 (1%)	80	93
All	All	808/831 (97%)	791 (98%)	17 (2%)	61	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	LYS
1	A	201	LYS
1	A	210	GLN
1	A	284	GLN
1	A	322	CYS
1	A	333	CYS
1	A	350	SER
1	A	362	SER
1	A	380	ASN
1	A	505	PHE
2	H	106	ARG
2	H	112(B)	TYR
2	H	123	LEU
2	H	186	GLN
2	H	212	ASN
3	L	79	SER
3	L	219	SER

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

Mol	Chain	Res	Type
3	L	171	GLN

### 5.3.3 RNA ⓘ

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 [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	490/510 (96%)	-0.12	4 (0%) 87 76	38, 69, 103, 132	0
2	H	217/225 (96%)	-0.03	0 100 100	47, 68, 100, 117	0
3	L	214/214 (100%)	-0.01	1 (0%) 91 84	45, 64, 97, 133	0
All	All	921/949 (97%)	-0.08	5 (0%) 91 84	38, 68, 101, 133	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	SER	4.2
1	A	135	GLY	2.8
1	A	516	ILE	2.6
3	L	230	CYS	2.3
1	A	350	SER	2.2

### 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.