



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:08 PM UTC

PDB ID : 3HAG / pdb_00003hag
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

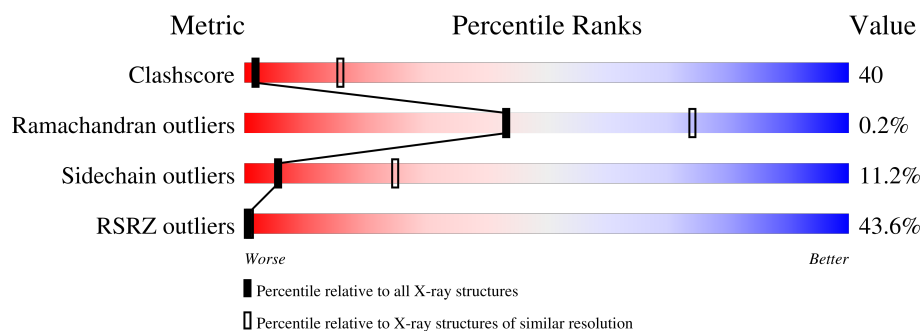
1 Overall quality at a glance

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	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	241.09Å 241.09Å 519.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.50) 94.5 (50.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.277 , 0.286 0.289 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 17.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.27	EDS
Total number of atoms	3589	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.88	8/3663 (0.2%)	1.34	48/5005 (1.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	ASP	N-CA	-8.47	1.35	1.46
1	A	123	PRO	C-N	-7.67	1.23	1.33
1	A	144	THR	C-N	6.38	1.41	1.33
1	A	531	GLN	C-N	-5.29	1.27	1.33
1	A	532	TYR	CA-C	5.24	1.60	1.52
1	A	143	LEU	C-N	5.15	1.40	1.33
1	A	396	PHE	N-CA	5.08	1.52	1.46
1	A	513	SER	C-N	-5.02	1.26	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ASP	N-CA-C	12.27	125.83	111.11
1	A	532	TYR	N-CA-C	9.54	127.11	111.37
1	A	355	PHE	N-CA-C	8.60	122.77	109.96
1	A	531	GLN	N-CA-C	-8.56	95.72	109.76
1	A	450	ASP	N-CA-C	7.35	122.08	113.18
1	A	514	LEU	N-CA-CB	-7.31	99.34	110.45
1	A	444	ASP	CA-CB-CG	6.98	119.58	112.60
1	A	127	SER	N-CA-C	6.92	120.61	108.56
1	A	506	GLY	N-CA-C	-6.78	105.70	114.85
1	A	503	VAL	N-CA-C	6.73	116.88	110.42
1	A	514	LEU	N-CA-C	6.68	119.57	110.55
1	A	391	ALA	N-CA-C	-6.67	107.02	114.62
1	A	151	THR	N-CA-C	6.55	119.69	111.24
1	A	294	THR	CB-CA-C	-6.54	101.48	112.00
1	A	370	LEU	N-CA-C	-6.51	100.20	109.96
1	A	531	GLN	CA-C-N	-6.50	111.07	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	531	GLN	C-N-CA	-6.50	111.07	120.82
1	A	334	GLY	CA-C-N	6.49	127.96	119.84
1	A	334	GLY	C-N-CA	6.49	127.96	119.84
1	A	310	ASN	N-CA-C	6.47	119.15	109.25
1	A	233	ARG	N-CA-C	6.35	119.76	109.40
1	A	513	SER	N-CA-C	6.35	120.23	112.23
1	A	489	THR	CA-C-N	-6.27	112.89	122.42
1	A	489	THR	C-N-CA	-6.27	112.89	122.42
1	A	141	SER	N-CA-C	-6.11	101.22	110.39
1	A	481	ASP	N-CA-C	-5.92	101.24	110.42
1	A	312	THR	CA-C-N	5.85	127.16	119.84
1	A	312	THR	C-N-CA	5.85	127.16	119.84
1	A	200	SER	N-CA-C	5.78	118.33	111.33
1	A	479	GLU	N-CA-C	5.78	117.92	108.55
1	A	494	VAL	CA-C-N	-5.73	114.35	122.94
1	A	494	VAL	C-N-CA	-5.73	114.35	122.94
1	A	327	ALA	N-CA-C	5.60	115.51	108.45
1	A	176	ALA	N-CA-C	-5.54	104.10	111.24
1	A	212	TRP	CA-C-N	5.49	125.01	119.19
1	A	212	TRP	C-N-CA	5.49	125.01	119.19
1	A	293	TYR	N-CA-C	5.47	117.64	108.23
1	A	558	PRO	CB-CA-C	5.32	120.33	111.56
1	A	124	ASP	CB-CA-C	5.30	120.18	109.68
1	A	124	ASP	N-CA-C	-5.29	99.71	108.75
1	A	164	LEU	CA-C-N	5.19	126.33	119.84
1	A	164	LEU	C-N-CA	5.19	126.33	119.84
1	A	392	GLY	N-CA-C	-5.11	101.06	113.18
1	A	580	CYS	N-CA-C	5.11	116.70	108.32
1	A	197	LEU	N-CA-C	-5.07	107.07	114.12
1	A	223	ASP	N-CA-C	-5.05	103.48	110.35
1	A	550	ALA	N-CA-C	5.04	118.19	111.75
1	A	350	MET	N-CA-C	5.03	117.66	111.82

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	282	0
All	All	3589	0	3539	282	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 40.

All (282) 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:HG22	1:A:586:THR:O	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:O	1:A:294:THR:OG1	1.73	0.99
1:A:586:THR:O	1:A:586:THR:CG2	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:HD13	1:A:174:ILE:H	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:475:LEU:HD23	1:A:498:VAL:HB	1.62	0.82
1:A:572:GLU:HB3	1:A:578:ARG:N	1.94	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:254:ARG:HH12	1:A:269:GLU:CD	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:254:ARG:NH1	1:A:269:GLU:CD	2.44	0.75
1:A:568:GLN:NE2	1:A:570:LEU:HD21	2.00	0.75
1:A:516:TRP:HA	1:A:519:VAL:HG23	1.70	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: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:254:ARG:NH1	1:A:269:GLU:CG	2.48	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:253:TYR:CD1	1:A:253:TYR:C	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:TYR:CG	1:A:308:PHE:HB3	2.31	0.64
1:A:122:VAL:HG21	1:A:125:VAL:HB	1.80	0.64
1:A:364:VAL:HG12	1:A:401:VAL:HG22	1.79	0.64
1:A:233:ARG:O	1:A:233:ARG:HG2	1.96	0.63
1:A:222:VAL:HG12	1:A:277:MET:HE1	1.79	0.63
1:A:511:SER:HA	1:A:516:TRP:HZ2	1.64	0.63
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:432:ASP:OD1	1:A:432:ASP:C	2.41	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:146:THR:C	1:A:147:ILE:HD13	2.25	0.61
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: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:218:THR:CG2	1:A:390:SER:O	2.49	0.59
1:A:521:LEU:CD1	1:A:604:HIS:HB2	2.32	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:350:MET:HE3	1:A:400:PRO:HB2	1.85	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: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:N	1:A:473:LEU:HD12	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:VAL:CG1	1:A:202:VAL:HB	2.34	0.56
1:A:201:ALA:HB2	1:A:288:TYR:CE1	2.39	0.56
1:A:198:VAL:HG23	1:A:297:LEU:O	2.05	0.56
1:A:557:TYR:O	1:A:583:THR:HA	2.04	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
1:A:197:LEU:HD11	1:A:299:LEU:HD22	1.86	0.56
1:A:198:VAL:HG11	1:A:202:VAL:HB	1.88	0.56
1:A:505:THR:HG21	1:A:507:ALA:HB2	1.88	0.56
1:A:549:GLU:HB2	1:A:588:LEU:CD1	2.36	0.56
1:A:560:ASN:HB3	1:A:563:THR:OG1	2.06	0.55
1:A:263:THR:HG21	1:A:444:ASP:HA	1.88	0.55
1:A:572:GLU:CB	1:A:578:ARG:H	2.02	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:278:LEU:HD13	1:A:278:LEU:C	2.32	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:CD1	1:A:253:TYR:O	2.60	0.54
1:A:427:ILE:HD11	1:A:431:ILE:HG13	1.89	0.54
1:A:570:LEU:C	1:A:571:ILE:HG13	2.31	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:173:HIS:HD2	1:A:175:MET:HB3	1.72	0.54
1:A:511:SER:HA	1:A:516:TRP:CZ2	2.43	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: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:222:VAL:HG12	1:A:277:MET:CE	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:GLN:HE21	1:A:570:LEU:HD21	1.73	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:268:GLU:HA	1:A:443:TYR:HH	1.75	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:531:GLN:O	1:A:532:TYR:C	2.52	0.50
1:A:188:VAL:HG22	1:A:305:GLU:HB3	1.92	0.50
1:A:559:TYR:HA	1:A:584:TYR:HB2	1.93	0.50
1:A:225:ASN:C	1:A:228:THR:HG22	2.37	0.50
1:A:173:HIS:CD2	1:A:175:MET:HB3	2.46	0.50
1:A:268:GLU:O	1:A:272:THR:HG22	2.11	0.50
1:A:258:TRP:C	1:A:259:ARG:HD3	2.35	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: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:604:HIS:O	1:A:605:SER:HB2	2.11	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:293:TYR:CE2	1:A:295:GLY:C	2.90	0.49
1:A:480:TYR:OH	1:A:491:PRO:HB3	2.13	0.49
1:A:251:LEU:HD12	1:A:251:LEU:N	2.28	0.49
1:A:299:LEU:N	1:A:299:LEU:HD23	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:515:ASP:O	1:A:515:ASP:CG	2.57	0.48
1:A:390:SER:HB3	1:A:395:LEU:O	2.14	0.48
1:A:461:PRO:C	1:A:464:VAL:HG12	2.37	0.48
1:A:369:ALA:HB1	1:A:441:GLN:O	2.14	0.47
1:A:450:ASP:C	1:A:452:PRO:HD3	2.40	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:293:TYR:O	1:A:293:TYR:CD2	2.68	0.47
1:A:541:LEU:HD21	1:A:569:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:C	1:A:138:LEU:HD13	2.40	0.47
1:A:179:ALA:O	1:A:180:SER:C	2.57	0.47
1:A:542:ARG:HH21	1:A:603:PRO:CD	2.27	0.47
1:A:401:VAL:HG12	1:A:402:VAL:N	2.29	0.47
1:A:524:ARG:HH11	1:A:604:HIS:HD2	1.64	0.46
1:A:585:THR:HG22	1:A:587:ASN:OD1	2.16	0.46
1:A:476:THR:O	1:A:476:THR:HG22	2.15	0.46
1:A:122:VAL:O	1:A:122:VAL:HG23	2.15	0.46
1:A:412:LEU:HD12	1:A:412:LEU:HA	1.79	0.46
1:A:472:TRP:C	1:A:473:LEU:HD12	2.41	0.46
1:A:314:GLY:O	1:A:315:ASN:C	2.57	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:263:THR:CG2	1:A:444:ASP:HA	2.45	0.45
1:A:289:THR:HG22	1:A:289:THR:O	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:236:VAL:HG12	1:A:240:ILE:CG1	2.46	0.45
1:A:536:PHE:HA	1:A:571:ILE:O	2.16	0.45
1:A:179:ALA:CA	1:A:308:PHE:CE2	3.00	0.45
1:A:498:VAL:HG13	1:A:511:SER:OG	2.17	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: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:HG13	1:A:240:ILE:O	2.17	0.44
1:A:385:THR:O	1:A:386:GLU:C	2.61	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:405:ASN:O	1:A:406:GLY:C	2.60	0.43
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:231:ASP:OD2	1:A:250:ARG:NH1	2.50	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:557:TYR:HD1	1:A:587:ASN:CG	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASN:ND2	1:A:314:GLY:H	2.14	0.43
1:A:167:GLN:HB2	1:A:171:ASN:ND2	2.33	0.43
1:A:254:ARG:NH2	1:A:269:GLU:HB3	2.33	0.43
1:A:476:THR:O	1:A:476:THR:CG2	2.66	0.43
1:A:188:VAL:CG2	1:A:305:GLU:HB3	2.49	0.43
1:A:157:ALA:HB2	1:A:277:MET:HG3	2.01	0.43
1:A:341:LEU:HD12	1:A:342:THR:H	1.81	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:450:ASP:O	1:A:452:PRO:HD3	2.19	0.43
1:A:453:THR:O	1:A:454:PRO:C	2.60	0.43
1:A:331:LEU:HB2	1:A:431:ILE:HB	1.99	0.42
1:A:549:GLU:OE1	1:A:554:LYS:HD2	2.19	0.42
1:A:164:LEU:O	1:A:173:HIS:HE1	2.02	0.42
1:A:146:THR:O	1:A:146:THR:HG22	2.20	0.42
1:A:493:TYR:O	1:A:580:CYS:CA	2.58	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:548:TRP:CE2	1:A:596:SER:HB2	2.54	0.42
1:A:167:GLN:HB2	1:A:171:ASN:HD22	1.84	0.42
1:A:188:VAL:HA	1:A:252:HIS:HE1	1.84	0.42
1:A:251:LEU:N	1:A:251:LEU:CD1	2.83	0.42
1:A:195:ARG:HA	1:A:196:PRO:HD3	1.88	0.42
1:A:253:TYR:CE1	1:A:254:ARG:HB2	2.55	0.42
1:A:375:LEU:H	1:A:375:LEU:CD1	2.08	0.42
1:A:492:MET:HE2	1:A:580:CYS:HB2	2.02	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:211:PHE:HB3	1:A:232:VAL:CG1	2.51	0.41
1:A:224:MET:O	1:A:228:THR:HG22	2.20	0.41
1:A:413:TYR:CD2	1:A:419:ALA:HA	2.56	0.41
1:A:475:LEU:HD23	1:A:498:VAL:CG2	2.51	0.41
1:A:192:ILE:HG22	1:A:300:LEU:HD22	2.03	0.41
1:A:155:LEU:HD23	1:A:155:LEU:N	2.36	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:187:VAL:HG22	1:A:306:LEU:HD22	2.03	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:197:LEU:HG	1:A:298:GLY:HA2	2.02	0.40
1:A:351:LYS:O	1:A:448:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LYS:HD3	1:A:413:TYR:OH	2.22	0.40
1:A:218:THR:HG21	1:A:395:LEU:HB3	2.03	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%)	43 74

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%)	355 (89%)	45 (11%)	5 25

All (45) 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	139	SER
1	A	155	LEU
1	A	161	SER
1	A	174	ILE
1	A	178	GLU
1	A	210	SER
1	A	215	THR
1	A	232	VAL
1	A	236	VAL
1	A	243	GLU
1	A	248	SER
1	A	270	GLU
1	A	272	THR
1	A	294	THR
1	A	299	LEU
1	A	326	SER
1	A	344	THR
1	A	374	ASN
1	A	375	LEU
1	A	386	GLU
1	A	390	SER
1	A	394	GLN
1	A	395	LEU
1	A	412	LEU
1	A	414	THR
1	A	432	ASP
1	A	435	GLU
1	A	436	SER
1	A	439	VAL
1	A	444	ASP
1	A	473	LEU
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	581	ILE
1	A	583	THR

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Mol	Chain	Res	Type
1	A	586	THR
1	A	587	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	137	ASN
1	A	152	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
1	A	449	GLN
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 oligosaccharides 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, 95th 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 ²)	Q<0.9
1	A	468/504 (92%)	2.07	204 (43%) 0 1	40, 69, 128, 137	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	ASP	7.3
1	A	481	ASP	7.3
1	A	605	SER	7.3
1	A	449	GLN	6.6
1	A	127	SER	6.2
1	A	496	ASP	5.9
1	A	512	ARG	5.7
1	A	489	THR	5.5
1	A	577	HIS	5.5
1	A	556	GLY	5.5
1	A	458	PRO	5.4
1	A	513	SER	5.3
1	A	482	GLN	5.2
1	A	480	TYR	5.2
1	A	525	PRO	5.2
1	A	562	ASN	5.0
1	A	363	GLU	4.9
1	A	530	GLN	4.9
1	A	560	ASN	4.9
1	A	564	THR	4.9
1	A	532	TYR	4.8
1	A	567	ASP	4.8
1	A	533	SER	4.8
1	A	491	PRO	4.6
1	A	604	HIS	4.5
1	A	551	GLY	4.4
1	A	583	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	565	ALA	4.3
1	A	568	GLN	4.2
1	A	146	THR	4.2
1	A	478	ALA	4.2
1	A	572	GLU	4.2
1	A	128	ARG	4.2
1	A	168	ASP	4.1
1	A	124	ASP	4.1
1	A	573	ASN	4.1
1	A	559	TYR	4.0
1	A	534	LYS	4.0
1	A	404	ALA	3.9
1	A	524	ARG	3.8
1	A	459	SER	3.8
1	A	356	THR	3.8
1	A	468	ASN	3.7
1	A	561	TYR	3.7
1	A	364	VAL	3.7
1	A	550	ALA	3.6
1	A	490	ASN	3.6
1	A	319	ARG	3.6
1	A	145	SER	3.6
1	A	479	GLU	3.6
1	A	240	ILE	3.6
1	A	421	GLN	3.5
1	A	531	GLN	3.5
1	A	457	ALA	3.5
1	A	563	THR	3.5
1	A	118	ASP	3.4
1	A	130	ALA	3.4
1	A	265	GLY	3.4
1	A	150	GLY	3.4
1	A	554	LYS	3.4
1	A	389	SER	3.4
1	A	257	GLY	3.4
1	A	493	TYR	3.4
1	A	466	ARG	3.4
1	A	241	ALA	3.4
1	A	288	TYR	3.4
1	A	351	LYS	3.3
1	A	452	PRO	3.3
1	A	314	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	282	GLY	3.2
1	A	522	ASP	3.2
1	A	467	ALA	3.2
1	A	497	THR	3.2
1	A	498	VAL	3.2
1	A	242	SER	3.2
1	A	290	ASN	3.2
1	A	584	TYR	3.2
1	A	324	SER	3.1
1	A	121	PRO	3.1
1	A	477	ALA	3.1
1	A	492	MET	3.1
1	A	237	GLN	3.1
1	A	129	GLY	3.1
1	A	504	ALA	3.0
1	A	547	PHE	3.0
1	A	508	GLN	3.0
1	A	495	SER	3.0
1	A	566	SER	3.0
1	A	190	ALA	3.0
1	A	526	LEU	3.0
1	A	578	ARG	3.0
1	A	519	VAL	3.0
1	A	501	VAL	3.0
1	A	340	GLU	2.9
1	A	214	GLN	2.9
1	A	518	LYS	2.9
1	A	286	ASN	2.9
1	A	195	ARG	2.9
1	A	407	GLU	2.9
1	A	517	SER	2.9
1	A	543	GLY	2.9
1	A	527	THR	2.9
1	A	125	VAL	2.9
1	A	361	VAL	2.9
1	A	586	THR	2.9
1	A	529	ILE	2.9
1	A	243	GLU	2.9
1	A	542	ARG	2.9
1	A	255	ASN	2.8
1	A	141	SER	2.8
1	A	448	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	555	ALA	2.8
1	A	436	SER	2.8
1	A	510	VAL	2.7
1	A	549	GLU	2.7
1	A	139	SER	2.7
1	A	422	ASP	2.7
1	A	289	THR	2.7
1	A	403	SER	2.7
1	A	541	LEU	2.7
1	A	461	PRO	2.6
1	A	336	ASP	2.6
1	A	270	GLU	2.6
1	A	328	ARG	2.6
1	A	287	SER	2.6
1	A	239	GLY	2.6
1	A	430	ASP	2.6
1	A	320	VAL	2.6
1	A	516	TRP	2.6
1	A	494	VAL	2.6
1	A	354	HIS	2.6
1	A	552	THR	2.6
1	A	475	LEU	2.6
1	A	292	PRO	2.6
1	A	376	ALA	2.6
1	A	603	PRO	2.5
1	A	514	LEU	2.5
1	A	460	ARG	2.5
1	A	268	GLU	2.5
1	A	434	GLY	2.5
1	A	537	PHE	2.5
1	A	472	TRP	2.4
1	A	167	GLN	2.4
1	A	463	SER	2.4
1	A	185	TYR	2.4
1	A	544	LYS	2.4
1	A	305	GLU	2.4
1	A	218	THR	2.4
1	A	515	ASP	2.4
1	A	252	HIS	2.4
1	A	333	ARG	2.4
1	A	428	PRO	2.4
1	A	122	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	238	PRO	2.4
1	A	367	GLY	2.4
1	A	582	SER	2.4
1	A	597	ALA	2.4
1	A	427	ILE	2.3
1	A	279	CYS	2.3
1	A	262	GLU	2.3
1	A	219	PRO	2.3
1	A	408	PRO	2.3
1	A	456	PRO	2.3
1	A	327	ALA	2.3
1	A	557	TYR	2.3
1	A	281	HIS	2.3
1	A	186	ARG	2.3
1	A	332	ARG	2.3
1	A	570	LEU	2.3
1	A	196	PRO	2.3
1	A	377	ASP	2.3
1	A	251	LEU	2.3
1	A	425	ILE	2.3
1	A	362	GLY	2.3
1	A	317	ASN	2.2
1	A	307	GLU	2.2
1	A	366	ARG	2.2
1	A	406	GLY	2.2
1	A	538	VAL	2.2
1	A	206	ALA	2.2
1	A	471	LEU	2.2
1	A	309	ARG	2.2
1	A	329	HIS	2.2
1	A	599	GLY	2.1
1	A	217	THR	2.1
1	A	152	ASN	2.1
1	A	511	SER	2.1
1	A	191	THR	2.1
1	A	216	THR	2.1
1	A	587	ASN	2.1
1	A	284	PRO	2.1
1	A	585	THR	2.1
1	A	189	ARG	2.1
1	A	147	ILE	2.1
1	A	423	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	596	SER	2.1
1	A	450	ASP	2.1
1	A	140	THR	2.1
1	A	536	PHE	2.1
1	A	143	LEU	2.1
1	A	465	LEU	2.1
1	A	509	GLY	2.0
1	A	476	THR	2.0
1	A	173	HIS	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 oligosaccharides 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.