



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:07 AM GMT

PDB ID : 3HAG  
Title : Crystal structure of the Hepatitis E Virus-like Particle  
Authors : Guu, T.S.Y.; Liu, Z.; Ye, Q.; Mata, D.A.; Li, K.; Yin, C.; Zhang, J.; Tao, Y.J.  
Deposited on : 2009-05-01  
Resolution : 3.50 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.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

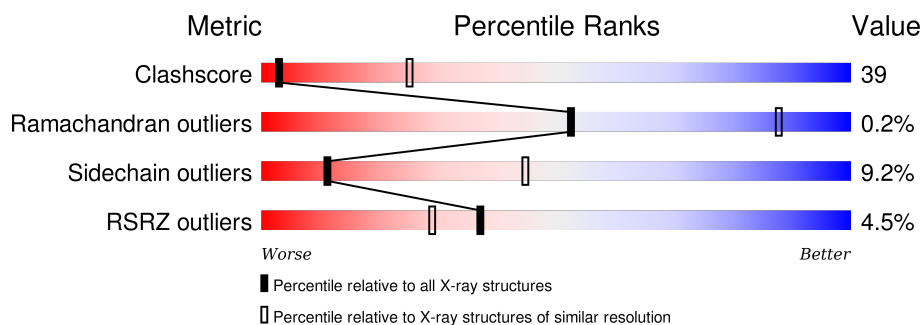
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	504	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3589 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3589	2254	622	706	7			

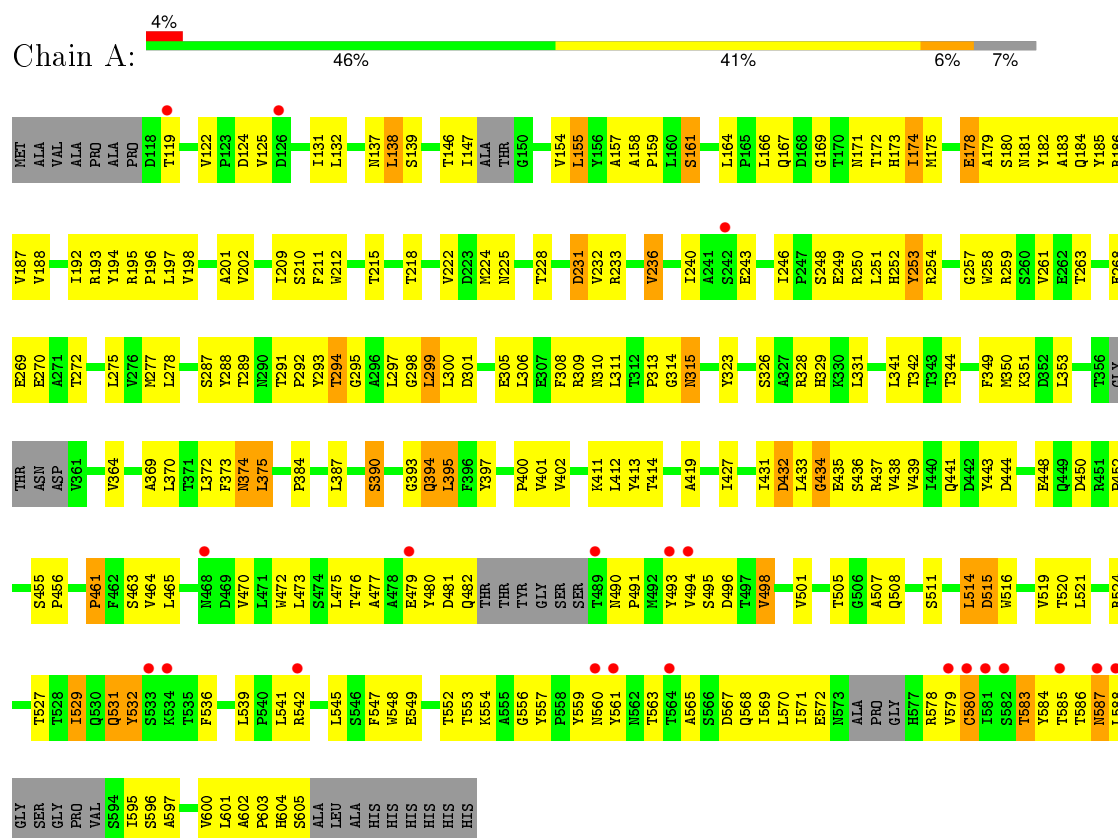
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	SER	PRO	see remark 999	UNP Q8JVV3
A	200	SER	ASN	see remark 999	UNP Q8JVV3
A	360	ASP	GLY	see remark 999	UNP Q8JVV3
A	575	PRO	ALA	see remark 999	UNP Q8JVV3
A	609	HIS	-	EXPRESSION TAG	UNP Q8JVV3
A	610	HIS	-	EXPRESSION TAG	UNP Q8JVV3
A	611	HIS	-	EXPRESSION TAG	UNP Q8JVV3
A	612	HIS	-	EXPRESSION TAG	UNP Q8JVV3
A	613	HIS	-	EXPRESSION TAG	UNP Q8JVV3
A	614	HIS	-	EXPRESSION TAG	UNP Q8JVV3

### 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: Capsid protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	241.09 Å   241.09 Å   519.86 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	50.00 – 3.50 58.34 – 3.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.50) 94.4 (58.34-3.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 3.49 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.277 ,   0.286 0.294 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	73.1	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 39.5	EDS
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 203094 reflections	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	3589	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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	0.63	1/3663 (0.0%)	0.93	6/5005 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	ASP	N-CA	-5.32	1.35	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	TYR	N-CA-C	5.97	127.11	111.00
1	A	531	GLN	N-CA-C	-5.66	95.72	111.00
1	A	514	LEU	N-CA-CB	-5.53	99.34	110.40
1	A	231	ASP	N-CA-C	5.49	125.83	111.00
1	A	561	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	A	328	ARG	CD-NE-CZ	5.19	130.86	123.60

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	3589	0	3539	277	0
All	All	3589	0	3539	277	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 39.

All (277) 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:254:ARG:HH12	1:A:269:GLU:CG	1.62	1.11
1:A:586:THR:O	1:A:586:THR:HG22	1.35	1.11
1:A:183:ALA:HB3	1:A:310:ASN:HB2	1.28	1.09
1:A:572:GLU:HB3	1:A:578:ARG:H	1.10	1.06
1:A:294:THR:OG1	1:A:294:THR:O	1.73	0.99
1:A:586:THR:CG2	1:A:586:THR:O	2.12	0.98
1:A:158:ALA:O	1:A:275:LEU:HD12	1.63	0.96
1:A:557:TYR:O	1:A:583:THR:HG22	1.67	0.95
1:A:475:LEU:HD22	1:A:495:SER:HB2	1.49	0.94
1:A:375:LEU:HD12	1:A:375:LEU:H	1.31	0.94
1:A:505:THR:HG22	1:A:507:ALA:H	1.35	0.91
1:A:225:ASN:HA	1:A:228:THR:HG22	1.52	0.91
1:A:225:ASN:HA	1:A:228:THR:CG2	2.01	0.91
1:A:174:ILE:H	1:A:174:ILE:HD13	1.37	0.89
1:A:493:TYR:O	1:A:580:CYS:HA	1.74	0.88
1:A:372:LEU:HB2	1:A:439:VAL:CG1	2.04	0.87
1:A:254:ARG:NH1	1:A:269:GLU:HB3	1.92	0.84
1:A:373:PHE:HB2	1:A:393:GLY:O	1.76	0.84
1:A:254:ARG:HH12	1:A:269:GLU:CB	1.91	0.83
1:A:186:ARG:HG3	1:A:257:GLY:O	1.78	0.83
1:A:494:VAL:HA	1:A:579:VAL:O	1.78	0.83
1:A:521:LEU:HD12	1:A:604:HIS:HB2	1.60	0.82
1:A:461:PRO:O	1:A:464:VAL:HG12	1.79	0.82
1:A:572:GLU:HB3	1:A:578:ARG:N	1.94	0.82
1:A:475:LEU:HD23	1:A:498:VAL:HB	1.62	0.82
1:A:475:LEU:HD22	1:A:495:SER:CB	2.09	0.82
1:A:201:ALA:HB1	1:A:287:SER:HB3	1.61	0.80
1:A:353:LEU:CD1	1:A:448:GLU:HA	2.11	0.80
1:A:179:ALA:CB	1:A:308:PHE:CE2	2.65	0.79
1:A:479:GLU:O	1:A:493:TYR:HA	1.83	0.79
1:A:557:TYR:O	1:A:583:THR:CG2	2.31	0.78
1:A:384:PRO:HD2	1:A:387:LEU:HD12	1.64	0.78
1:A:218:THR:HG22	1:A:390:SER:O	1.84	0.76
1:A:401:VAL:HG21	1:A:411:LYS:HB2	1.68	0.76
1:A:480:TYR:CZ	1:A:491:PRO:HB3	2.21	0.76
1:A:179:ALA:CB	1:A:308:PHE:HE2	1.98	0.75
1:A:568:GLN:NE2	1:A:570:LEU:HD21	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:TRP:HA	1:A:519:VAL:HG23	1.70	0.74
1:A:254:ARG:HH12	1:A:269:GLU:CD	1.89	0.74
1:A:427:ILE:HD11	1:A:431:ILE:CG1	2.17	0.74
1:A:563:THR:HG22	1:A:565:ALA:H	1.51	0.74
1:A:477:ALA:HB3	1:A:496:ASP:OD1	1.87	0.74
1:A:548:TRP:O	1:A:595:ILE:HG23	1.86	0.73
1:A:254:ARG:HH12	1:A:269:GLU:HG3	1.52	0.72
1:A:179:ALA:HB2	1:A:308:PHE:CE2	2.24	0.72
1:A:201:ALA:O	1:A:287:SER:HB2	1.90	0.71
1:A:435:GLU:OE1	1:A:435:GLU:HA	1.90	0.71
1:A:524:ARG:HD2	1:A:604:HIS:CD2	2.26	0.71
1:A:470:VAL:HG22	1:A:600:VAL:HG22	1.72	0.71
1:A:139:SER:HB3	1:A:301:ASP:OD2	1.90	0.71
1:A:254:ARG:NH1	1:A:269:GLU:CD	2.44	0.70
1:A:254:ARG:NH1	1:A:269:GLU:CG	2.48	0.70
1:A:159:PRO:HB2	1:A:272:THR:OG1	1.91	0.70
1:A:505:THR:HG22	1:A:507:ALA:N	2.06	0.70
1:A:524:ARG:HD2	1:A:604:HIS:HD2	1.57	0.70
1:A:427:ILE:HD11	1:A:431:ILE:HG12	1.72	0.70
1:A:183:ALA:N	1:A:310:ASN:O	2.23	0.69
1:A:455:SER:HB2	1:A:456:PRO:HD3	1.73	0.69
1:A:498:VAL:HG11	1:A:579:VAL:HG21	1.74	0.69
1:A:225:ASN:CA	1:A:228:THR:HG22	2.22	0.69
1:A:268:GLU:HA	1:A:443:TYR:OH	1.93	0.69
1:A:183:ALA:CB	1:A:310:ASN:HB2	2.16	0.68
1:A:552:THR:OG1	1:A:554:LYS:HG3	1.93	0.68
1:A:541:LEU:HD23	1:A:568:GLN:HA	1.75	0.68
1:A:174:ILE:O	1:A:178:GLU:HB2	1.93	0.68
1:A:557:TYR:CD1	1:A:587:ASN:OD1	2.47	0.67
1:A:198:VAL:CG2	1:A:297:LEU:HA	2.25	0.66
1:A:184:GLN:OE1	1:A:309:ARG:HD3	1.96	0.66
1:A:254:ARG:NH1	1:A:269:GLU:CB	2.56	0.65
1:A:547:PHE:HZ	1:A:583:THR:CG2	2.10	0.65
1:A:131:ILE:HG13	1:A:309:ARG:O	1.97	0.65
1:A:258:TRP:O	1:A:259:ARG:HD3	1.97	0.65
1:A:341:LEU:HD12	1:A:342:THR:N	2.11	0.64
1:A:182:TYR:CG	1:A:308:PHE:HB3	2.31	0.64
1:A:364:VAL:HG12	1:A:401:VAL:HG22	1.79	0.64
1:A:122:VAL:HG21	1:A:125:VAL:HB	1.80	0.64
1:A:233:ARG:HG2	1:A:233:ARG:O	1.96	0.63
1:A:511:SER:HA	1:A:516:TRP:HZ2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:VAL:CG2	1:A:411:LYS:HB2	2.29	0.63
1:A:254:ARG:NH1	1:A:269:GLU:OE2	2.31	0.63
1:A:254:ARG:CZ	1:A:269:GLU:HB3	2.29	0.62
1:A:375:LEU:HD23	1:A:433:LEU:HD22	1.81	0.62
1:A:461:PRO:O	1:A:464:VAL:CG1	2.46	0.62
1:A:249:GLU:O	1:A:253:TYR:HB3	2.00	0.62
1:A:158:ALA:O	1:A:275:LEU:CD1	2.44	0.62
1:A:125:VAL:O	1:A:125:VAL:HG22	1.99	0.61
1:A:254:ARG:HH12	1:A:269:GLU:HB3	1.55	0.61
1:A:253:TYR:CD1	1:A:253:TYR:C	2.74	0.61
1:A:210:SER:HB2	1:A:212:TRP:CZ3	2.36	0.61
1:A:516:TRP:HA	1:A:519:VAL:CG2	2.30	0.61
1:A:180:SER:O	1:A:315:ASN:HB3	2.00	0.60
1:A:225:ASN:HA	1:A:228:THR:HG21	1.83	0.60
1:A:232:VAL:HG12	1:A:232:VAL:O	2.02	0.60
1:A:184:GLN:HB2	1:A:309:ARG:HB3	1.83	0.60
1:A:494:VAL:HG22	1:A:580:CYS:HB3	1.83	0.60
1:A:172:THR:HG22	1:A:173:HIS:N	2.17	0.59
1:A:154:VAL:N	1:A:394:GLN:OE1	2.34	0.59
1:A:521:LEU:CD1	1:A:604:HIS:HB2	2.32	0.59
1:A:218:THR:CG2	1:A:390:SER:O	2.49	0.59
1:A:372:LEU:HB2	1:A:439:VAL:HG13	1.84	0.59
1:A:209:ILE:HG12	1:A:278:LEU:HD23	1.85	0.59
1:A:557:TYR:HD1	1:A:587:ASN:OD1	1.86	0.58
1:A:181:ASN:HD22	1:A:314:GLY:H	1.51	0.58
1:A:258:TRP:CH2	1:A:309:ARG:HD2	2.39	0.58
1:A:572:GLU:HB2	1:A:578:ARG:HB2	1.85	0.58
1:A:494:VAL:HG13	1:A:579:VAL:O	2.04	0.58
1:A:432:ASP:C	1:A:432:ASP:OD1	2.41	0.58
1:A:125:VAL:O	1:A:125:VAL:HG13	2.02	0.57
1:A:179:ALA:HB1	1:A:308:PHE:HE2	1.67	0.57
1:A:473:LEU:HD12	1:A:473:LEU:N	2.19	0.57
1:A:146:THR:C	1:A:147:ILE:HD13	2.25	0.57
1:A:353:LEU:HD12	1:A:448:GLU:HA	1.84	0.57
1:A:549:GLU:HB2	1:A:588:LEU:HD11	1.87	0.57
1:A:201:ALA:HB2	1:A:288:TYR:CE1	2.39	0.56
1:A:198:VAL:CG1	1:A:202:VAL:HB	2.34	0.56
1:A:557:TYR:O	1:A:583:THR:HA	2.04	0.56
1:A:198:VAL:HG23	1:A:297:LEU:O	2.05	0.56
1:A:372:LEU:HB2	1:A:439:VAL:HG12	1.85	0.56
1:A:475:LEU:HD12	1:A:595:ILE:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:HD11	1:A:299:LEU:HD22	1.86	0.56
1:A:549:GLU:HB2	1:A:588:LEU:CD1	2.36	0.56
1:A:505:THR:HG21	1:A:507:ALA:HB2	1.88	0.56
1:A:198:VAL:HG11	1:A:202:VAL:HB	1.88	0.56
1:A:560:ASN:HB3	1:A:563:THR:OG1	2.06	0.55
1:A:572:GLU:CB	1:A:578:ARG:H	2.02	0.55
1:A:263:THR:HG21	1:A:444:ASP:HA	1.88	0.55
1:A:370:LEU:HD23	1:A:397:TYR:CE2	2.42	0.55
1:A:155:LEU:HB2	1:A:278:LEU:HD12	1.87	0.55
1:A:542:ARG:HH21	1:A:603:PRO:HD3	1.71	0.55
1:A:465:LEU:HD13	1:A:601:LEU:HD11	1.88	0.55
1:A:253:TYR:O	1:A:253:TYR:CD1	2.60	0.54
1:A:427:ILE:HD11	1:A:431:ILE:HG13	1.89	0.54
1:A:293:TYR:CZ	1:A:295:GLY:HA3	2.42	0.54
1:A:539:LEU:O	1:A:541:LEU:HD22	2.08	0.54
1:A:194:TYR:HB2	1:A:209:ILE:HD11	1.90	0.54
1:A:511:SER:HA	1:A:516:TRP:CZ2	2.43	0.54
1:A:173:HIS:HD2	1:A:175:MET:HB3	1.72	0.54
1:A:122:VAL:CG2	1:A:125:VAL:HB	2.37	0.53
1:A:475:LEU:HD23	1:A:498:VAL:CB	2.36	0.53
1:A:547:PHE:CZ	1:A:583:THR:CG2	2.92	0.53
1:A:498:VAL:HG11	1:A:579:VAL:CG2	2.38	0.53
1:A:559:TYR:HD2	1:A:584:TYR:HA	1.74	0.53
1:A:174:ILE:O	1:A:178:GLU:N	2.33	0.53
1:A:222:VAL:HG12	1:A:277:MET:CE	2.39	0.53
1:A:198:VAL:HG22	1:A:297:LEU:HA	1.91	0.52
1:A:146:THR:O	1:A:147:ILE:HD13	2.09	0.52
1:A:138:LEU:HB3	1:A:166:LEU:CD1	2.40	0.52
1:A:463:SER:O	1:A:519:VAL:HG13	2.10	0.52
1:A:545:LEU:HD11	1:A:597:ALA:HB1	1.92	0.52
1:A:542:ARG:HG3	1:A:602:ALA:HB2	1.92	0.51
1:A:568:GLN:HE21	1:A:570:LEU:HD21	1.73	0.51
1:A:236:VAL:HG12	1:A:240:ILE:HG13	1.93	0.51
1:A:349:PHE:CZ	1:A:400:PRO:HD3	2.45	0.51
1:A:222:VAL:HG12	1:A:277:MET:HE3	1.92	0.51
1:A:501:VAL:HG22	1:A:508:GLN:HB3	1.92	0.51
1:A:494:VAL:CA	1:A:579:VAL:O	2.54	0.51
1:A:373:PHE:CD1	1:A:438:VAL:HG22	2.45	0.51
1:A:169:GLY:HA2	1:A:323:TYR:CE2	2.46	0.51
1:A:514:LEU:HD23	1:A:515:ASP:N	2.26	0.51
1:A:559:TYR:HA	1:A:584:TYR:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:VAL:HG22	1:A:305:GLU:HB3	1.92	0.50
1:A:570:LEU:C	1:A:571:ILE:HG13	2.31	0.50
1:A:268:GLU:O	1:A:272:THR:HG22	2.11	0.50
1:A:173:HIS:CD2	1:A:175:MET:HB3	2.46	0.50
1:A:278:LEU:C	1:A:278:LEU:HD13	2.32	0.50
1:A:541:LEU:CD2	1:A:568:GLN:HA	2.42	0.50
1:A:138:LEU:HB3	1:A:166:LEU:HD13	1.93	0.49
1:A:604:HIS:O	1:A:605:SER:HB2	2.11	0.49
1:A:179:ALA:HB2	1:A:308:PHE:CZ	2.47	0.49
1:A:384:PRO:HD2	1:A:387:LEU:CD1	2.37	0.49
1:A:481:ASP:OD1	1:A:482:GLN:N	2.44	0.49
1:A:179:ALA:HA	1:A:308:PHE:CE2	2.47	0.49
1:A:246:ILE:HG21	1:A:251:LEU:HD11	1.93	0.49
1:A:183:ALA:O	1:A:261:VAL:HG23	2.12	0.49
1:A:480:TYR:OH	1:A:491:PRO:HB3	2.13	0.49
1:A:251:LEU:N	1:A:251:LEU:HD12	2.28	0.49
1:A:299:LEU:HD23	1:A:299:LEU:N	2.28	0.49
1:A:246:ILE:CG2	1:A:251:LEU:HD11	2.43	0.48
1:A:210:SER:HB2	1:A:212:TRP:CH2	2.48	0.48
1:A:172:THR:CG2	1:A:173:HIS:N	2.76	0.48
1:A:185:TYR:CE1	1:A:259:ARG:HB2	2.49	0.48
1:A:390:SER:HB3	1:A:395:LEU:O	2.14	0.48
1:A:401:VAL:HG12	1:A:402:VAL:N	2.29	0.47
1:A:369:ALA:HB1	1:A:441:GLN:O	2.14	0.47
1:A:529:ILE:HG22	1:A:529:ILE:O	2.14	0.47
1:A:536:PHE:CD2	1:A:571:ILE:O	2.68	0.47
1:A:139:SER:HB2	1:A:299:LEU:HD12	1.96	0.47
1:A:541:LEU:HD21	1:A:569:ILE:HG13	1.96	0.47
1:A:293:TYR:CD2	1:A:293:TYR:O	2.68	0.47
1:A:542:ARG:HH21	1:A:603:PRO:CD	2.27	0.47
1:A:531:GLN:O	1:A:532:TYR:C	2.52	0.47
1:A:585:THR:HG22	1:A:587:ASN:OD1	2.16	0.46
1:A:524:ARG:HH11	1:A:604:HIS:HD2	1.64	0.46
1:A:476:THR:HG22	1:A:476:THR:O	2.15	0.46
1:A:122:VAL:O	1:A:122:VAL:HG23	2.15	0.46
1:A:412:LEU:HA	1:A:412:LEU:HD12	1.79	0.46
1:A:198:VAL:HG23	1:A:297:LEU:HA	1.96	0.46
1:A:548:TRP:HD1	1:A:549:GLU:O	1.99	0.45
1:A:225:ASN:C	1:A:228:THR:HG22	2.37	0.45
1:A:258:TRP:C	1:A:259:ARG:HD3	2.35	0.45
1:A:263:THR:CG2	1:A:444:ASP:HA	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:THR:O	1:A:289:THR:HG22	2.14	0.45
1:A:329:HIS:O	1:A:433:LEU:N	2.44	0.45
1:A:174:ILE:H	1:A:174:ILE:CD1	2.10	0.45
1:A:536:PHE:HA	1:A:571:ILE:O	2.16	0.45
1:A:236:VAL:HG12	1:A:240:ILE:CG1	2.46	0.45
1:A:498:VAL:HG13	1:A:511:SER:OG	2.17	0.45
1:A:179:ALA:CA	1:A:308:PHE:CE2	3.00	0.45
1:A:210:SER:CB	1:A:212:TRP:CZ3	3.00	0.45
1:A:547:PHE:CE1	1:A:556:GLY:HA3	2.52	0.45
1:A:531:GLN:OE1	1:A:531:GLN:HA	2.17	0.45
1:A:293:TYR:CE2	1:A:295:GLY:C	2.90	0.45
1:A:309:ARG:HB3	1:A:310:ASN:H	1.62	0.44
1:A:491:PRO:HD2	1:A:583:THR:O	2.17	0.44
1:A:548:TRP:CD1	1:A:549:GLU:O	2.70	0.44
1:A:250:ARG:HA	1:A:250:ARG:HD3	1.68	0.44
1:A:547:PHE:CZ	1:A:583:THR:HG23	2.52	0.44
1:A:240:ILE:O	1:A:240:ILE:HG13	2.17	0.44
1:A:184:GLN:HB2	1:A:309:ARG:CB	2.47	0.44
1:A:464:VAL:O	1:A:464:VAL:HG13	2.18	0.44
1:A:536:PHE:HB2	1:A:570:LEU:HD12	2.00	0.44
1:A:193:ARG:NH1	1:A:243:GLU:OE2	2.47	0.43
1:A:311:LEU:HG	1:A:313:PRO:HD3	2.01	0.43
1:A:258:TRP:CZ3	1:A:309:ARG:HD2	2.54	0.43
1:A:375:LEU:CD2	1:A:433:LEU:HD22	2.48	0.43
1:A:231:ASP:OD2	1:A:250:ARG:NH1	2.50	0.43
1:A:181:ASN:ND2	1:A:314:GLY:H	2.14	0.43
1:A:254:ARG:NH2	1:A:269:GLU:HB3	2.33	0.43
1:A:476:THR:CG2	1:A:476:THR:O	2.66	0.43
1:A:167:GLN:HB2	1:A:171:ASN:ND2	2.33	0.43
1:A:461:PRO:C	1:A:464:VAL:HG12	2.37	0.43
1:A:515:ASP:O	1:A:515:ASP:CG	2.57	0.43
1:A:188:VAL:CG2	1:A:305:GLU:HB3	2.49	0.43
1:A:341:LEU:HD12	1:A:342:THR:H	1.81	0.43
1:A:157:ALA:HB2	1:A:277:MET:HG3	2.01	0.43
1:A:374:ASN:HB2	1:A:437:ARG:HB3	2.01	0.43
1:A:161:SER:O	1:A:164:LEU:HB2	2.18	0.43
1:A:222:VAL:CG1	1:A:277:MET:HE3	2.48	0.43
1:A:450:ASP:O	1:A:452:PRO:HD3	2.19	0.43
1:A:450:ASP:C	1:A:452:PRO:HD3	2.40	0.43
1:A:549:GLU:OE1	1:A:554:LYS:HD2	2.19	0.42
1:A:331:LEU:HB2	1:A:431:ILE:HB	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:O	1:A:173:HIS:HE1	2.02	0.42
1:A:493:TYR:O	1:A:580:CYS:CA	2.58	0.42
1:A:146:THR:O	1:A:146:THR:HG22	2.20	0.42
1:A:548:TRP:CE2	1:A:596:SER:HB2	2.54	0.42
1:A:179:ALA:O	1:A:180:SER:C	2.57	0.42
1:A:539:LEU:HD12	1:A:601:LEU:HD21	2.02	0.42
1:A:541:LEU:HD13	1:A:601:LEU:HD23	2.02	0.42
1:A:137:ASN:C	1:A:138:LEU:HD13	2.40	0.42
1:A:188:VAL:HA	1:A:252:HIS:HE1	1.84	0.42
1:A:167:GLN:HB2	1:A:171:ASN:HD22	1.84	0.42
1:A:251:LEU:N	1:A:251:LEU:CD1	2.83	0.42
1:A:253:TYR:CE1	1:A:254:ARG:HB2	2.55	0.42
1:A:195:ARG:HA	1:A:196:PRO:HD3	1.88	0.42
1:A:375:LEU:CD1	1:A:375:LEU:H	2.08	0.42
1:A:472:TRP:C	1:A:473:LEU:HD12	2.41	0.41
1:A:433:LEU:O	1:A:434:GLY:O	2.39	0.41
1:A:521:LEU:HD12	1:A:604:HIS:CB	2.41	0.41
1:A:475:LEU:HD23	1:A:498:VAL:CG2	2.51	0.41
1:A:224:MET:O	1:A:228:THR:HG22	2.20	0.41
1:A:314:GLY:O	1:A:315:ASN:C	2.57	0.41
1:A:413:TYR:CD2	1:A:419:ALA:HA	2.56	0.41
1:A:211:PHE:HB3	1:A:232:VAL:CG1	2.51	0.41
1:A:192:ILE:HG22	1:A:300:LEU:HD22	2.03	0.41
1:A:253:TYR:O	1:A:253:TYR:HD1	2.04	0.41
1:A:372:LEU:HD22	1:A:394:GLN:O	2.21	0.41
1:A:155:LEU:HD23	1:A:155:LEU:N	2.36	0.41
1:A:259:ARG:HD3	1:A:259:ARG:HA	1.82	0.41
1:A:505:THR:CG2	1:A:507:ALA:HB2	2.50	0.41
1:A:187:VAL:HG22	1:A:306:LEU:HD22	2.03	0.41
1:A:351:LYS:O	1:A:448:GLU:HG3	2.22	0.40
1:A:411:LYS:HD3	1:A:413:TYR:OH	2.22	0.40
1:A:197:LEU:HG	1:A:298:GLY:HA2	2.02	0.40
1:A:218:THR:HG21	1:A:395:LEU:HB3	2.03	0.40
1:A:350:MET:CE	1:A:400:PRO:HB2	2.52	0.40
1:A:291:THR:HG22	1:A:292:PRO:CD	2.52	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	456/504 (90%)	418 (92%)	37 (8%)	1 (0%)	52	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLY

### 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	400/424 (94%)	363 (91%)	37 (9%)	11	45

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	THR
1	A	132	LEU
1	A	138	LEU
1	A	155	LEU
1	A	161	SER
1	A	174	ILE
1	A	178	GLU
1	A	215	THR
1	A	236	VAL
1	A	248	SER

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Mol	Chain	Res	Type
1	A	253	TYR
1	A	270	GLU
1	A	294	THR
1	A	299	LEU
1	A	315	ASN
1	A	326	SER
1	A	344	THR
1	A	374	ASN
1	A	375	LEU
1	A	390	SER
1	A	394	GLN
1	A	395	LEU
1	A	414	THR
1	A	432	ASP
1	A	436	SER
1	A	461	PRO
1	A	490	ASN
1	A	498	VAL
1	A	515	ASP
1	A	520	THR
1	A	527	THR
1	A	529	ILE
1	A	553	THR
1	A	567	ASP
1	A	580	CYS
1	A	583	THR
1	A	587	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	152	ASN
1	A	171	ASN
1	A	173	HIS
1	A	181	ASN
1	A	252	HIS
1	A	315	ASN
1	A	374	ASN
1	A	405	ASN
1	A	418	ASN
1	A	420	GLN

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Mol	Chain	Res	Type
1	A	447	HIS
1	A	449	GLN
1	A	490	ASN
1	A	568	GLN
1	A	604	HIS

### 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 [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	468/504 (92%)	0.12	21 (4%) 37 29	40, 69, 128, 137	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	588	LEU	4.2
1	A	533	SER	4.0
1	A	493	TYR	4.0
1	A	494	VAL	3.3
1	A	119	THR	3.2
1	A	582	SER	3.0
1	A	579	VAL	2.9
1	A	479	GLU	2.9
1	A	468	ASN	2.5
1	A	126	ASP	2.5
1	A	560	ASN	2.5
1	A	585	THR	2.2
1	A	242	SER	2.2
1	A	561	TYR	2.2
1	A	489	THR	2.1
1	A	581	ILE	2.1
1	A	534	LYS	2.1
1	A	542	ARG	2.0
1	A	587	ASN	2.0
1	A	564	THR	2.0
1	A	580	CYS	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.