



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:11 PM UTC

PDB ID : 3T6J / pdb_00003t6j
Title : Structure of human DPPIII in complex with the opioid peptide Tynorphin, at 3.0 Angstroms
Authors : Bezerra, G.A.; Gruber, K.
Deposited on : 2011-07-28
Resolution : 2.98 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

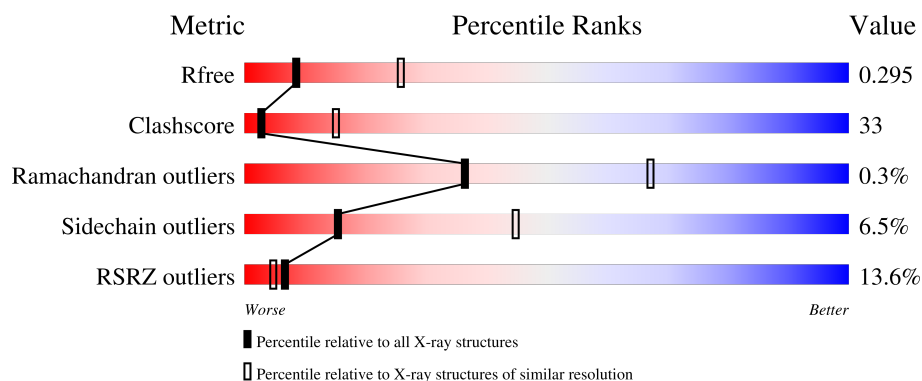
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	726	
2	B	5	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5787 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 Dipeptidyl peptidase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	722	Total	C	N	O	S	0	0	0
			5732	3655	968	1096	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	451	ALA	GLU	engineered mutation	UNP Q9NY33

- Molecule 2 is a protein called Tynorphin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	0	0	0
			48	35	6	7			

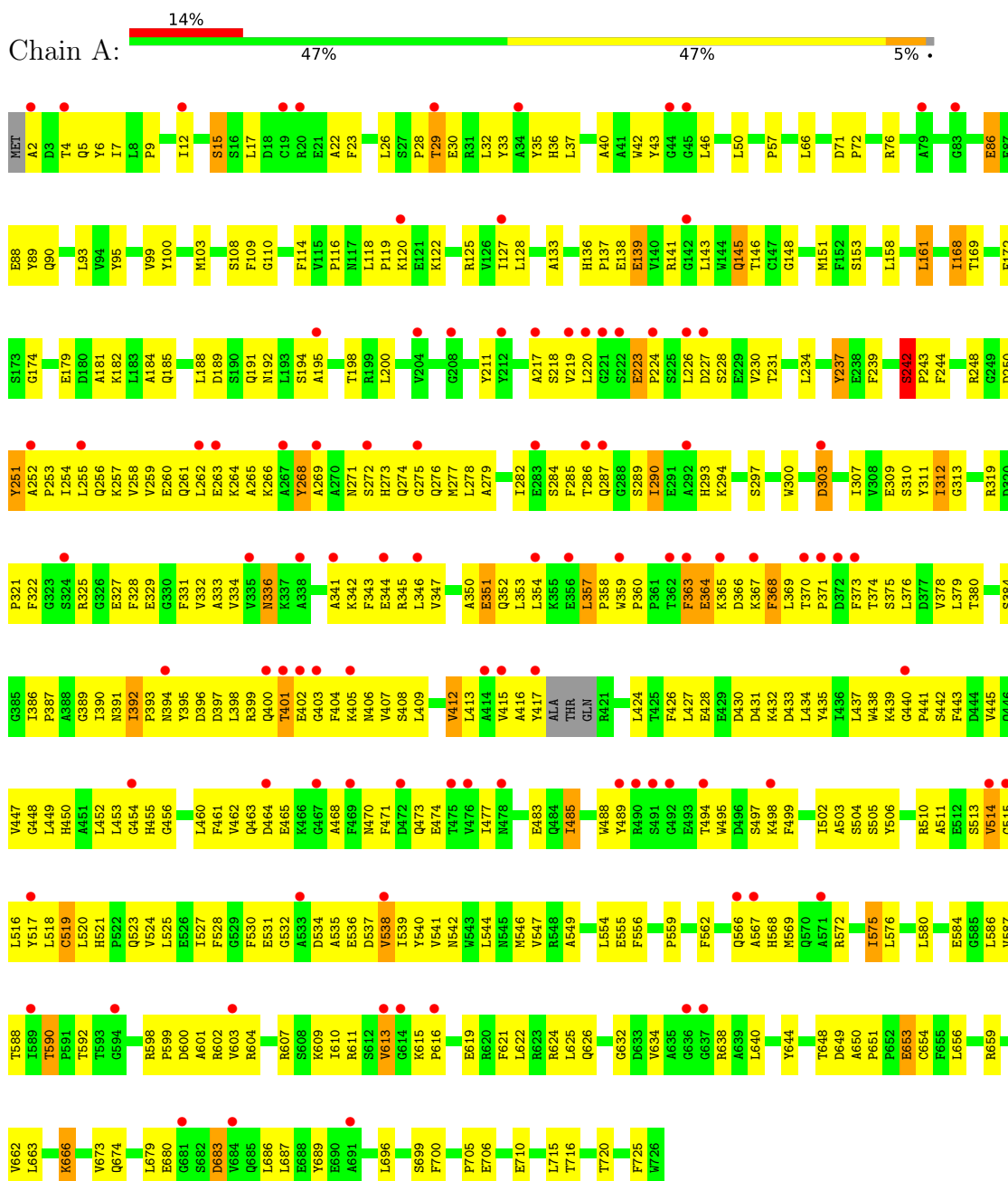
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		

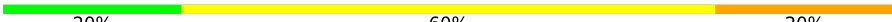
3 Residue-property plots

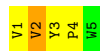
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dipeptidyl peptidase 3



- Molecule 2: Tynorphin

Chain B:  20% 60% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.01Å 107.27Å 65.48Å 90.00° 93.67° 90.00°	Depositor
Resolution (Å)	19.60 – 2.98 19.60 – 2.98	Depositor EDS
% Data completeness (in resolution range)	96.1 (19.60-2.98) 95.9 (19.60-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.98Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.237 , 0.268 0.258 , 0.295	Depositor DCC
R_{free} test set	833 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5787	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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	0.31	0/5863	0.78	9/7941 (0.1%)
2	B	0.29	0/51	0.79	1/70 (1.4%)
All	All	0.31	0/5914	0.78	10/8011 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	GLU	CA-C-N	-6.70	112.59	119.83
1	A	223	GLU	C-N-CA	-6.70	112.59	119.83
1	A	357	LEU	CA-C-N	5.92	125.62	119.82
1	A	357	LEU	C-N-CA	5.92	125.62	119.82
1	A	366	ASP	N-CA-C	5.63	117.42	111.28
1	A	242	SER	CA-C-N	5.60	126.08	120.14
1	A	242	SER	C-N-CA	5.60	126.08	120.14
2	B	2	VAL	N-CA-C	5.29	116.41	109.21
1	A	360	PRO	CA-C-N	5.05	124.71	119.56
1	A	360	PRO	C-N-CA	5.05	124.71	119.56

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	5732	0	5604	377	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	46	10	0
3	A	7	0	0	4	0
All	All	5787	0	5650	377	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 33.

All (377) 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:118:LEU:HD12	1:A:119:PRO:HD2	1.35	1.08
1:A:342:LYS:HD2	1:A:345:ARG:HH21	1.26	1.00
1:A:394:ASN:HA	1:A:399:ARG:HH22	1.33	0.92
1:A:531:GLU:HA	1:A:535:ALA:HB2	1.52	0.90
1:A:88:GLU:HB3	1:A:118:LEU:HD13	1.51	0.90
1:A:397:ASP:O	1:A:401:THR:HG22	1.72	0.89
1:A:219:VAL:HG22	1:A:286:THR:HA	1.56	0.88
1:A:40:ALA:HB2	1:A:261:GLN:HB2	1.57	0.85
1:A:223:GLU:HB3	1:A:224:PRO:HD2	1.57	0.85
1:A:9:PRO:HD2	1:A:12:ILE:HD11	1.59	0.84
1:A:290:ILE:HD12	1:A:290:ILE:H	1.39	0.84
1:A:260:GLU:O	1:A:263:GLU:HG2	1.78	0.84
1:A:211:TYR:HD2	1:A:243:PRO:HG2	1.43	0.83
1:A:17:LEU:HD21	1:A:378:VAL:HB	1.60	0.81
1:A:9:PRO:O	1:A:12:ILE:HG12	1.84	0.78
1:A:119:PRO:HB2	1:A:122:LYS:HG3	1.65	0.78
1:A:367:LYS:HG3	1:A:368:PHE:H	1.47	0.78
1:A:33:TYR:O	1:A:37:LEU:HD13	1.83	0.77
1:A:211:TYR:CD2	1:A:243:PRO:HG2	2.19	0.77
1:A:424:LEU:HD12	1:A:432:LYS:HB3	1.66	0.77
1:A:103:MET:HA	1:A:103:MET:HE2	1.67	0.76
1:A:266:LYS:HZ1	1:A:279:ALA:HB2	1.50	0.75
1:A:2:ALA:HA	1:A:5:GLN:HG3	1.68	0.75
1:A:406:ASN:ND2	1:A:452:LEU:HD12	2.01	0.74
1:A:266:LYS:NZ	1:A:279:ALA:HB2	2.03	0.74
1:A:428:GLU:O	1:A:430:ASP:O	2.05	0.74
1:A:194:SER:HB3	1:A:290:ILE:HG12	1.70	0.73
1:A:435:TYR:O	1:A:439:LYS:HB2	1.88	0.73
1:A:28:PRO:O	1:A:32:LEU:HD12	1.89	0.72
1:A:534:ASP:O	1:A:536:GLU:O	2.08	0.71
1:A:394:ASN:C	1:A:399:ARG:HH12	1.98	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:HD11	1:A:265:ALA:HB1	1.72	0.70
1:A:453:LEU:HD22	1:A:518:LEU:CD2	2.21	0.70
1:A:364:GLU:HG3	1:A:365:LYS:N	2.06	0.69
1:A:616:PRO:HA	1:A:619:GLU:OE1	1.93	0.69
1:A:136:HIS:HB3	1:A:139:GLU:HG2	1.75	0.69
1:A:392:ILE:HB	1:A:393:PRO:HA	1.75	0.68
1:A:402:GLU:HG2	1:A:403:GLY:N	2.08	0.68
1:A:118:LEU:HD12	1:A:119:PRO:CD	2.21	0.68
1:A:397:ASP:HA	1:A:400:GLN:NE2	2.10	0.67
1:A:376:LEU:HD13	1:A:407:VAL:HG13	1.75	0.66
1:A:387:PRO:HB3	2:B:2:VAL:HG13	1.77	0.66
1:A:523:GLN:HE22	1:A:527:ILE:HG13	1.59	0.66
1:A:346:LEU:HD21	1:A:452:LEU:HD22	1.76	0.66
1:A:498:LYS:NZ	1:A:632:GLY:HA3	2.09	0.66
1:A:392:ILE:HG23	2:B:1:VAL:H1	1.61	0.65
1:A:515:GLY:O	1:A:519:CYS:HB3	1.97	0.65
1:A:394:ASN:HA	1:A:399:ARG:NH2	2.08	0.65
1:A:367:LYS:CG	1:A:368:PHE:H	2.07	0.65
1:A:568:HIS:CD2	2:B:4:PRO:HD3	2.31	0.65
1:A:538:VAL:HG13	1:A:539:ILE:H	1.61	0.65
1:A:511:ALA:O	1:A:514:VAL:HG22	1.97	0.64
1:A:364:GLU:HG3	1:A:365:LYS:H	1.63	0.64
1:A:95:TYR:CD2	1:A:116:PRO:HG3	2.32	0.64
1:A:513:SER:HB3	1:A:575:ILE:HD11	1.80	0.64
1:A:375:SER:HA	1:A:408:SER:O	1.97	0.63
1:A:450:HIS:CD2	2:B:3:TYR:HB2	2.34	0.63
1:A:470:ASN:OD1	1:A:471:PHE:HD1	1.80	0.63
1:A:255:LEU:HD23	1:A:285:PHE:HB3	1.79	0.63
1:A:263:GLU:HA	1:A:266:LYS:HG3	1.79	0.63
1:A:649:ASP:HB2	1:A:656:LEU:HD12	1.81	0.63
1:A:663:LEU:O	1:A:666:LYS:HE2	1.99	0.62
1:A:311:TYR:HB3	1:A:331:PHE:CE2	2.34	0.62
1:A:450:HIS:O	1:A:454:GLY:HA3	1.98	0.62
1:A:462:VAL:HA	1:A:489:TYR:O	1.98	0.62
1:A:651:PRO:HA	1:A:653:GLU:H	1.65	0.62
1:A:369:LEU:HG	1:A:370:THR:N	2.15	0.61
1:A:4:THR:HG23	1:A:666:LYS:NZ	2.15	0.61
1:A:33:TYR:OH	1:A:274:GLN:HG2	2.01	0.61
1:A:351:GLU:HG2	1:A:352:GLN:H	1.66	0.61
1:A:663:LEU:O	1:A:666:LYS:HB3	2.01	0.61
1:A:549:ALA:HB1	1:A:572:ARG:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HD11	1:A:127:ILE:HG22	1.83	0.60
1:A:136:HIS:HB3	1:A:139:GLU:CG	2.32	0.60
1:A:342:LYS:HD2	1:A:345:ARG:NH2	2.08	0.60
1:A:452:LEU:O	1:A:456:GLY:HA3	2.01	0.60
1:A:615:LYS:HB3	1:A:616:PRO:HD3	1.83	0.60
1:A:430:ASP:O	1:A:431:ASP:HB2	2.01	0.60
1:A:401:THR:HG23	1:A:402:GLU:OE1	2.01	0.60
1:A:392:ILE:HG23	2:B:1:VAL:N	2.17	0.59
1:A:71:ASP:HB2	1:A:72:PRO:HD2	1.85	0.59
1:A:4:THR:HA	1:A:7:ILE:HG12	1.85	0.59
1:A:398:LEU:HA	1:A:401:THR:CG2	2.33	0.59
1:A:341:ALA:O	1:A:344:GLU:HG2	2.03	0.59
1:A:262:LEU:O	1:A:265:ALA:HB3	2.02	0.58
1:A:110:GLY:HA3	3:A:740:HOH:O	2.03	0.58
1:A:341:ALA:O	1:A:345:ARG:HG3	2.03	0.58
1:A:610:ILE:HG23	1:A:611:ARG:HG3	1.84	0.58
1:A:402:GLU:HG2	1:A:403:GLY:H	1.68	0.58
1:A:367:LYS:HG3	1:A:368:PHE:N	2.17	0.58
1:A:357:LEU:HD13	1:A:359:TRP:CZ2	2.39	0.58
1:A:256:GLN:O	1:A:260:GLU:HG3	2.04	0.58
1:A:373:PHE:CE2	1:A:448:GLY:HA2	2.39	0.58
1:A:46:LEU:HD23	1:A:715:LEU:HD11	1.86	0.57
1:A:369:LEU:C	1:A:371:PRO:HD3	2.29	0.57
1:A:260:GLU:O	1:A:264:LYS:HD3	2.04	0.57
1:A:494:THR:HG22	1:A:495:TRP:N	2.19	0.57
1:A:253:PRO:O	1:A:256:GLN:HB3	2.04	0.57
1:A:568:HIS:HB3	1:A:572:ARG:NH1	2.19	0.57
1:A:254:ILE:O	1:A:258:VAL:HG23	2.04	0.57
1:A:428:GLU:O	1:A:432:LYS:HG3	2.04	0.57
1:A:217:ALA:HA	1:A:250:ASP:HB3	1.86	0.57
1:A:15:SER:CB	1:A:415:VAL:HG13	2.35	0.56
1:A:413:LEU:N	1:A:413:LEU:HD23	2.19	0.56
1:A:621:PHE:HE1	1:A:644:TYR:CE2	2.23	0.56
1:A:271:ASN:OD1	1:A:274:GLN:OE1	2.24	0.56
1:A:386:ILE:HD11	1:A:674:GLN:HE21	1.70	0.56
1:A:371:PRO:HB3	1:A:404:PHE:O	2.05	0.56
1:A:42:TRP:CE2	1:A:380:THR:HG23	2.40	0.56
1:A:373:PHE:HE2	1:A:448:GLY:HA2	1.71	0.56
1:A:438:TRP:HB2	1:A:541:VAL:HG21	1.87	0.56
1:A:506:TYR:OH	1:A:625:LEU:HA	2.07	0.55
1:A:369:LEU:HG	1:A:370:THR:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:LYS:HZ1	1:A:632:GLY:HA3	1.71	0.55
1:A:4:THR:HG23	1:A:666:LYS:HZ1	1.70	0.55
1:A:358:PRO:HG2	1:A:359:TRP:CE3	2.42	0.55
1:A:346:LEU:CD2	1:A:452:LEU:HD22	2.36	0.55
1:A:510:ARG:O	1:A:514:VAL:HG13	2.07	0.55
1:A:76:ARG:NH1	1:A:86:GLU:OE1	2.40	0.55
1:A:427:LEU:O	1:A:602:ARG:NH1	2.39	0.55
1:A:514:VAL:HG12	1:A:622:LEU:HD22	1.89	0.55
1:A:369:LEU:HD22	1:A:402:GLU:O	2.06	0.55
1:A:424:LEU:CD1	1:A:432:LYS:HB3	2.36	0.55
1:A:602:ARG:HD3	3:A:741:HOH:O	2.07	0.55
1:A:502:ILE:HD13	1:A:638:ARG:HG2	1.89	0.54
1:A:274:GLN:HE22	1:A:303:ASP:HB2	1.71	0.54
1:A:290:ILE:HD12	1:A:290:ILE:N	2.17	0.54
1:A:268:TYR:N	1:A:268:TYR:CD2	2.75	0.54
1:A:15:SER:HB3	1:A:415:VAL:HG13	1.88	0.54
1:A:37:LEU:N	1:A:37:LEU:HD12	2.21	0.54
1:A:43:TYR:O	1:A:46:LEU:HD13	2.08	0.54
1:A:413:LEU:O	1:A:415:VAL:N	2.41	0.54
1:A:413:LEU:O	1:A:416:ALA:N	2.40	0.54
1:A:521:HIS:CE1	1:A:523:GLN:HB2	2.42	0.54
1:A:556:PHE:CD1	1:A:569:MET:HG3	2.43	0.54
1:A:376:LEU:HD12	1:A:376:LEU:N	2.23	0.53
1:A:673:VAL:HG22	1:A:696:LEU:HB2	1.89	0.53
1:A:705:PRO:HG2	1:A:706:GLU:OE2	2.09	0.53
1:A:525:LEU:HD23	1:A:535:ALA:HA	1.90	0.53
1:A:613:VAL:O	1:A:616:PRO:HD2	2.09	0.53
1:A:452:LEU:HD23	1:A:453:LEU:CD1	2.38	0.53
1:A:89:TYR:CZ	1:A:93:LEU:HD21	2.43	0.53
1:A:191:GLN:O	1:A:192:ASN:OD1	2.27	0.53
1:A:544:LEU:O	1:A:547:VAL:HG22	2.08	0.53
1:A:23:PHE:CE2	1:A:686:LEU:HB2	2.44	0.53
1:A:494:THR:CG2	1:A:495:TRP:N	2.72	0.53
1:A:433:ASP:O	1:A:437:LEU:HD13	2.09	0.52
1:A:284:SER:OG	1:A:293:HIS:HB2	2.09	0.52
1:A:300:TRP:CH2	1:A:405:LYS:HD3	2.45	0.52
1:A:336:ASN:OD1	1:A:336:ASN:C	2.52	0.52
1:A:353:LEU:HB2	1:A:453:LEU:HD21	1.91	0.52
1:A:367:LYS:O	1:A:368:PHE:HB2	2.09	0.52
1:A:659:ARG:O	1:A:663:LEU:HD13	2.10	0.52
1:A:520:LEU:HD21	1:A:610:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:TYR:O	1:A:99:VAL:HG23	2.10	0.52
1:A:161:LEU:HG	1:A:168:ILE:O	2.09	0.52
1:A:184:ALA:O	1:A:188:LEU:HG	2.10	0.52
1:A:359:TRP:CD2	1:A:626:GLN:HG2	2.44	0.52
1:A:257:LYS:O	1:A:260:GLU:HB2	2.09	0.52
1:A:312:ILE:HG13	1:A:329:GLU:O	2.10	0.52
1:A:525:LEU:HB3	1:A:530:PHE:O	2.09	0.52
1:A:716:THR:O	1:A:720:THR:HG23	2.10	0.52
1:A:71:ASP:HB2	1:A:72:PRO:CD	2.40	0.52
1:A:100:TYR:HB3	1:A:700:PHE:CE2	2.45	0.52
1:A:22:ALA:O	1:A:26:LEU:HD13	2.10	0.51
1:A:616:PRO:HA	1:A:619:GLU:CD	2.35	0.51
1:A:412:VAL:HG13	1:A:413:LEU:HD23	1.92	0.51
1:A:453:LEU:HD22	1:A:518:LEU:HD22	1.93	0.51
1:A:390:ILE:HG22	2:B:2:VAL:HA	1.91	0.51
1:A:223:GLU:HB3	1:A:224:PRO:CD	2.35	0.51
1:A:536:GLU:HA	1:A:536:GLU:OE1	2.10	0.51
1:A:584:GLU:O	1:A:609:LYS:HE3	2.11	0.51
1:A:181:ALA:O	1:A:185:GLN:HB2	2.10	0.51
1:A:6:TYR:O	1:A:114:PHE:HA	2.10	0.51
1:A:424:LEU:HB2	1:A:432:LYS:NZ	2.26	0.51
1:A:531:GLU:O	1:A:534:ASP:HB2	2.11	0.51
1:A:153:SER:OG	1:A:158:LEU:HD12	2.11	0.50
1:A:389:GLY:HA2	1:A:407:VAL:O	2.11	0.50
1:A:371:PRO:HG2	1:A:404:PHE:CZ	2.46	0.50
1:A:453:LEU:HD22	1:A:518:LEU:HD21	1.93	0.50
1:A:523:GLN:NE2	1:A:527:ILE:HG13	2.27	0.50
1:A:610:ILE:HG23	1:A:611:ARG:N	2.27	0.50
1:A:333:ALA:CB	1:A:378:VAL:HA	2.41	0.50
1:A:29:THR:CG2	1:A:30:GLU:N	2.75	0.50
1:A:499:PHE:HB2	1:A:503:ALA:HB2	1.93	0.50
1:A:648:THR:HG23	1:A:650:ALA:H	1.76	0.50
1:A:683:ASP:OD1	1:A:683:ASP:N	2.45	0.50
1:A:274:GLN:HA	1:A:277:MET:HG2	1.93	0.50
1:A:290:ILE:H	1:A:290:ILE:CD1	2.16	0.50
1:A:391:ASN:ND2	1:A:406:ASN:OD1	2.45	0.50
1:A:464:ASP:OD1	1:A:464:ASP:N	2.44	0.50
1:A:141:ARG:O	1:A:145:GLN:HB2	2.12	0.49
1:A:431:ASP:O	1:A:434:LEU:N	2.45	0.49
1:A:516:LEU:HD11	1:A:546:MET:HG2	1.94	0.49
1:A:50:LEU:HD12	1:A:57:PRO:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLN:CD	1:A:473:GLN:H	2.20	0.49
1:A:473:GLN:HG2	1:A:474:GLU:N	2.27	0.49
1:A:599:PRO:O	1:A:600:ASP:HB2	2.12	0.49
1:A:36:HIS:HB3	1:A:261:GLN:O	2.12	0.49
1:A:412:VAL:HG13	1:A:413:LEU:H	1.78	0.49
1:A:554:LEU:HD12	1:A:662:VAL:HG21	1.94	0.49
1:A:555:GLU:HA	1:A:663:LEU:HD11	1.93	0.49
1:A:148:GLY:O	1:A:151:MET:HB3	2.12	0.48
1:A:226:LEU:O	1:A:227:ASP:HB3	2.12	0.48
1:A:363:PHE:CE2	1:A:461:PHE:HE2	2.31	0.48
1:A:427:LEU:O	1:A:602:ARG:CZ	2.61	0.48
1:A:462:VAL:H	1:A:470:ASN:ND2	2.12	0.48
1:A:230:VAL:CG2	1:A:287:GLN:HB3	2.44	0.48
1:A:333:ALA:HB2	1:A:378:VAL:HA	1.94	0.48
1:A:547:VAL:HG23	1:A:603:VAL:HG11	1.96	0.48
1:A:256:GLN:O	1:A:259:VAL:HG22	2.13	0.48
1:A:272:SER:O	1:A:276:GLN:HG2	2.13	0.48
1:A:442:SER:HB2	1:A:538:VAL:HG23	1.94	0.48
1:A:390:ILE:HA	2:B:1:VAL:O	2.14	0.48
1:A:455:HIS:CD2	2:B:1:VAL:HG11	2.49	0.48
1:A:251:TYR:O	1:A:255:LEU:HD13	2.14	0.48
1:A:440:GLY:N	1:A:441:PRO:HD2	2.29	0.48
1:A:277:MET:HG3	1:A:278:LEU:N	2.28	0.47
1:A:294:LYS:O	1:A:297:SER:HB2	2.14	0.47
1:A:158:LEU:HD22	1:A:168:ILE:HD11	1.96	0.47
1:A:537:ASP:O	1:A:538:VAL:C	2.58	0.47
1:A:218:SER:HB2	1:A:286:THR:O	2.15	0.47
1:A:359:TRP:CE2	1:A:626:GLN:HG2	2.49	0.47
1:A:598:ARG:HB3	1:A:599:PRO:HD2	1.97	0.47
1:A:237:TYR:N	1:A:237:TYR:CD2	2.82	0.47
1:A:274:GLN:HE22	1:A:303:ASP:CB	2.27	0.47
1:A:350:ALA:HB3	1:A:368:PHE:HZ	1.79	0.47
1:A:392:ILE:HB	1:A:393:PRO:CA	2.43	0.47
1:A:438:TRP:NE1	1:A:537:ASP:HB3	2.28	0.47
1:A:609:LYS:HB3	1:A:613:VAL:CG2	2.45	0.47
1:A:546:MET:CG	1:A:575:ILE:HG21	2.45	0.47
1:A:341:ALA:HA	1:A:344:GLU:CD	2.40	0.47
1:A:412:VAL:HG13	1:A:413:LEU:N	2.30	0.47
1:A:505:SER:HA	1:A:567:ALA:HB1	1.97	0.47
1:A:689:TYR:CZ	1:A:699:SER:HA	2.49	0.47
1:A:369:LEU:CG	1:A:370:THR:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:PRO:CB	1:A:404:PHE:O	2.64	0.46
1:A:463:GLN:HB2	1:A:488:TRP:NE1	2.30	0.46
1:A:537:ASP:H	1:A:607:ARG:HH22	1.62	0.46
1:A:279:ALA:HA	1:A:282:ILE:HD13	1.96	0.46
1:A:312:ILE:HG12	1:A:313:GLY:N	2.31	0.46
1:A:387:PRO:O	1:A:409:LEU:HD12	2.15	0.46
1:A:471:PHE:HZ	1:A:485:ILE:CD1	2.28	0.46
1:A:412:VAL:O	1:A:415:VAL:HB	2.15	0.46
1:A:538:VAL:HG13	1:A:539:ILE:N	2.28	0.46
1:A:580:LEU:HD23	1:A:587:VAL:HG23	1.97	0.46
1:A:499:PHE:HB3	1:A:502:ILE:HG13	1.97	0.46
1:A:312:ILE:HD11	1:A:328:PHE:HZ	1.80	0.46
1:A:343:PHE:HD2	1:A:373:PHE:CD2	2.34	0.46
1:A:447:VAL:HG22	2:B:3:TYR:CE2	2.51	0.46
1:A:531:GLU:H	1:A:534:ASP:HB2	1.80	0.46
1:A:189:ASP:OD2	1:A:497:SER:HB2	2.16	0.46
1:A:182:LYS:O	1:A:185:GLN:HB3	2.17	0.45
1:A:452:LEU:HD23	1:A:453:LEU:HD11	1.99	0.45
1:A:230:VAL:O	1:A:234:LEU:HG	2.16	0.45
1:A:396:ASP:O	1:A:399:ARG:HB2	2.17	0.45
1:A:613:VAL:C	1:A:616:PRO:HD2	2.41	0.45
1:A:137:PRO:HB2	3:A:743:HOH:O	2.15	0.45
1:A:218:SER:OG	1:A:248:ARG:HB2	2.17	0.45
1:A:230:VAL:HG21	1:A:287:GLN:HB3	1.98	0.45
1:A:369:LEU:CG	1:A:370:THR:H	2.29	0.45
1:A:143:LEU:O	1:A:146:THR:N	2.47	0.45
1:A:354:LEU:N	1:A:354:LEU:HD12	2.31	0.45
1:A:263:GLU:HA	1:A:266:LYS:CG	2.46	0.45
1:A:447:VAL:HG22	2:B:3:TYR:CD2	2.51	0.45
1:A:438:TRP:CD1	1:A:537:ASP:HB3	2.52	0.45
1:A:242:SER:HA	1:A:243:PRO:HD3	1.66	0.45
1:A:279:ALA:O	1:A:282:ILE:HB	2.16	0.45
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.80	0.45
1:A:536:GLU:O	1:A:537:ASP:HB2	2.17	0.45
1:A:363:PHE:HE2	1:A:461:PHE:HE2	1.65	0.44
1:A:432:LYS:HG3	1:A:432:LYS:H	1.63	0.44
1:A:445:VAL:HG22	1:A:528:PHE:CD2	2.52	0.44
1:A:673:VAL:HG13	1:A:696:LEU:HA	1.99	0.44
1:A:138:GLU:HB2	1:A:139:GLU:OE1	2.18	0.44
1:A:575:ILE:HG22	1:A:576:LEU:N	2.32	0.44
1:A:266:LYS:NZ	1:A:275:GLY:O	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:THR:HG23	1:A:402:GLU:H	1.82	0.44
1:A:449:LEU:HD11	1:A:524:VAL:HG11	1.99	0.44
1:A:57:PRO:HB3	1:A:715:LEU:HB3	1.99	0.44
1:A:331:PHE:HA	1:A:380:THR:O	2.18	0.44
1:A:598:ARG:HB3	1:A:599:PRO:CD	2.47	0.44
1:A:122:LYS:O	1:A:125:ARG:HB2	2.18	0.44
1:A:319:ARG:HD3	1:A:327:GLU:OE2	2.18	0.44
1:A:35:TYR:C	1:A:35:TYR:CD2	2.95	0.44
1:A:294:LYS:HG2	1:A:395:TYR:CE2	2.52	0.44
1:A:397:ASP:OD1	1:A:397:ASP:N	2.51	0.44
1:A:689:TYR:CE2	1:A:699:SER:HA	2.53	0.44
1:A:464:ASP:O	1:A:465:GLU:C	2.60	0.44
1:A:696:LEU:O	1:A:696:LEU:HD23	2.17	0.44
1:A:108:SER:HB2	1:A:384:SER:HB2	2.00	0.43
1:A:37:LEU:HD11	1:A:265:ALA:CB	2.46	0.43
1:A:354:LEU:HD12	1:A:354:LEU:H	1.83	0.43
1:A:426:PHE:HA	1:A:601:ALA:O	2.18	0.43
1:A:37:LEU:N	1:A:37:LEU:CD1	2.82	0.43
1:A:89:TYR:CE2	1:A:93:LEU:HD11	2.53	0.43
1:A:179:GLU:OE1	1:A:179:GLU:N	2.48	0.43
1:A:192:ASN:OD1	1:A:192:ASN:O	2.36	0.43
1:A:274:GLN:HG3	1:A:277:MET:HE2	2.00	0.43
1:A:461:PHE:O	1:A:488:TRP:HB2	2.18	0.43
1:A:169:THR:HG21	1:A:321:PRO:HG2	1.99	0.43
1:A:409:LEU:HB2	1:A:412:VAL:CG1	2.48	0.43
1:A:609:LYS:O	1:A:613:VAL:HG23	2.19	0.43
1:A:540:TYR:CD1	1:A:607:ARG:HB3	2.54	0.43
1:A:354:LEU:H	1:A:354:LEU:CD1	2.31	0.43
1:A:431:ASP:O	1:A:432:LYS:C	2.60	0.43
1:A:449:LEU:HD23	1:A:518:LEU:HB2	2.00	0.43
1:A:30:GLU:OE2	1:A:307:ILE:HG21	2.19	0.43
1:A:271:ASN:OD1	1:A:273:HIS:HB2	2.19	0.43
1:A:438:TRP:CE2	1:A:537:ASP:HB3	2.54	0.43
1:A:517:TYR:HE2	1:A:615:LYS:HE2	1.84	0.43
1:A:413:LEU:C	1:A:415:VAL:N	2.76	0.42
1:A:471:PHE:HZ	1:A:485:ILE:HD13	1.84	0.42
1:A:586:LEU:HD22	1:A:613:VAL:HG23	2.00	0.42
1:A:95:TYR:CG	1:A:116:PRO:HG3	2.53	0.42
1:A:604:ARG:HG2	1:A:604:ARG:HH21	1.83	0.42
1:A:228:SER:O	1:A:231:THR:HB	2.19	0.42
1:A:409:LEU:HB2	1:A:412:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:GLN:HG2	1:A:569:MET:H	1.83	0.42
1:A:649:ASP:OD1	1:A:654:CYS:HB3	2.19	0.42
1:A:680:GLU:HA	1:A:680:GLU:OE1	2.19	0.42
1:A:42:TRP:HA	1:A:42:TRP:CE3	2.53	0.42
1:A:100:TYR:HB3	1:A:700:PHE:CD2	2.54	0.42
1:A:185:GLN:HG2	1:A:322:PHE:CZ	2.55	0.42
1:A:195:ALA:O	1:A:325:ARG:HA	2.19	0.42
1:A:464:ASP:OD1	1:A:468:ALA:O	2.37	0.42
1:A:358:PRO:HG2	1:A:359:TRP:CZ3	2.54	0.42
1:A:368:PHE:CG	1:A:369:LEU:N	2.86	0.42
1:A:40:ALA:HB1	1:A:258:VAL:HG13	2.00	0.42
1:A:90:GLN:HA	1:A:93:LEU:HD12	2.02	0.42
1:A:430:ASP:O	1:A:432:LYS:N	2.52	0.42
1:A:309:GLU:HG2	1:A:376:LEU:HD21	2.02	0.42
1:A:109:PHE:CE1	1:A:566:GLN:NE2	2.82	0.42
1:A:443:PHE:O	1:A:447:VAL:HG23	2.20	0.42
1:A:431:ASP:O	1:A:433:ASP:N	2.53	0.41
1:A:536:GLU:O	1:A:538:VAL:N	2.53	0.41
1:A:602:ARG:NH1	3:A:741:HOH:O	2.51	0.41
1:A:37:LEU:CD1	1:A:265:ALA:CB	2.98	0.41
1:A:172:PHE:CD1	1:A:200:LEU:HB3	2.55	0.41
1:A:219:VAL:HG23	1:A:220:LEU:N	2.33	0.41
1:A:417:TYR:HE1	1:A:440:GLY:HA2	1.85	0.41
1:A:120:LYS:HZ1	1:A:148:GLY:C	2.27	0.41
1:A:42:TRP:CZ2	1:A:380:THR:HG23	2.55	0.41
1:A:424:LEU:HD23	1:A:424:LEU:HA	1.73	0.41
1:A:686:LEU:O	1:A:687:LEU:HD23	2.21	0.41
1:A:223:GLU:O	1:A:224:PRO:C	2.61	0.41
1:A:400:GLN:HG2	1:A:401:THR:N	2.36	0.41
1:A:477:ILE:HG23	1:A:483:GLU:O	2.20	0.41
1:A:537:ASP:O	1:A:540:TYR:N	2.53	0.41
1:A:580:LEU:HA	1:A:587:VAL:CG2	2.51	0.41
1:A:621:PHE:CE1	1:A:644:TYR:CE2	3.07	0.41
1:A:109:PHE:CZ	1:A:569:MET:HE2	2.55	0.41
1:A:269:ALA:HB1	1:A:274:GLN:HB2	2.02	0.41
1:A:371:PRO:HB3	1:A:404:PHE:H	1.84	0.41
1:A:35:TYR:CZ	1:A:679:LEU:HB2	2.55	0.41
1:A:312:ILE:CG1	1:A:313:GLY:N	2.83	0.41
1:A:230:VAL:HG21	1:A:287:GLN:O	2.21	0.41
1:A:263:GLU:HG3	1:A:264:LYS:HD2	2.03	0.41
1:A:347:VAL:HG12	1:A:370:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:PRO:HG2	1:A:404:PHE:CE1	2.55	0.41
1:A:590:THR:O	1:A:592:THR:HG23	2.19	0.41
1:A:624:ARG:NH2	1:A:640:LEU:HD22	2.36	0.41
1:A:239:PHE:HB2	1:A:244:PHE:HD1	1.86	0.41
1:A:263:GLU:HA	1:A:266:LYS:CD	2.51	0.41
1:A:390:ILE:HG12	1:A:407:VAL:HB	2.02	0.41
1:A:502:ILE:O	1:A:503:ALA:C	2.64	0.41
1:A:174:GLY:HA3	1:A:725:PHE:O	2.21	0.40
1:A:230:VAL:HG13	1:A:289:SER:OG	2.21	0.40
1:A:252:ALA:N	1:A:253:PRO:HD2	2.36	0.40
1:A:343:PHE:O	1:A:346:LEU:N	2.54	0.40
1:A:532:GLY:C	1:A:534:ASP:H	2.29	0.40
1:A:539:ILE:O	1:A:542:ASN:HB3	2.21	0.40
1:A:540:TYR:CE1	1:A:607:ARG:HB3	2.56	0.40
1:A:634:VAL:O	1:A:638:ARG:HG3	2.21	0.40
1:A:686:LEU:C	1:A:687:LEU:HD23	2.46	0.40
1:A:128:LEU:O	1:A:133:ALA:HB3	2.21	0.40
1:A:559:PRO:O	1:A:562:PHE:CD1	2.74	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	718/726 (99%)	634 (88%)	82 (11%)	2 (0%)	36	67
2	B	3/5 (60%)	3 (100%)	0	0	100	100
All	All	721/731 (99%)	637 (88%)	82 (11%)	2 (0%)	36	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	PHE
1	A	538	VAL

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	606/609 (100%)	566 (93%)	40 (7%)	15	44
2	B	5/5 (100%)	5 (100%)	0	100	100
All	All	611/614 (100%)	571 (94%)	40 (6%)	15	45

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	29	THR
1	A	86	GLU
1	A	139	GLU
1	A	145	GLN
1	A	161	LEU
1	A	168	ILE
1	A	198	THR
1	A	237	TYR
1	A	242	SER
1	A	251	TYR
1	A	268	TYR
1	A	290	ILE
1	A	303	ASP
1	A	310	SER
1	A	312	ILE
1	A	332	VAL
1	A	334	VAL
1	A	336	ASN
1	A	351	GLU
1	A	363	PHE
1	A	364	GLU

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Mol	Chain	Res	Type
1	A	374	THR
1	A	379	LEU
1	A	392	ILE
1	A	401	THR
1	A	412	VAL
1	A	460	LEU
1	A	485	ILE
1	A	504	SER
1	A	514	VAL
1	A	519	CYS
1	A	575	ILE
1	A	588	THR
1	A	590	THR
1	A	613	VAL
1	A	653	GLU
1	A	666	LYS
1	A	683	ASP
1	A	710	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	160	HIS
1	A	274	GLN
1	A	391	ASN
1	A	406	ASN
1	A	545	ASN
1	A	674	GLN

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 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	722/726 (99%)	1.01	99 (13%) 6 5	8, 64, 132, 234	0
2	B	5/5 (100%)	0.99	0 100 100	39, 46, 63, 80	0
All	All	727/731 (99%)	1.01	99 (13%) 7 5	8, 64, 132, 234	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	GLY	5.0
1	A	533	ALA	4.6
1	A	491	SER	4.5
1	A	567	ALA	4.2
1	A	589	ILE	3.9
1	A	370	THR	3.9
1	A	403	GLY	3.9
1	A	341	ALA	3.8
1	A	283	GLU	3.7
1	A	262	LEU	3.7
1	A	19	CYS	3.6
1	A	417	TYR	3.6
1	A	195	ALA	3.5
1	A	492	GLY	3.5
1	A	414	ALA	3.4
1	A	346	LEU	3.4
1	A	571	ALA	3.3
1	A	83	GLY	3.3
1	A	405	LYS	3.3
1	A	224	PRO	3.2
1	A	691	ALA	3.2
1	A	373	PHE	3.2
1	A	324	SER	3.2
1	A	489	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	269	ALA	3.1
1	A	227	ASP	3.1
1	A	372	ASP	3.1
1	A	469	PHE	3.1
1	A	494	THR	3.0
1	A	226	LEU	3.0
1	A	684	VAL	3.0
1	A	354	LEU	3.0
1	A	498	LYS	3.0
1	A	120	LYS	2.9
1	A	219	VAL	2.9
1	A	79	ALA	2.9
1	A	616	PRO	2.9
1	A	255	LEU	2.8
1	A	603	VAL	2.8
1	A	362	THR	2.8
1	A	681	GLY	2.8
1	A	454	GLY	2.7
1	A	20	ARG	2.7
1	A	212	TYR	2.7
1	A	517	TYR	2.7
1	A	359	TRP	2.6
1	A	402	GLU	2.6
1	A	263	GLU	2.6
1	A	356	GLU	2.6
1	A	400	GLN	2.5
1	A	394	ASN	2.5
1	A	636	GLY	2.5
1	A	252	ALA	2.5
1	A	475	THR	2.5
1	A	515	GLY	2.5
1	A	538	VAL	2.5
1	A	490	ARG	2.5
1	A	401	THR	2.5
1	A	44	GLY	2.4
1	A	222	SER	2.4
1	A	363	PHE	2.4
1	A	415	VAL	2.4
1	A	267	ALA	2.4
1	A	367	LYS	2.4
1	A	221	GLY	2.3
1	A	29	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	127	ILE	2.3
1	A	637	GLY	2.3
1	A	478	ASN	2.3
1	A	217	ALA	2.3
1	A	440	GLY	2.2
1	A	566	GLN	2.2
1	A	338	ALA	2.2
1	A	613	VAL	2.2
1	A	4	THR	2.2
1	A	45	GLY	2.2
1	A	594	GLY	2.2
1	A	365	LYS	2.2
1	A	34	ALA	2.2
1	A	292	ALA	2.2
1	A	476	VAL	2.2
1	A	142	GLY	2.2
1	A	220	LEU	2.2
1	A	464	ASP	2.1
1	A	208	GLY	2.1
1	A	287	GLN	2.1
1	A	204	VAL	2.1
1	A	335	VAL	2.1
1	A	614	GLY	2.1
1	A	272	SER	2.1
1	A	303	ASP	2.1
1	A	2	ALA	2.1
1	A	12	ILE	2.0
1	A	472	ASP	2.0
1	A	344	GLU	2.0
1	A	514	VAL	2.0
1	A	371	PRO	2.0
1	A	467	GLY	2.0
1	A	286	THR	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.