



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 10:24 AM EDT

PDB ID : 2IOQ  
Title : Crystal Structure of full-length HTPG, the Escherichia coli HSP90  
Authors : Shiau, A.K.; Harris, S.F.; Agard, D.A.  
Deposited on : 2006-10-10  
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

<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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

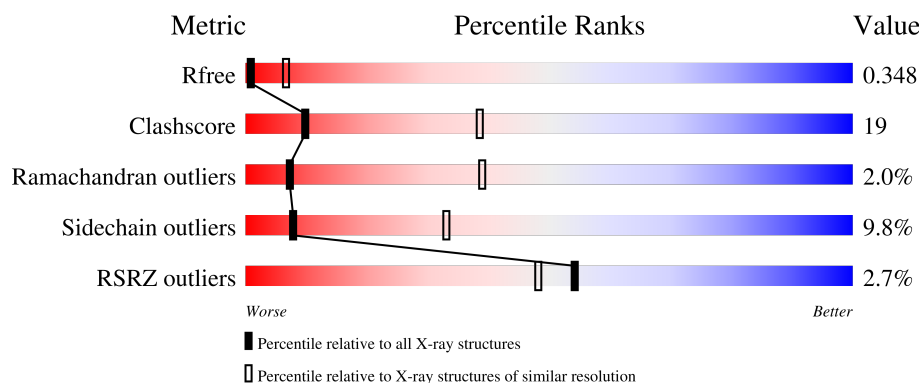
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	624	
1	B	624	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9007 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.

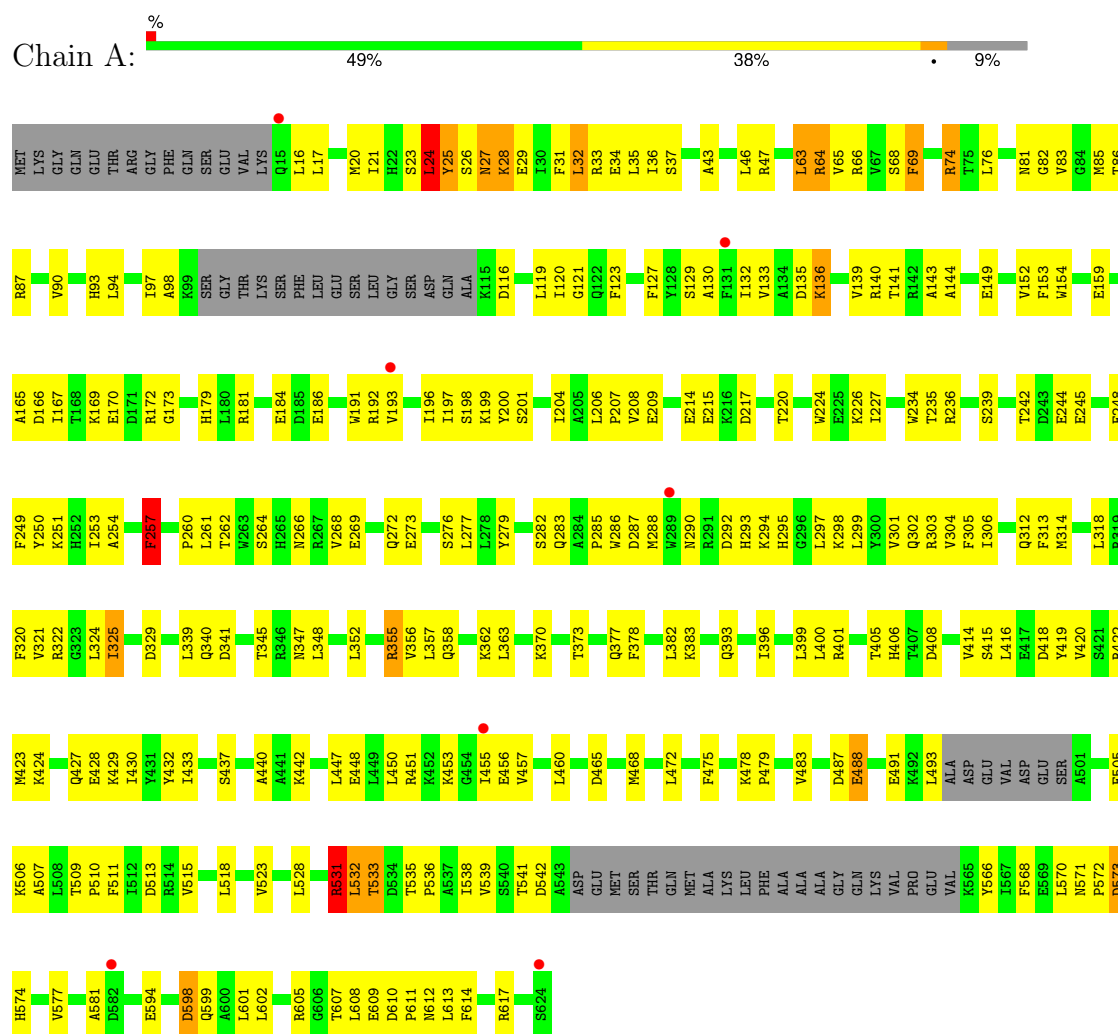
- Molecule 1 is a protein called Chaperone protein htpG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	567	Total	C	N	O	S	0	0	0
			4474	2829	773	862	10			
1	B	577	Total	C	N	O	S	0	0	0
			4533	2865	787	872	9			

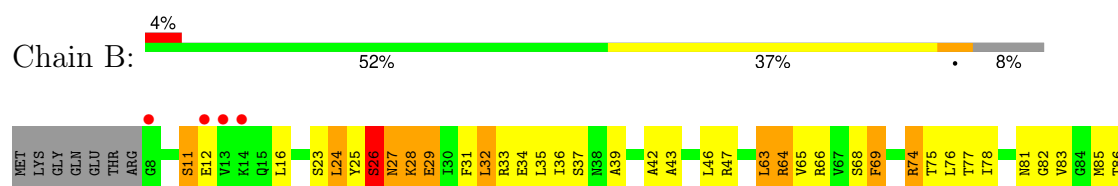
### 3 Residue-property plots [i](#)

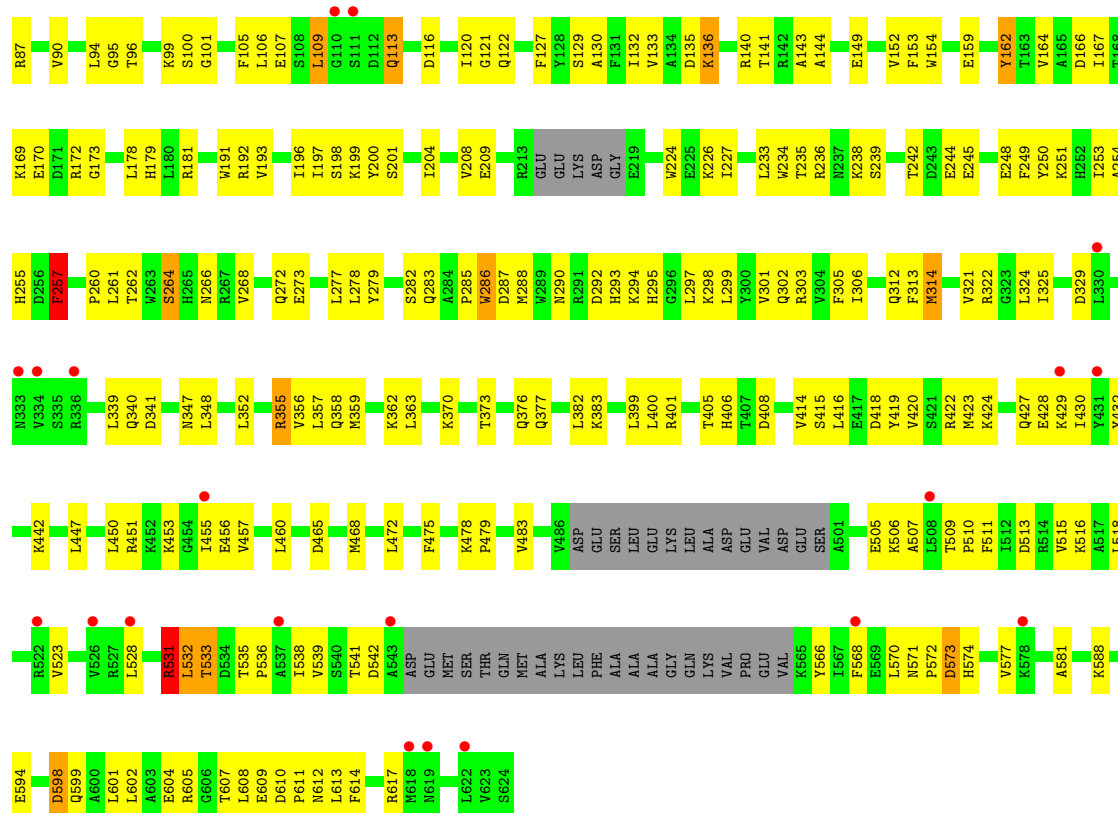
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Chaperone protein htpG



#### • Molecule 1: Chaperone protein htpG





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.12Å 105.12Å 531.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.70 – 3.50 58.28 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (58.70-3.50) 98.8 (58.28-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.329 , 0.370 0.311 , 0.348	Depositor DCC
$R_{free}$ test set	1109 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	124.1	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 81.2	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	0.89	EDS
Total number of atoms	9007	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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

### 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	0.21	0/4556	0.44	1/6165 (0.0%)
1	B	0.22	0/4617	0.43	1/6251 (0.0%)
All	All	0.22	0/9173	0.43	2/12416 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
All	All	0	7

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	28	LYS	N-CA-C	5.66	126.29	111.00
1	B	26	SER	CB-CA-C	-5.03	100.54	110.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	SER	Peptide
1	A	257	PHE	Peptide
1	A	27	ASN	Peptide
1	A	293	HIS	Peptide
1	B	257	PHE	Peptide
1	B	27	ASN	Peptide
1	B	293	HIS	Peptide

## 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	4474	0	4308	167	0
1	B	4533	0	4347	173	0
All	All	9007	0	8655	339	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 19.

All (339) 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:B:153:PHE:HB2	1:B:167:ILE:HD13	1.54	0.89
1:A:528:LEU:HD12	1:A:572:PRO:HG3	1.61	0.81
1:B:528:LEU:HD12	1:B:572:PRO:HG3	1.63	0.80
1:A:294:LYS:HD2	1:A:322:ARG:HH22	1.47	0.79
1:A:215:GLU:HG3	1:A:220:THR:HG23	1.64	0.78
1:A:201:SER:HA	1:A:204:ILE:HD12	1.66	0.78
1:B:294:LYS:HD2	1:B:322:ARG:HH22	1.49	0.78
1:A:24:LEU:HD23	1:A:26:SER:N	2.00	0.77
1:A:153:PHE:HB2	1:A:167:ILE:HD13	1.66	0.76
1:A:90:VAL:HG13	1:A:94:LEU:HD12	1.69	0.75
1:B:460:LEU:HD23	1:B:465:ASP:HB3	1.68	0.74
1:A:460:LEU:HD23	1:A:465:ASP:HB3	1.70	0.74
1:B:11:SER:HA	1:B:286:TRP:NE1	2.03	0.73
1:B:90:VAL:HG13	1:B:94:LEU:HD12	1.71	0.73
1:A:455:ILE:HG22	1:A:456:GLU:H	1.55	0.71
1:B:201:SER:HA	1:B:204:ILE:HD12	1.71	0.71
1:A:249:PHE:O	1:A:253:ILE:HG13	1.91	0.71
1:A:488:GLU:HA	1:A:491:GLU:HB2	1.74	0.70
1:B:455:ILE:HG22	1:B:456:GLU:H	1.55	0.69
1:B:249:PHE:O	1:B:253:ILE:HG13	1.93	0.69
1:A:32:LEU:O	1:A:36:ILE:HG13	1.95	0.67
1:A:242:THR:HG23	1:A:245:GLU:H	1.59	0.67
1:B:32:LEU:O	1:B:36:ILE:HG13	1.94	0.66
1:A:294:LYS:HD2	1:A:322:ARG:NH2	2.12	0.65
1:B:533:THR:HG23	1:B:535:THR:H	1.62	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:GLU:HB3	1:B:617:ARG:NH1	2.12	0.64
1:B:242:THR:HG23	1:B:245:GLU:H	1.63	0.64
1:A:533:THR:HG23	1:A:535:THR:H	1.62	0.63
1:A:594:GLU:HB3	1:A:617:ARG:NH1	2.13	0.63
1:B:294:LYS:HD2	1:B:322:ARG:NH2	2.14	0.62
1:A:250:TYR:HA	1:A:253:ILE:HD11	1.82	0.62
1:A:24:LEU:HD23	1:A:26:SER:H	1.61	0.61
1:B:140:ARG:O	1:B:169:LYS:HE2	2.00	0.61
1:B:248:GLU:HA	1:B:251:LYS:HD2	1.84	0.60
1:A:25:TYR:C	1:A:27:ASN:H	2.05	0.60
1:B:420:VAL:HA	1:B:423:MET:HG3	1.85	0.59
1:B:429:LYS:HG2	1:B:479:PRO:HG2	1.85	0.58
1:A:429:LYS:HG2	1:A:479:PRO:HG2	1.84	0.58
1:B:257:PHE:HD1	1:B:257:PHE:H	1.51	0.58
1:A:370:LYS:O	1:A:373:THR:HB	2.04	0.58
1:A:257:PHE:HD1	1:A:257:PHE:H	1.52	0.58
1:B:136:LYS:NZ	1:B:179:HIS:HB2	2.18	0.57
1:A:405:THR:HG22	1:A:451:ARG:HH21	1.69	0.57
1:A:428:GLU:O	1:A:479:PRO:HD2	2.05	0.57
1:B:405:THR:HG22	1:B:451:ARG:HH21	1.69	0.56
1:A:248:GLU:HA	1:A:251:LYS:HD2	1.86	0.56
1:A:509:THR:OG1	1:A:510:PRO:HD3	2.04	0.56
1:B:370:LYS:O	1:B:373:THR:HB	2.04	0.56
1:B:509:THR:OG1	1:B:510:PRO:HD3	2.04	0.56
1:B:11:SER:HA	1:B:286:TRP:CE2	2.41	0.56
1:B:428:GLU:O	1:B:479:PRO:HD2	2.05	0.56
1:A:144:ALA:HA	1:A:172:ARG:HG3	1.87	0.56
1:B:250:TYR:HA	1:B:253:ILE:HD11	1.88	0.56
1:B:253:ILE:HG22	1:B:298:LYS:NZ	2.21	0.56
1:A:140:ARG:O	1:A:169:LYS:HE2	2.07	0.55
1:A:268:VAL:O	1:A:273:GLU:HA	2.06	0.55
1:B:355:ARG:HG3	1:B:355:ARG:HH11	1.70	0.55
1:A:86:THR:O	1:A:90:VAL:HG23	2.07	0.55
1:B:16:LEU:HD11	1:B:101:GLY:HA3	1.89	0.55
1:B:523:VAL:HG11	1:B:568:PHE:HB2	1.88	0.55
1:A:523:VAL:HG11	1:A:568:PHE:HB2	1.87	0.55
1:A:193:VAL:O	1:A:197:ILE:HG12	2.07	0.55
1:A:420:VAL:HA	1:A:423:MET:HG3	1.88	0.55
1:B:46:LEU:HD22	1:B:82:GLY:O	2.07	0.55
1:A:85:MET:C	1:A:143:ALA:HB2	2.28	0.54
1:A:136:LYS:NZ	1:A:179:HIS:HB2	2.22	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:MET:C	1:B:143:ALA:HB2	2.28	0.54
1:A:64:ARG:HD3	1:A:81:ASN:HD21	1.72	0.54
1:A:24:LEU:C	1:A:26:SER:H	2.10	0.54
1:B:66:ARG:HD3	1:B:224:TRP:CD2	2.43	0.54
1:B:144:ALA:HA	1:B:172:ARG:HG3	1.88	0.54
1:B:172:ARG:HG2	1:B:173:GLY:N	2.23	0.54
1:A:355:ARG:HG3	1:A:355:ARG:HH11	1.73	0.54
1:B:268:VAL:O	1:B:273:GLU:HA	2.07	0.54
1:B:400:LEU:O	1:B:401:ARG:HG2	2.08	0.53
1:B:152:VAL:HG12	1:B:153:PHE:N	2.22	0.53
1:A:192:ARG:O	1:A:196:ILE:HG12	2.09	0.53
1:B:192:ARG:O	1:B:196:ILE:HG12	2.09	0.53
1:A:283:GLN:HA	1:A:377:GLN:OE1	2.09	0.53
1:A:571:ASN:O	1:A:577:VAL:HG21	2.09	0.53
1:B:64:ARG:HD3	1:B:81:ASN:HD21	1.74	0.53
1:B:193:VAL:O	1:B:197:ILE:HG12	2.09	0.53
1:B:312:GLN:HE21	1:B:340:GLN:HB2	1.74	0.53
1:B:506:LYS:O	1:B:510:PRO:CD	2.58	0.52
1:B:566:TYR:OH	1:B:605:ARG:HD3	2.08	0.52
1:A:506:LYS:O	1:A:510:PRO:CD	2.57	0.52
1:A:172:ARG:HG2	1:A:173:GLY:N	2.24	0.52
1:A:533:THR:HG23	1:A:535:THR:N	2.25	0.52
1:B:299:LEU:HD22	1:B:339:LEU:HD11	1.92	0.52
1:A:261:LEU:HG	1:A:282:SER:HA	1.92	0.52
1:B:261:LEU:HG	1:B:282:SER:HA	1.91	0.52
1:B:418:ASP:O	1:B:422:ARG:HG3	2.10	0.52
1:B:352:LEU:O	1:B:356:VAL:HG23	2.10	0.52
1:A:152:VAL:HG12	1:A:153:PHE:N	2.24	0.51
1:B:571:ASN:O	1:B:577:VAL:HG21	2.10	0.51
1:A:93:HIS:O	1:A:97:ILE:HG13	2.10	0.51
1:A:400:LEU:O	1:A:401:ARG:HG2	2.11	0.51
1:B:533:THR:HG23	1:B:535:THR:N	2.25	0.51
1:A:299:LEU:HD22	1:A:339:LEU:HD11	1.92	0.51
1:A:383:LYS:HG2	1:A:468:MET:SD	2.51	0.51
1:A:135:ASP:HB3	1:A:181:ARG:HG2	1.93	0.51
1:A:418:ASP:O	1:A:422:ARG:HG3	2.09	0.51
1:A:566:TYR:OH	1:A:605:ARG:HD3	2.09	0.51
1:A:250:TYR:HB2	1:A:279:TYR:CD2	2.46	0.51
1:B:24:LEU:HG	1:B:25:TYR:N	2.25	0.51
1:B:64:ARG:HG2	1:B:64:ARG:HH11	1.76	0.51
1:B:419:TYR:CE2	1:B:430:ILE:HG23	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ALA:C	1:A:510:PRO:HD2	2.31	0.51
1:B:135:ASP:HB3	1:B:181:ARG:HG2	1.92	0.51
1:B:87:ARG:HH12	1:B:166:ASP:H	1.59	0.50
1:B:86:THR:O	1:B:90:VAL:HG23	2.11	0.50
1:A:66:ARG:HD3	1:A:224:TRP:CD2	2.46	0.50
1:A:236:ARG:HH22	1:A:245:GLU:CD	2.15	0.50
1:B:507:ALA:C	1:B:510:PRO:HD2	2.32	0.50
1:A:352:LEU:O	1:A:356:VAL:HG23	2.11	0.50
1:A:24:LEU:C	1:A:26:SER:N	2.64	0.50
1:A:419:TYR:CE2	1:A:430:ILE:HG23	2.45	0.50
1:B:283:GLN:HA	1:B:377:GLN:OE1	2.11	0.50
1:B:450:LEU:HB3	1:B:455:ILE:HB	1.93	0.50
1:A:87:ARG:HH12	1:A:166:ASP:H	1.59	0.50
1:A:116:ASP:O	1:A:120:ILE:HG13	2.12	0.50
1:B:509:THR:HG1	1:B:510:PRO:HD3	1.75	0.50
1:B:406:HIS:HB2	1:B:456:GLU:OE1	2.11	0.49
1:B:257:PHE:N	1:B:257:PHE:CD1	2.80	0.49
1:A:25:TYR:C	1:A:27:ASN:N	2.66	0.49
1:B:31:PHE:CG	1:B:32:LEU:N	2.80	0.49
1:A:144:ALA:HB2	1:A:172:ARG:HD2	1.94	0.49
1:A:234:TRP:CD2	1:A:324:LEU:HD11	2.46	0.49
1:A:505:GLU:O	1:A:509:THR:HG23	2.12	0.49
1:A:574:HIS:HB3	1:A:577:VAL:HG23	1.95	0.49
1:A:432:TYR:O	1:A:483:VAL:HG22	2.13	0.49
1:B:12:GLU:CB	1:B:105:PHE:HB2	2.43	0.49
1:A:31:PHE:CG	1:A:32:LEU:N	2.81	0.49
1:B:416:LEU:HB3	1:B:475:PHE:CE2	2.47	0.49
1:B:236:ARG:HH22	1:B:245:GLU:CD	2.16	0.49
1:A:139:VAL:HB	1:A:154:TRP:HB3	1.95	0.49
1:A:450:LEU:HB3	1:A:455:ILE:HB	1.94	0.49
1:A:415:SER:H	1:A:418:ASP:HB2	1.78	0.48
1:B:505:GLU:O	1:B:509:THR:HG23	2.12	0.48
1:A:312:GLN:HE21	1:A:340:GLN:HB2	1.78	0.48
1:B:415:SER:H	1:B:418:ASP:HB2	1.78	0.48
1:A:416:LEU:HB3	1:A:475:PHE:CE2	2.48	0.48
1:A:253:ILE:HG22	1:A:298:LYS:NZ	2.28	0.48
1:A:257:PHE:HD1	1:A:257:PHE:N	2.12	0.48
1:B:68:SER:O	1:B:76:LEU:HD12	2.13	0.48
1:A:257:PHE:N	1:A:257:PHE:CD1	2.81	0.48
1:A:448:GLU:HB3	1:A:533:THR:HA	1.95	0.48
1:B:66:ARG:HB3	1:B:224:TRP:CZ3	2.49	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ASN:HB3	1:B:355:ARG:NH2	2.29	0.48
1:A:325:ILE:HD13	1:A:325:ILE:O	2.13	0.48
1:A:357:LEU:HD23	1:A:399:LEU:CD1	2.44	0.48
1:B:234:TRP:CD2	1:B:324:LEU:HD11	2.48	0.48
1:B:574:HIS:HB3	1:B:577:VAL:HG23	1.96	0.48
1:A:46:LEU:HD22	1:A:82:GLY:O	2.13	0.47
1:A:66:ARG:HB3	1:A:224:TRP:CZ3	2.49	0.47
1:A:295:HIS:CD2	1:A:295:HIS:H	2.31	0.47
1:A:541:THR:HG22	1:A:542:ASP:H	1.79	0.47
1:B:144:ALA:HB2	1:B:172:ARG:HD2	1.95	0.47
1:B:355:ARG:HG3	1:B:355:ARG:NH1	2.29	0.47
1:A:262:THR:CG2	1:A:363:LEU:HD22	2.44	0.47
1:A:285:PRO:HD2	1:A:288:MET:HE1	1.95	0.47
1:A:297:LEU:HD12	1:A:313:PHE:HB2	1.95	0.47
1:B:198:SER:C	1:B:200:TYR:H	2.17	0.47
1:B:136:LYS:CE	1:B:179:HIS:HB2	2.44	0.47
1:B:297:LEU:HD12	1:B:313:PHE:HB2	1.95	0.47
1:A:268:VAL:HG12	1:A:272:GLN:O	2.14	0.47
1:B:541:THR:HG22	1:B:542:ASP:H	1.80	0.47
1:B:69:PHE:N	1:B:69:PHE:CD2	2.83	0.47
1:A:25:TYR:O	1:A:26:SER:CB	2.63	0.47
1:B:250:TYR:CD2	1:B:260:PRO:HD3	2.49	0.47
1:B:268:VAL:HG12	1:B:272:GLN:O	2.15	0.47
1:A:17:LEU:O	1:A:21:ILE:HG13	2.15	0.47
1:A:455:ILE:HG22	1:A:456:GLU:N	2.27	0.47
1:B:107:GLU:C	1:B:109:LEU:H	2.18	0.47
1:B:129:SER:O	1:B:132:ILE:HB	2.15	0.47
1:B:250:TYR:HD2	1:B:260:PRO:HD3	1.79	0.47
1:B:295:HIS:H	1:B:295:HIS:CD2	2.32	0.47
1:A:65:VAL:HG13	1:A:208:VAL:HA	1.97	0.47
1:B:242:THR:HG22	1:B:245:GLU:OE1	2.15	0.47
1:B:314:MET:HG3	1:B:321:VAL:HB	1.97	0.47
1:B:357:LEU:HD23	1:B:399:LEU:CD1	2.45	0.47
1:B:511:PHE:O	1:B:515:VAL:HG23	2.15	0.46
1:A:119:LEU:O	1:A:123:PHE:HB2	2.15	0.46
1:A:511:PHE:O	1:A:515:VAL:HG23	2.15	0.46
1:B:116:ASP:O	1:B:120:ILE:HG13	2.15	0.46
1:B:455:ILE:HG22	1:B:456:GLU:N	2.28	0.46
1:A:612:ASN:H	1:A:612:ASN:ND2	2.14	0.46
1:A:136:LYS:CE	1:A:179:HIS:HB2	2.45	0.46
1:B:96:THR:HG21	1:B:116:ASP:OD1	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLU:O	1:A:37:SER:HB3	2.16	0.46
1:A:447:LEU:HD22	1:A:457:VAL:HG11	1.98	0.46
1:A:29:GLU:CD	1:A:29:GLU:H	2.18	0.46
1:B:528:LEU:HD13	1:B:570:LEU:HB2	1.98	0.46
1:A:314:MET:HG3	1:A:321:VAL:HB	1.98	0.46
1:A:406:HIS:HB2	1:A:456:GLU:OE1	2.15	0.46
1:B:250:TYR:HB2	1:B:279:TYR:CD2	2.51	0.46
1:A:528:LEU:HD13	1:A:570:LEU:HB2	1.98	0.45
1:B:83:VAL:O	1:B:143:ALA:HA	2.16	0.45
1:B:288:MET:HB2	1:B:288:MET:HE3	1.78	0.45
1:A:532:LEU:HD12	1:A:573:ASP:OD1	2.16	0.45
1:B:113:GLN:HE21	1:B:113:GLN:HA	1.79	0.45
1:B:612:ASN:ND2	1:B:612:ASN:H	2.13	0.45
1:B:432:TYR:O	1:B:483:VAL:HG22	2.15	0.45
1:B:602:LEU:HB2	1:B:608:LEU:HD21	1.97	0.45
1:A:598:ASP:HA	1:A:601:LEU:HD12	1.98	0.45
1:A:599:GLN:HE21	1:A:614:PHE:HZ	1.64	0.45
1:A:69:PHE:N	1:A:69:PHE:CD2	2.84	0.45
1:B:65:VAL:HG13	1:B:208:VAL:HA	1.99	0.45
1:B:598:ASP:HA	1:B:601:LEU:HD12	1.98	0.45
1:B:24:LEU:C	1:B:26:SER:N	2.70	0.45
1:B:305:PHE:O	1:B:306:ILE:HD13	2.17	0.45
1:A:83:VAL:O	1:A:143:ALA:HA	2.17	0.45
1:B:34:GLU:O	1:B:37:SER:HB3	2.16	0.45
1:B:227:ILE:O	1:B:227:ILE:HG22	2.17	0.45
1:A:266:ASN:HB3	1:A:355:ARG:NH2	2.32	0.45
1:A:288:MET:HB2	1:A:288:MET:HE3	1.80	0.45
1:A:355:ARG:HG3	1:A:355:ARG:NH1	2.32	0.45
1:B:447:LEU:HD22	1:B:457:VAL:HG11	1.98	0.45
1:A:129:SER:O	1:A:132:ILE:HB	2.17	0.44
1:B:63:LEU:HA	1:B:81:ASN:ND2	2.31	0.44
1:B:69:PHE:N	1:B:69:PHE:HD2	2.15	0.44
1:B:257:PHE:HD1	1:B:257:PHE:N	2.11	0.44
1:B:610:ASP:CG	1:B:613:LEU:HB2	2.38	0.44
1:B:532:LEU:HD12	1:B:573:ASP:OD1	2.18	0.44
1:B:43:ALA:O	1:B:46:LEU:HB3	2.17	0.44
1:B:262:THR:CG2	1:B:363:LEU:HD22	2.48	0.44
1:B:285:PRO:HD2	1:B:288:MET:HE1	1.99	0.44
1:B:424:LYS:H	1:B:427:GLN:NE2	2.15	0.44
1:B:511:PHE:HE1	1:B:581:ALA:HA	1.82	0.44
1:B:588:LYS:HA	1:B:588:LYS:HD3	1.68	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:VAL:O	1:B:302:GLN:HB2	2.18	0.44
1:A:250:TYR:CD2	1:A:260:PRO:HD3	2.52	0.44
1:A:609:GLU:O	1:A:611:PRO:HD3	2.18	0.44
1:B:506:LYS:O	1:B:510:PRO:HD2	2.18	0.44
1:A:453:LYS:HG2	1:A:493:LEU:HD22	1.98	0.44
1:A:227:ILE:HG22	1:A:227:ILE:O	2.18	0.44
1:A:447:LEU:CD2	1:A:457:VAL:HG11	2.48	0.44
1:A:506:LYS:O	1:A:510:PRO:HD3	2.17	0.44
1:A:511:PHE:HE1	1:A:581:ALA:HA	1.82	0.44
1:A:305:PHE:O	1:A:306:ILE:HD13	2.18	0.44
1:B:401:ARG:HG2	1:B:401:ARG:HH11	1.83	0.44
1:B:506:LYS:O	1:B:510:PRO:HD3	2.18	0.44
1:B:609:GLU:O	1:B:611:PRO:HD3	2.18	0.44
1:A:242:THR:HG22	1:A:245:GLU:OE1	2.18	0.44
1:A:301:VAL:O	1:A:302:GLN:HB2	2.17	0.44
1:A:602:LEU:HB2	1:A:608:LEU:HD21	1.99	0.44
1:A:250:TYR:HB2	1:A:279:TYR:CE2	2.52	0.43
1:A:262:THR:HG22	1:A:363:LEU:HD22	2.00	0.43
1:B:63:LEU:HA	1:B:81:ASN:HD21	1.83	0.43
1:B:74:ARG:HE	1:B:74:ARG:HB3	1.42	0.43
1:A:506:LYS:O	1:A:510:PRO:HD2	2.17	0.43
1:B:277:LEU:HD12	1:B:277:LEU:C	2.39	0.43
1:B:536:PRO:HB3	1:B:574:HIS:HD2	1.84	0.43
1:A:607:THR:O	1:A:608:LEU:HD23	2.19	0.43
1:A:250:TYR:HD2	1:A:260:PRO:HD3	1.84	0.43
1:A:253:ILE:HG13	1:A:253:ILE:H	1.65	0.43
1:A:424:LYS:H	1:A:427:GLN:NE2	2.15	0.43
1:B:290:ASN:HB3	1:B:292:ASP:H	1.83	0.43
1:B:447:LEU:CD2	1:B:457:VAL:HG11	2.48	0.43
1:A:290:ASN:HB3	1:A:292:ASP:H	1.83	0.43
1:A:487:ASP:OD1	1:A:487:ASP:N	2.50	0.43
1:A:531:ARG:O	1:A:533:THR:HG22	2.19	0.43
1:A:535:THR:HG23	1:A:536:PRO:HD2	2.01	0.43
1:B:191:TRP:CG	1:B:192:ARG:N	2.86	0.43
1:A:63:LEU:HA	1:A:81:ASN:ND2	2.33	0.43
1:A:68:SER:O	1:A:76:LEU:HD12	2.19	0.43
1:A:198:SER:C	1:A:200:TYR:H	2.21	0.43
1:B:162:TYR:HD1	1:B:162:TYR:H	1.66	0.43
1:B:277:LEU:HD12	1:B:278:LEU:N	2.34	0.43
1:A:437:SER:O	1:A:440:ALA:HB3	2.18	0.43
1:B:198:SER:C	1:B:200:TYR:N	2.72	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:O	1:A:133:VAL:HG22	2.19	0.43
1:A:408:ASP:HB2	1:A:442:LYS:HE3	2.00	0.43
1:B:233:LEU:CD1	1:B:245:GLU:HB3	2.48	0.43
1:B:27:ASN:O	1:B:29:GLU:N	2.51	0.43
1:B:264:SER:HB3	1:B:359:MET:HE2	2.00	0.43
1:A:253:ILE:HD12	1:A:254:ALA:N	2.34	0.43
1:A:357:LEU:HD23	1:A:399:LEU:HD11	2.01	0.43
1:B:68:SER:OG	1:B:77:THR:HB	2.19	0.42
1:A:610:ASP:CG	1:A:613:LEU:HB2	2.39	0.42
1:A:64:ARG:HD3	1:A:81:ASN:ND2	2.33	0.42
1:B:46:LEU:HD22	1:B:82:GLY:C	2.40	0.42
1:B:209:GLU:HA	1:B:226:LYS:HA	2.02	0.42
1:B:539:VAL:HB	1:B:566:TYR:HB3	2.02	0.42
1:A:165:ALA:O	1:A:167:ILE:HG23	2.18	0.42
1:A:269:GLU:HB2	1:B:164:VAL:HG13	2.01	0.42
1:B:78:ILE:HD12	1:B:78:ILE:N	2.34	0.42
1:B:531:ARG:O	1:B:533:THR:HG22	2.20	0.42
1:B:64:ARG:NH2	1:B:66:ARG:CZ	2.82	0.42
1:B:136:LYS:HZ2	1:B:179:HIS:HB2	1.83	0.42
1:B:238:LYS:HB3	1:B:238:LYS:HE2	1.77	0.42
1:B:253:ILE:HD12	1:B:254:ALA:N	2.35	0.42
1:B:16:LEU:HD23	1:B:16:LEU:HA	1.89	0.42
1:A:320:PHE:HB2	1:A:378:PHE:CE2	2.55	0.42
1:B:154:TRP:HE1	1:B:162:TYR:HD2	1.67	0.42
1:B:250:TYR:HB2	1:B:279:TYR:CE2	2.55	0.42
1:B:383:LYS:HG2	1:B:468:MET:SD	2.60	0.42
1:B:599:GLN:HE21	1:B:614:PHE:HZ	1.66	0.42
1:A:69:PHE:N	1:A:69:PHE:HD2	2.17	0.42
1:A:74:ARG:HE	1:A:74:ARG:HB3	1.41	0.42
1:B:453:LYS:HD2	1:B:453:LYS:HA	1.92	0.42
1:B:607:THR:O	1:B:608:LEU:HD23	2.20	0.42
1:A:277:LEU:C	1:A:277:LEU:HD12	2.40	0.41
1:A:430:ILE:HD12	1:A:430:ILE:N	2.35	0.41
1:A:64:ARG:HH11	1:A:64:ARG:HG2	1.85	0.41
1:A:539:VAL:HB	1:A:566:TYR:HB3	2.02	0.41
1:B:233:LEU:HD11	1:B:245:GLU:HB3	2.02	0.41
1:B:528:LEU:HD12	1:B:572:PRO:CG	2.44	0.41
1:B:75:THR:HA	1:B:178:LEU:O	2.20	0.41
1:B:95:GLY:O	1:B:99:LYS:HD3	2.21	0.41
1:B:535:THR:HG23	1:B:536:PRO:HD2	2.02	0.41
1:A:209:GLU:HA	1:A:226:LYS:HA	2.03	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ARG:HD3	1:B:224:TRP:CE2	2.54	0.41
1:B:130:ALA:O	1:B:133:VAL:HG22	2.19	0.41
1:A:16:LEU:O	1:A:20:MET:HG2	2.21	0.41
1:B:122:GLN:HB2	1:B:255:HIS:CD2	2.55	0.41
1:B:261:LEU:HD23	1:B:261:LEU:HA	1.92	0.41
1:A:401:ARG:HG2	1:A:401:ARG:HH11	1.86	0.41
1:B:253:ILE:HG13	1:B:253:ILE:H	1.65	0.41
1:B:314:MET:HE3	1:B:321:VAL:HG11	2.03	0.41
1:B:516:LYS:HE2	1:B:516:LYS:HB3	1.87	0.41
1:A:191:TRP:CG	1:A:192:ARG:N	2.89	0.41
1:A:304:VAL:O	1:A:306:ILE:HG12	2.21	0.41
1:A:536:PRO:HB3	1:A:574:HIS:HD2	1.85	0.41
1:B:408:ASP:HB2	1:B:442:LYS:HE3	2.01	0.41
1:B:248:GLU:O	1:B:251:LYS:HB2	2.21	0.41
1:B:604:GLU:O	1:B:604:GLU:HG3	2.20	0.41
1:A:184:GLU:C	1:A:186:GLU:N	2.75	0.40
1:A:248:GLU:O	1:A:251:LYS:HB2	2.22	0.40
1:A:63:LEU:HA	1:A:81:ASN:HD21	1.86	0.40
1:A:94:LEU:HB3	1:A:154:TRP:CE2	2.57	0.40
1:A:318:LEU:O	1:A:321:VAL:HG23	2.21	0.40
1:B:39:ALA:O	1:B:42:ALA:HB3	2.21	0.40
1:B:357:LEU:HD23	1:B:399:LEU:HD11	2.03	0.40
1:A:43:ALA:O	1:A:46:LEU:HB3	2.21	0.40
1:A:206:LEU:HA	1:A:207:PRO:HD3	1.94	0.40
1:A:313:PHE:HE1	1:A:345:THR:HG23	1.86	0.40
1:A:393:GLN:HA	1:A:396:ILE:HD12	2.03	0.40
1:B:191:TRP:CD1	1:B:192:ARG:N	2.90	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	559/624 (90%)	467 (84%)	81 (14%)	11 (2%)	7	39
1	B	569/624 (91%)	470 (83%)	87 (15%)	12 (2%)	7	38
All	All	1128/1248 (90%)	937 (83%)	168 (15%)	23 (2%)	7	39

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	28	LYS
1	A	98	ALA
1	B	28	LYS
1	B	100	SER
1	A	533	THR
1	B	109	LEU
1	B	533	THR
1	A	25	TYR
1	B	26	SER
1	B	159	GLU
1	B	199	LYS
1	A	127	PHE
1	A	159	GLU
1	A	217	ASP
1	A	531	ARG
1	B	24	LEU
1	B	127	PHE
1	B	531	ARG
1	A	199	LYS
1	B	11	SER
1	B	121	GLY
1	A	121	GLY

### 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	464/547 (85%)	420 (90%)	44 (10%)	8	34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	467/547 (85%)	420 (90%)	47 (10%)	7	32
All	All	931/1094 (85%)	840 (90%)	91 (10%)	8	33

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	32	LEU
1	A	33	ARG
1	A	35	LEU
1	A	47	ARG
1	A	63	LEU
1	A	64	ARG
1	A	69	PHE
1	A	74	ARG
1	A	136	LYS
1	A	141	THR
1	A	149	GLU
1	A	170	GLU
1	A	214	GLU
1	A	235	THR
1	A	239	SER
1	A	244	GLU
1	A	257	PHE
1	A	264	SER
1	A	276	SER
1	A	286	TRP
1	A	287	ASP
1	A	303	ARG
1	A	325	ILE
1	A	329	ASP
1	A	341	ASP
1	A	347	ASN
1	A	348	LEU
1	A	355	ARG
1	A	358	GLN
1	A	362	LYS
1	A	382	LEU
1	A	414	VAL
1	A	433	ILE
1	A	472	LEU
1	A	478	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	488	GLU
1	A	513	ASP
1	A	518	LEU
1	A	531	ARG
1	A	532	LEU
1	A	538	ILE
1	A	573	ASP
1	A	598	ASP
1	B	23	SER
1	B	28	LYS
1	B	29	GLU
1	B	32	LEU
1	B	33	ARG
1	B	35	LEU
1	B	47	ARG
1	B	63	LEU
1	B	64	ARG
1	B	69	PHE
1	B	74	ARG
1	B	106	LEU
1	B	113	GLN
1	B	136	LYS
1	B	141	THR
1	B	149	GLU
1	B	162	TYR
1	B	170	GLU
1	B	235	THR
1	B	239	SER
1	B	244	GLU
1	B	257	PHE
1	B	264	SER
1	B	286	TRP
1	B	287	ASP
1	B	303	ARG
1	B	314	MET
1	B	325	ILE
1	B	329	ASP
1	B	341	ASP
1	B	347	ASN
1	B	348	LEU
1	B	355	ARG
1	B	358	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	362	LYS
1	B	376	GLN
1	B	382	LEU
1	B	414	VAL
1	B	472	LEU
1	B	478	LYS
1	B	513	ASP
1	B	518	LEU
1	B	531	ARG
1	B	532	LEU
1	B	538	ILE
1	B	573	ASP
1	B	598	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	HIS
1	A	347	ASN
1	A	392	ASN
1	A	427	GLN
1	A	599	GLN
1	A	612	ASN
1	B	113	GLN
1	B	255	HIS
1	B	295	HIS
1	B	347	ASN
1	B	392	ASN
1	B	427	GLN
1	B	446	HIS
1	B	599	GLN
1	B	612	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	567/624 (90%)	-0.14	7 (1%) 79 73	23, 121, 182, 227	0
1	B	577/624 (92%)	-0.06	24 (4%) 36 32	25, 120, 200, 223	0
All	All	1144/1248 (91%)	-0.10	31 (2%) 54 48	23, 121, 191, 227	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	VAL	4.8
1	B	12	GLU	4.6
1	B	13	VAL	4.1
1	B	14	LYS	4.0
1	B	622	LEU	3.9
1	B	111	SER	3.7
1	B	336	ARG	3.5
1	B	429	LYS	3.3
1	B	330	LEU	3.1
1	B	537	ALA	3.0
1	B	110	GLY	3.0
1	A	455	ILE	2.9
1	B	526	VAL	2.8
1	B	568	PHE	2.8
1	B	618	MET	2.8
1	A	624	SER	2.7
1	A	15	GLN	2.7
1	A	582	ASP	2.6
1	B	455	ILE	2.5
1	B	543	ALA	2.5
1	B	431	TYR	2.4
1	B	8	GLY	2.3
1	A	131	PHE	2.3
1	B	528	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	289	TRP	2.2
1	A	193	VAL	2.2
1	B	522	ARG	2.2
1	B	333	ASN	2.2
1	B	508	LEU	2.1
1	B	578	LYS	2.0
1	B	619	ASN	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 monosaccharides 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.