



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:55 AM UTC

PDB ID : 2IOQ / pdb_00002ioq
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

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

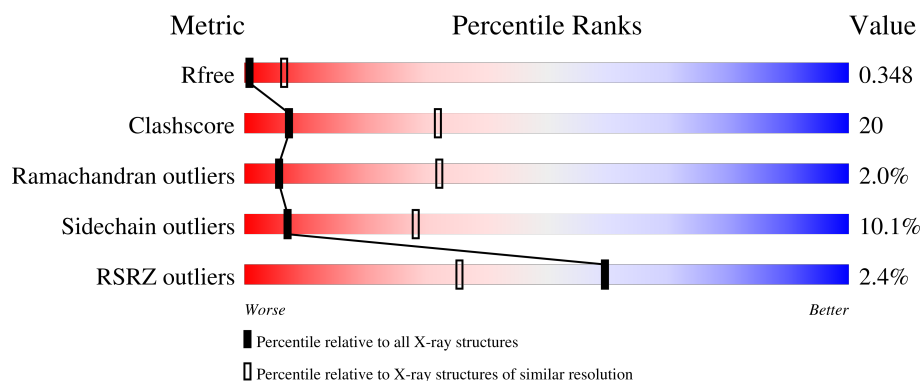
1 Overall quality at a glance

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))
R_{free}	180053	1085 (3.54-3.46)
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	624	2% 49% 38% • 9%
1	B	624	2% 51% 36% • • 8%

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.

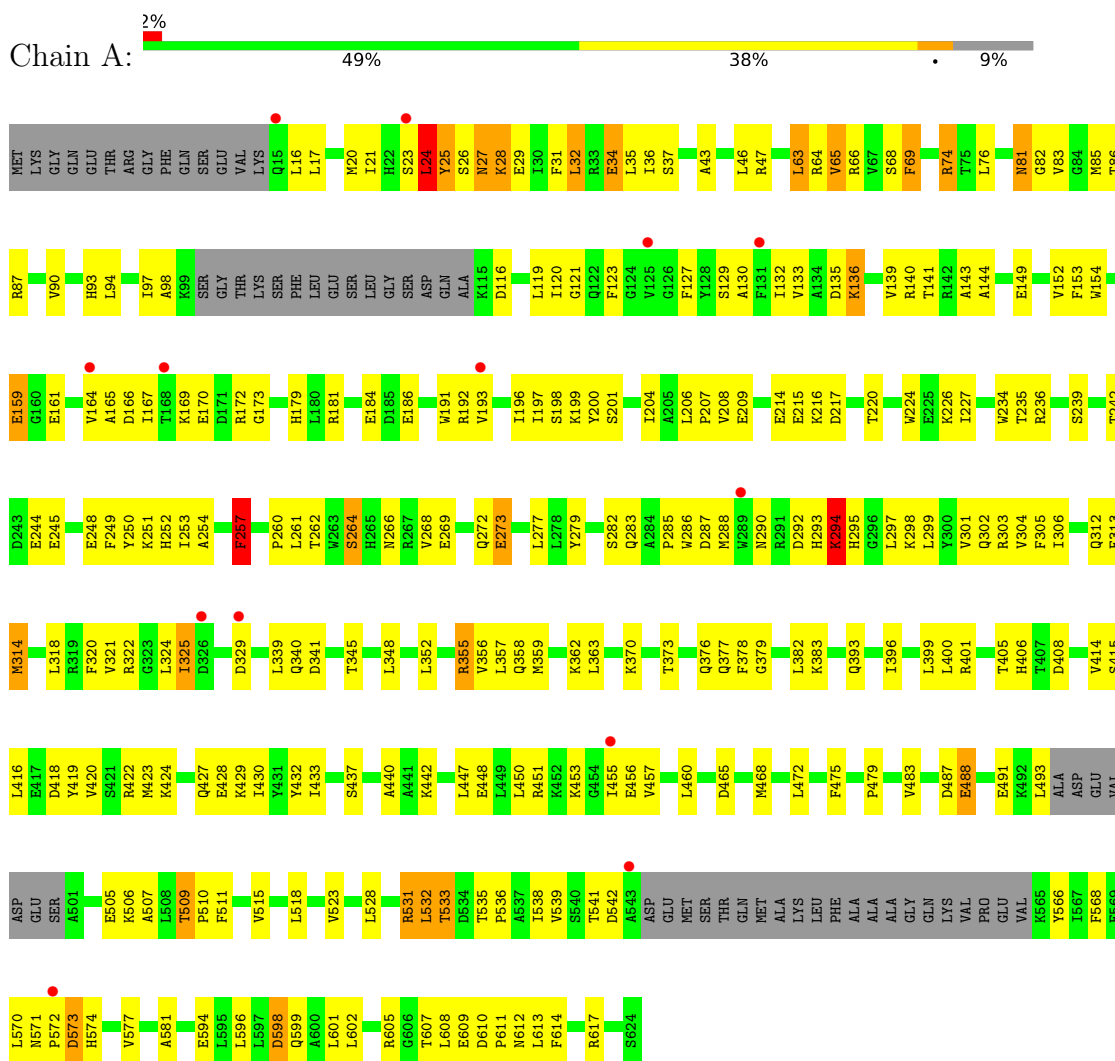
- Molecule 1 is a protein called Chaperone protein htpG.

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			

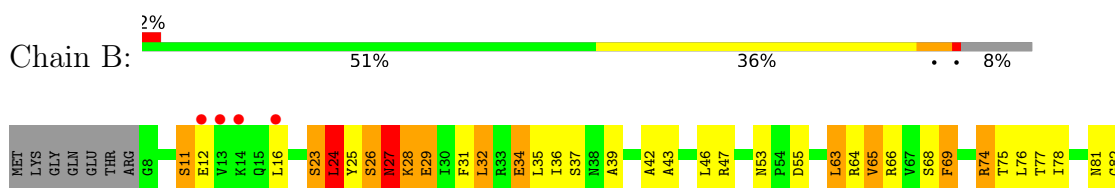
3 Residue-property plots

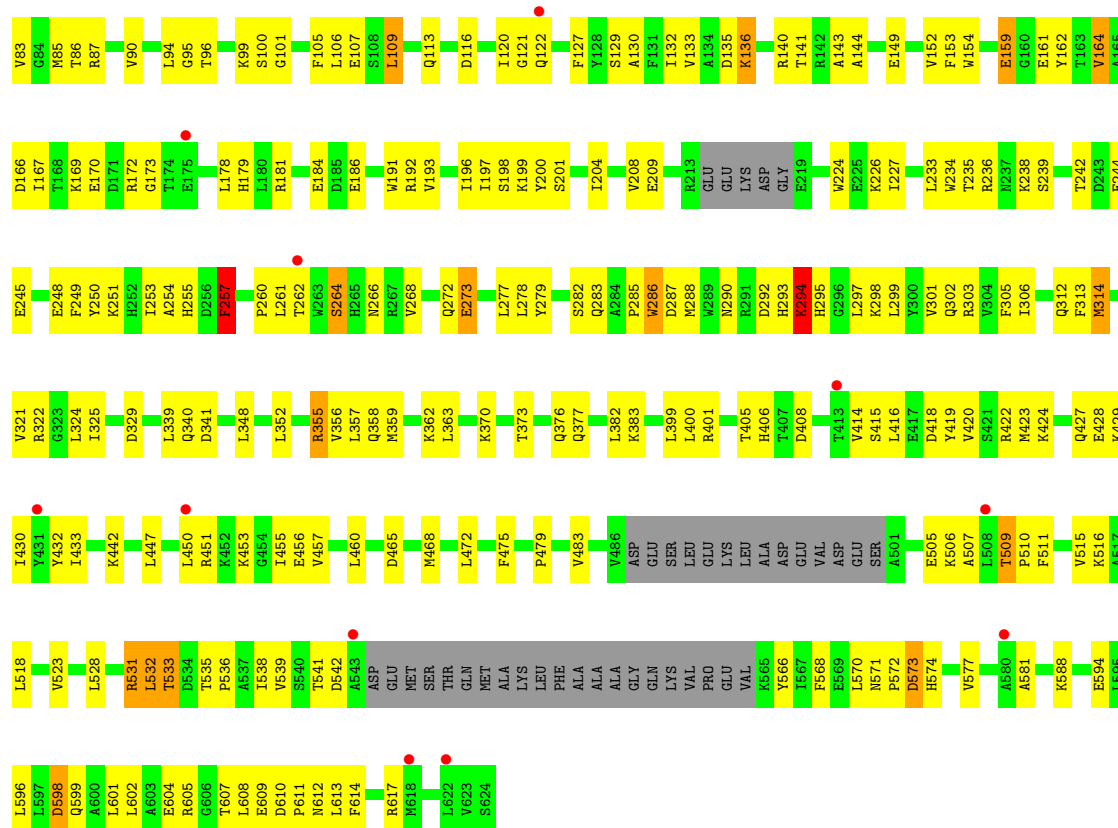
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	105.12Å 105.12Å 531.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.70 – 3.50 58.70 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (58.70-3.50) 98.8 (58.70-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	124.1	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 86.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

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 [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	0.25	0/4556	0.74	4/6165 (0.1%)
1	B	0.25	0/4617	0.73	5/6251 (0.1%)
All	All	0.25	0/9173	0.74	9/12416 (0.1%)

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 (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	509	THR	CA-C-N	-8.68	109.42	119.05
1	A	509	THR	C-N-CA	-8.68	109.42	119.05
1	B	509	THR	CA-C-N	-8.66	109.44	119.05
1	B	509	THR	C-N-CA	-8.66	109.44	119.05
1	A	28	LYS	N-CA-C	7.27	126.29	110.80
1	B	294	LYS	N-CA-C	-6.82	106.15	114.75
1	A	294	LYS	N-CA-C	-6.82	106.15	114.75
1	B	23	SER	N-CA-C	-5.68	106.01	114.64
1	B	27	ASN	N-CA-C	-5.27	104.44	111.87

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 [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	4474	0	4308	179	0
1	B	4533	0	4347	184	0
All	All	9007	0	8655	362	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 20.

All (362) 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:B:314:MET:HE3	1:B:321:VAL:HG11	1.61	0.82
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:A:314:MET:HE3	1:A:321:VAL:HG11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:423:MET:HE2	1:A:427:GLN:HG2	1.76	0.67
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:25:TYR:C	1:A:27:ASN:H	2.05	0.65
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
1:B:423:MET:HE2	1:B:427:GLN:HG2	1.79	0.64
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:285:PRO:HD2	1:A:288:MET:HE3	1.81	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:24:LEU:C	1:A:26:SER:H	2.10	0.60
1:B:285:PRO:HD2	1:B:288:MET:HE3	1.84	0.59
1:B:420:VAL:HA	1:B:423:MET:HG3	1.85	0.59
1:A:85:MET:C	1:A:143:ALA:HB2	2.28	0.59
1:B:85:MET:C	1:B:143:ALA:HB2	2.28	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:B:297:LEU:HD11	1:B:314:MET:HE2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:THR:OG1	1:A:510:PRO:HD3	2.04	0.56
1:B:264:SER:HB3	1:B:359:MET:HE2	1.87	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:A:507:ALA:C	1:A:510:PRO:HD2	2.31	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:236:ARG:HH22	1:A:245:GLU:CD	2.15	0.55
1:A:523:VAL:HG11	1:A:568:PHE:HB2	1.87	0.55
1:B:507:ALA:C	1:B:510:PRO:HD2	2.32	0.55
1:A:24:LEU:C	1:A:26:SER:N	2.64	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:25:TYR:C	1:A:27:ASN:N	2.66	0.54
1:A:136:LYS:NZ	1:A:179:HIS:HB2	2.22	0.54
1:A:64:ARG:HD3	1:A:81:ASN:HD21	1.72	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:236:ARG:HH22	1:B:245:GLU:CD	2.16	0.54
1:B:268:VAL:O	1:B:273:GLU:HA	2.07	0.54
1:A:297:LEU:HD11	1:A:314:MET:HE2	1.90	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:198:SER:C	1:B:200:TYR:H	2.17	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:107:GLU:C	1:B:109:LEU:H	2.18	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:29:GLU:CD	1:A:29:GLU:H	2.18	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
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:352:LEU:O	1:A:356:VAL:HG23	2.11	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:24:LEU:C	1:B:26:SER:N	2.70	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:PHE:CG	1:B:32:LEU:N	2.80	0.49
1:B:610:ASP:CG	1:B:613:LEU:HB2	2.38	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:A:139:VAL:HB	1:A:154:TRP:HB3	1.95	0.49
1:A:264:SER:HB3	1:A:359:MET:HE2	1.94	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:B:277:LEU:HD12	1:B:277:LEU:C	2.39	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
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:198:SER:C	1:A:200:TYR:H	2.21	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:297:LEU:HD12	1:A:313:PHE:HB2	1.95	0.47
1:B:136:LYS:CE	1:B:179:HIS:HB2	2.44	0.47
1:B:198:SER:C	1:B:200:TYR:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:610:ASP:CG	1:A:613:LEU:HB2	2.39	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: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:277:LEU:C	1:A:277:LEU:HD12	2.40	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:288:MET:HE3	1:B:288:MET:HB2	1.88	0.46
1:B:455:ILE:HG22	1:B:456:GLU:N	2.28	0.46
1:B:46:LEU:HD22	1:B:82:GLY:C	2.40	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
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: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:419:TYR:HE2	1:A:423:MET:HE3	1.80	0.45
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: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:419:TYR:HE2	1:B:423:MET:HE3	1.81	0.45
1:B:612:ASN:ND2	1:B:612:ASN:H	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
1:A:198:SER:C	1:A:200:TYR:N	2.75	0.44
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:159:GLU:C	1:A:161:GLU:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:252:HIS:ND1	1:A:252:HIS:C	2.76	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: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:B:74:ARG:HH22	1:B:181:ARG:C	2.26	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:B:25:TYR:C	1:B:27:ASN:H	2.27	0.43
1:B:162:TYR:HD1	1:B:162:TYR:H	1.66	0.43
1:B:184:GLU:C	1:B:186:GLU:N	2.75	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: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: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:64:ARG:HD3	1:A:81:ASN:ND2	2.33	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:25:TYR:C	1:B:27:ASN:N	2.77	0.42
1:B:78:ILE:HD12	1:B:78:ILE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:GLU:C	1:B:161:GLU:H	2.27	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: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:A:184:GLU:C	1:A:186:GLU:N	2.75	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:24:LEU:C	1:B:26:SER:H	2.27	0.42
1:A:378:PHE:O	1:A:379:GLY:C	2.62	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: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:B:400:LEU:C	1:B:401:ARG:HG2	2.45	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
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:A:74:ARG:HH22	1:A:181:ARG:C	2.28	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:516:LYS:HE2	1:B:516:LYS:HB3	1.87	0.41
1:A:46:LEU:HD22	1:A:82:GLY:C	2.45	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:400:LEU:C	1:A:401:ARG:HG2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:PRO:HB3	1:A:574:HIS:HD2	1.85	0.41
1:B:107:GLU:C	1:B:109:LEU:N	2.79	0.41
1:B:408:ASP:HB2	1:B:442:LYS:HE3	2.01	0.41
1:A:184:GLU:C	1:A:186:GLU:H	2.29	0.41
1:B:248:GLU:O	1:B:251:LYS:HB2	2.21	0.41
1:B:253:ILE:HG22	1:B:298:LYS:HZ3	1.84	0.41
1:B:604:GLU:O	1:B:604:GLU:HG3	2.20	0.41
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:B:53:ASN:C	1:B:55:ASP:H	2.30	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 [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	559/624 (90%)	467 (84%)	81 (14%)	11 (2%)	6	32
1	B	569/624 (91%)	470 (83%)	87 (15%)	12 (2%)	5	31
All	All	1128/1248 (90%)	937 (83%)	168 (15%)	23 (2%)	6	32

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%)	417 (90%)	47 (10%)	7	28
1	B	467/547 (85%)	420 (90%)	47 (10%)	7	28
All	All	931/1094 (85%)	837 (90%)	94 (10%)	7	28

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU

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Mol	Chain	Res	Type
1	A	32	LEU
1	A	34	GLU
1	A	35	LEU
1	A	47	ARG
1	A	63	LEU
1	A	65	VAL
1	A	69	PHE
1	A	74	ARG
1	A	81	ASN
1	A	136	LYS
1	A	141	THR
1	A	149	GLU
1	A	164	VAL
1	A	170	GLU
1	A	214	GLU
1	A	216	LYS
1	A	235	THR
1	A	239	SER
1	A	244	GLU
1	A	257	PHE
1	A	264	SER
1	A	273	GLU
1	A	286	TRP
1	A	287	ASP
1	A	294	LYS
1	A	303	ARG
1	A	314	MET
1	A	325	ILE
1	A	329	ASP
1	A	341	ASP
1	A	348	LEU
1	A	355	ARG
1	A	358	GLN
1	A	362	LYS
1	A	376	GLN
1	A	382	LEU
1	A	414	VAL
1	A	433	ILE
1	A	472	LEU
1	A	488	GLU
1	A	518	LEU
1	A	532	LEU

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Mol	Chain	Res	Type
1	A	538	ILE
1	A	573	ASP
1	A	596	LEU
1	A	598	ASP
1	B	23	SER
1	B	24	LEU
1	B	28	LYS
1	B	29	GLU
1	B	32	LEU
1	B	34	GLU
1	B	35	LEU
1	B	47	ARG
1	B	63	LEU
1	B	65	VAL
1	B	69	PHE
1	B	74	ARG
1	B	106	LEU
1	B	136	LYS
1	B	141	THR
1	B	149	GLU
1	B	164	VAL
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	273	GLU
1	B	286	TRP
1	B	287	ASP
1	B	294	LYS
1	B	303	ARG
1	B	314	MET
1	B	325	ILE
1	B	329	ASP
1	B	341	ASP
1	B	348	LEU
1	B	355	ARG
1	B	358	GLN
1	B	362	LYS
1	B	376	GLN
1	B	382	LEU

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Mol	Chain	Res	Type
1	B	414	VAL
1	B	433	ILE
1	B	472	LEU
1	B	518	LEU
1	B	532	LEU
1	B	538	ILE
1	B	573	ASP
1	B	596	LEU
1	B	598	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	HIS
1	A	302	GLN
1	A	347	ASN
1	A	392	ASN
1	A	427	GLN
1	A	446	HIS
1	A	599	GLN
1	A	612	ASN
1	B	38	ASN
1	B	113	GLN
1	B	203	HIS
1	B	255	HIS
1	B	295	HIS
1	B	302	GLN
1	B	347	ASN
1	B	392	ASN
1	B	427	GLN
1	B	571	ASN
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 [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	567/624 (90%)	0.20	13 (2%) 61 37	23, 121, 182, 227	0
1	B	577/624 (92%)	0.18	15 (2%) 57 33	25, 120, 200, 223	0
All	All	1144/1248 (91%)	0.19	28 (2%) 59 35	23, 121, 191, 227	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	622	LEU	5.6
1	B	12	GLU	3.6
1	B	618	MET	3.4
1	B	14	LYS	3.4
1	A	329	ASP	3.3
1	B	508	LEU	3.1
1	B	450	LEU	2.8
1	A	168	THR	2.8
1	A	125	VAL	2.6
1	A	543	ALA	2.6
1	B	431	TYR	2.6
1	A	455	ILE	2.6
1	B	175	GLU	2.5
1	B	262	THR	2.5
1	A	193	VAL	2.5
1	B	13	VAL	2.4
1	B	413	THR	2.3
1	A	15	GLN	2.2
1	A	326	ASP	2.2
1	B	16	LEU	2.2
1	A	131	PHE	2.2
1	B	122	GLN	2.2
1	B	580	ALA	2.1
1	A	164	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	543	ALA	2.1
1	A	572	PRO	2.1
1	A	289	TRP	2.0
1	A	23	SER	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.