



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 10:29 PM EDT

PDB ID : 1GXR / pdb_00001gxr
Title : WD40 Region of Human Groucho/TLE1
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Deposited on : 2002-04-10
Resolution : 1.65 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

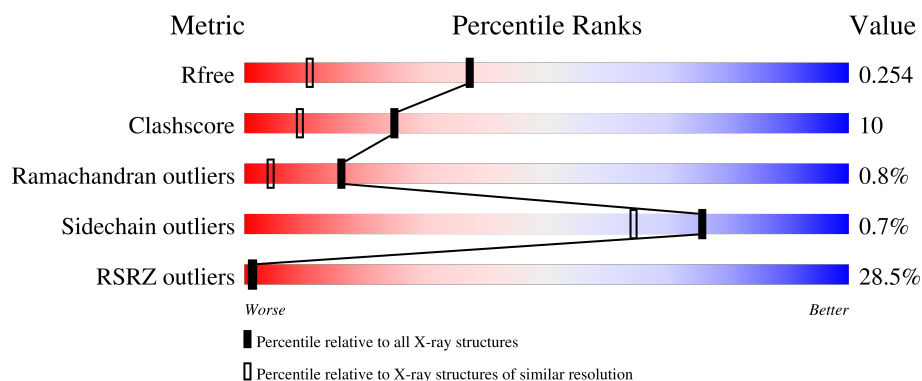
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	337	15% 79% 19% ..
1	B	337	41% 74% 21% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5594 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 TRANSDUCIN-LIKE ENHANCER PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2562	1613	442	490	17			
1	B	324	Total	C	N	O	S	0	0	0
			2467	1558	422	471	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	464	ASP	THR	SEE REMARK 999	UNP Q04724
A	465	ALA	PRO	SEE REMARK 999	UNP Q04724
B	464	ASP	THR	SEE REMARK 999	UNP Q04724
B	465	ALA	PRO	SEE REMARK 999	UNP Q04724

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

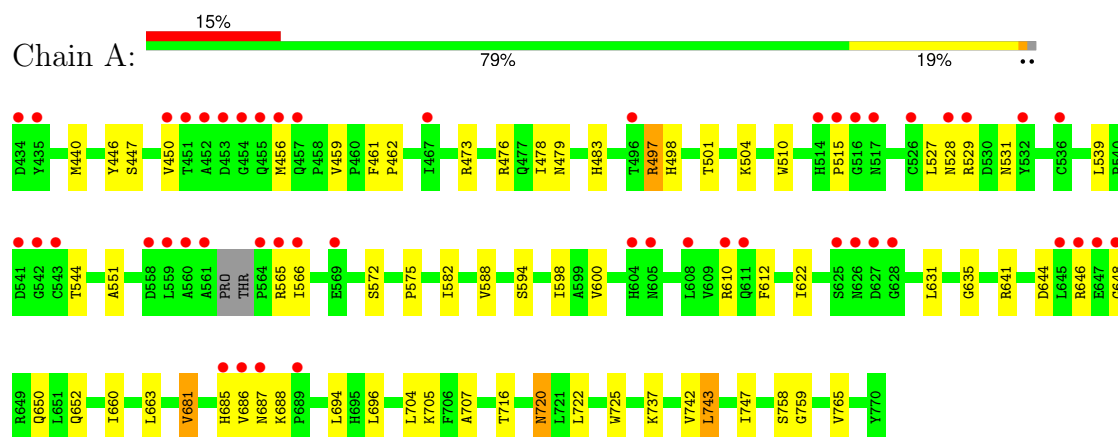
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	335	Total	O	0	0
			335	335		
3	B	229	Total	O	0	0
			229	229		

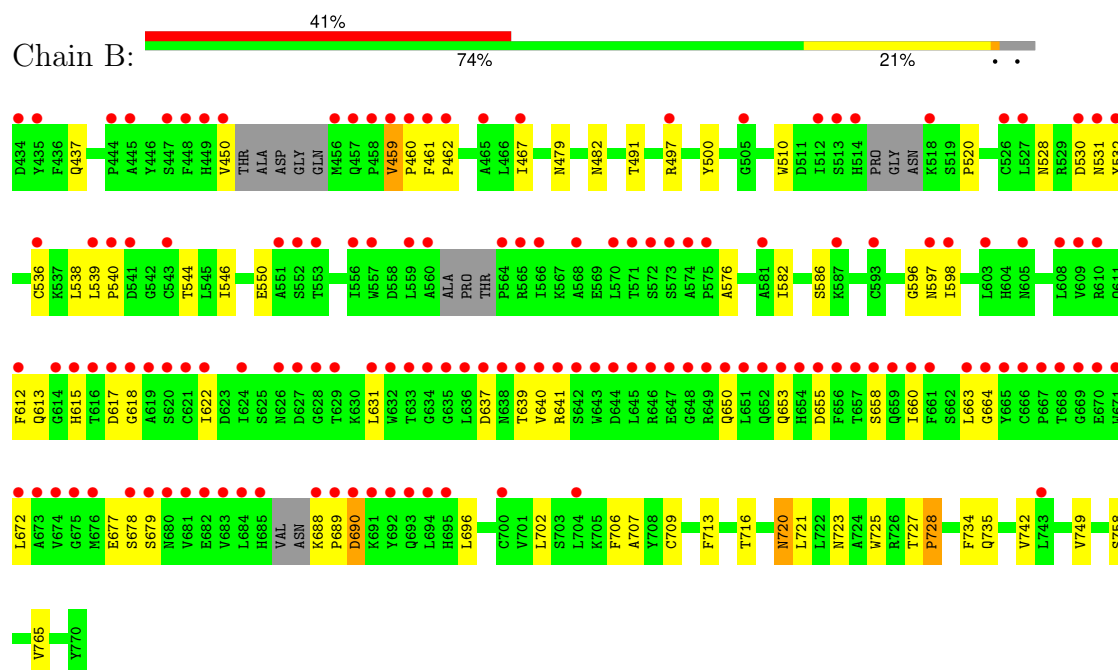
3 Residue-property plots

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: TRANSDUCIN-LIKE ENHANCER PROTEIN 1



• Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.41 Å 56.66 Å 102.03 Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	40.45 – 1.65 40.45 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.45-1.65) 100.0 (40.45-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 1.60 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.256 0.229 , 0.254	Depositor DCC
R_{free} test set	4185 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5594	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.33% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.35	0/2626	0.93	8/3573 (0.2%)
1	B	0.31	0/2525	0.85	6/3429 (0.2%)
All	All	0.33	0/5151	0.89	14/7002 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	681	VAL	N-CA-C	-6.47	99.05	108.11
1	A	758	SER	N-CA-C	6.47	120.07	109.72
1	B	707	ALA	N-CA-C	-6.33	101.58	110.50
1	A	459	VAL	N-CA-C	6.22	113.98	108.63
1	B	459	VAL	N-CA-C	6.04	113.86	107.76
1	B	758	SER	N-CA-C	5.80	119.02	109.85
1	B	702	LEU	N-CA-C	5.77	117.65	111.36
1	A	707	ALA	N-CA-C	-5.75	102.40	110.50
1	A	759	GLY	N-CA-C	-5.71	108.39	114.67
1	B	721	LEU	N-CA-C	5.25	118.05	109.59
1	B	709	CYS	N-CA-C	-5.25	106.83	113.18
1	A	722	LEU	N-CA-C	-5.16	100.11	108.52
1	A	635	GLY	N-CA-C	5.12	118.57	111.10
1	A	473	ARG	N-CA-C	-5.08	107.21	113.41

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	2562	0	2471	48	0
1	B	2467	0	2357	52	0
2	A	1	0	0	0	0
3	A	335	0	0	9	0
3	B	229	0	0	4	0
All	All	5594	0	4828	97	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 10.

All (97) 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:447:SER:H	1:B:437:GLN:HE22	1.24	0.84
1:B:658:SER:HB2	1:B:677:GLU:HB3	1.59	0.83
1:B:749:VAL:HG22	3:B:2053:HOH:O	1.79	0.80
1:B:622:ILE:HD11	1:B:631:LEU:HD11	1.65	0.76
1:B:528:ASN:HB3	1:B:531:ASN:ND2	2.10	0.65
1:B:720:ASN:HD22	1:B:720:ASN:N	1.95	0.65
1:A:483:HIS:HD2	1:A:501:THR:OG1	1.81	0.62
1:B:696:LEU:HB2	1:B:725:TRP:HH2	1.66	0.61
1:B:491:THR:HG22	1:B:500:TYR:HB2	1.84	0.60
1:A:641:ARG:HH11	1:A:650:GLN:HE22	1.50	0.60
1:A:446:TYR:H	1:B:437:GLN:NE2	2.00	0.59
1:B:696:LEU:HB2	1:B:725:TRP:CH2	2.37	0.59
1:A:572:SER:HB2	3:A:2198:HOH:O	2.01	0.59
1:A:720:ASN:HD22	1:A:720:ASN:N	2.01	0.58
1:A:716:THR:HB	1:A:742:VAL:HB	1.86	0.58
1:A:598:ILE:HB	1:A:612:PHE:HB2	1.86	0.58
1:A:644:ASP:OD1	1:A:646:ARG:HG2	2.05	0.57
1:A:504:LYS:HG2	1:A:529:ARG:O	2.05	0.56
1:B:550:GLU:HA	1:B:576:ALA:HB1	1.88	0.56
1:A:528:ASN:HB3	1:A:531:ASN:ND2	2.21	0.55
1:A:622:ILE:HD11	1:A:631:LEU:HD11	1.88	0.55
1:B:598:ILE:HB	1:B:612:PHE:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:ASN:HD21	1:B:530:ASP:HB2	1.72	0.54
1:B:479:ASN:HB2	1:B:765:VAL:HB	1.89	0.54
1:B:639:THR:HB	1:B:653:GLN:NE2	2.23	0.54
1:A:483:HIS:HE1	3:A:2059:HOH:O	1.90	0.53
1:A:660:ILE:HD12	1:A:660:ILE:N	2.23	0.53
1:A:539:LEU:HD13	1:A:582:ILE:HG21	1.91	0.53
1:B:716:THR:HB	1:B:742:VAL:HB	1.90	0.53
1:B:639:THR:HB	1:B:653:GLN:HE22	1.73	0.52
1:A:478:ILE:HG13	1:A:479:ASN:HD22	1.75	0.52
1:A:575:PRO:HG2	1:A:594:SER:OG	2.10	0.52
1:B:641:ARG:HD3	1:B:650:GLN:CD	2.35	0.52
1:A:539:LEU:HD23	1:A:544:THR:HB	1.91	0.51
1:A:663:LEU:C	1:A:663:LEU:HD12	2.35	0.51
1:B:617:ASP:HB2	1:B:637:ASP:HB3	1.92	0.51
1:B:660:ILE:N	1:B:660:ILE:HD12	2.26	0.51
1:A:743:LEU:N	1:A:743:LEU:HD22	2.26	0.51
1:B:510:TRP:CH2	1:B:520:PRO:HG3	2.45	0.51
1:B:615:HIS:HB3	1:B:617:ASP:O	2.11	0.51
1:A:663:LEU:HA	1:A:704:LEU:HD21	1.92	0.50
1:B:640:VAL:CG2	1:B:660:ILE:HG12	2.42	0.50
1:B:655:ASP:HA	3:B:2143:HOH:O	2.11	0.50
1:A:479:ASN:HB2	1:A:765:VAL:HB	1.94	0.49
1:B:532:TYR:HB2	1:B:550:GLU:OE1	2.13	0.49
1:A:696:LEU:HB2	1:A:725:TRP:CH2	2.48	0.49
1:A:652:GLN:HG2	3:A:2194:HOH:O	2.13	0.49
1:B:546:ILE:HD12	1:B:582:ILE:HD11	1.95	0.48
1:B:640:VAL:HG23	1:B:660:ILE:HG12	1.94	0.48
1:B:596:GLY:N	1:B:618:GLY:HA2	2.29	0.48
1:A:565:ARG:HA	3:A:2113:HOH:O	2.15	0.47
1:B:500:TYR:CE1	1:B:538:LEU:HD11	2.50	0.47
1:B:531:ASN:HA	3:B:2071:HOH:O	2.13	0.47
1:B:550:GLU:HA	1:B:576:ALA:CB	2.44	0.47
1:B:641:ARG:HD3	1:B:650:GLN:OE1	2.15	0.46
1:B:536:CYS:HA	1:B:546:ILE:O	2.16	0.46
1:B:540:PRO:HG2	1:B:586:SER:OG	2.16	0.46
1:A:450:VAL:HG22	1:A:456:MET:HG2	1.97	0.46
1:A:743:LEU:HD22	1:A:743:LEU:H	1.81	0.45
1:A:476:ARG:NH1	1:A:478:ILE:HG22	2.32	0.45
1:A:528:ASN:HD22	1:A:529:ARG:H	1.64	0.45
1:A:588:VAL:HG11	1:A:600:VAL:HG13	1.98	0.45
1:A:497:ARG:HB3	3:A:2055:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ASN:ND2	3:A:2037:HOH:O	2.42	0.45
1:A:685:HIS:NE2	1:A:688:LYS:HD2	2.32	0.45
1:B:539:LEU:HD12	1:B:544:THR:HB	1.99	0.44
1:A:515:PRO:HB3	3:A:2068:HOH:O	2.16	0.44
1:B:688:LYS:HG2	1:B:689:PRO:N	2.33	0.44
1:B:723:ASN:ND2	1:B:735:GLN:HG2	2.32	0.44
1:B:450:VAL:O	1:B:690:ASP:HA	2.18	0.44
1:B:528:ASN:C	1:B:530:ASP:H	2.25	0.44
1:B:664:GLY:O	1:B:672:LEU:HD12	2.18	0.44
1:A:737:LYS:HE3	3:A:2304:HOH:O	2.17	0.44
1:B:637:ASP:O	1:B:639:THR:HG23	2.18	0.44
1:A:566:ILE:O	1:A:566:ILE:HG23	2.18	0.44
1:B:720:ASN:N	1:B:720:ASN:ND2	2.61	0.44
1:A:461:PHE:HA	1:A:462:PRO:HD3	1.89	0.44
1:B:482:ASN:ND2	3:B:2040:HOH:O	2.50	0.44
1:A:527:LEU:HD22	1:A:551:ALA:HB3	2.00	0.43
1:B:723:ASN:HD22	1:B:735:GLN:HG2	1.83	0.43
1:B:461:PHE:HA	1:B:462:PRO:HD3	1.90	0.43
1:B:459:VAL:HA	1:B:460:PRO:HD3	1.89	0.43
1:A:497:ARG:HE	1:A:498:HIS:CE1	2.36	0.43
1:A:504:LYS:HE2	3:A:2043:HOH:O	2.19	0.42
1:A:440:MET:HE3	1:B:467:ILE:HD11	2.01	0.42
1:B:734:PHE:C	1:B:734:PHE:CD1	2.97	0.42
1:A:681:VAL:HB	1:A:694:LEU:HB2	2.02	0.42
1:B:597:ASN:OD1	1:B:613:GLN:HG2	2.20	0.42
1:B:727:THR:HA	1:B:728:PRO:HA	1.88	0.41
1:A:610:ARG:CZ	1:A:648:GLY:HA3	2.50	0.41
1:B:706:PHE:HA	1:B:713:PHE:CB	2.51	0.41
1:A:498:HIS:HA	1:A:510:TRP:O	2.20	0.41
1:A:686:VAL:HG12	1:A:687:ASN:ND2	2.36	0.41
1:B:663:LEU:HD23	1:B:663:LEU:C	2.46	0.41
1:A:705:LYS:HZ2	1:A:747:ILE:H	1.69	0.41
1:A:610:ARG:HH11	1:A:610:ARG:HG2	1.85	0.41
1:A:497:ARG:HG3	1:A:498:HIS:ND1	2.37	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	331/337 (98%)	317 (96%)	13 (4%)	1 (0%)	36	21
1	B	314/337 (93%)	292 (93%)	18 (6%)	4 (1%)	9	1
All	All	645/674 (96%)	609 (94%)	31 (5%)	5 (1%)	16	4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	679	SER
1	B	678	SER
1	B	497	ARG
1	B	690	ASP
1	A	497	ARG

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	283/288 (98%)	281 (99%)	2 (1%)	76	64
1	B	268/288 (93%)	266 (99%)	2 (1%)	76	64
All	All	551/576 (96%)	547 (99%)	4 (1%)	76	64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	720	ASN

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Mol	Chain	Res	Type
1	A	743	LEU
1	B	720	ASN
1	B	728	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	479	ASN
1	A	483	HIS
1	A	528	ASN
1	A	531	ASN
1	A	650	GLN
1	A	652	GLN
1	A	680	ASN
1	A	687	ASN
1	A	720	ASN
1	A	735	GLN
1	B	437	GLN
1	B	477	GLN
1	B	482	ASN
1	B	523	GLN
1	B	528	ASN
1	B	531	ASN
1	B	605	ASN
1	B	606	GLN
1	B	652	GLN
1	B	654	HIS
1	B	659	GLN
1	B	720	ASN
1	B	723	ASN
1	B	735	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	335/337 (99%)	0.84	49 (14%) 6 6	15, 24, 47, 59	0
1	B	324/337 (96%)	1.80	139 (42%) 0 0	16, 35, 50, 58	0
All	All	659/674 (97%)	1.31	188 (28%) 1 1	15, 29, 50, 59	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	689	PRO	7.0
1	A	561	ALA	6.0
1	A	454	GLY	5.9
1	B	683	VAL	5.7
1	A	452	ALA	5.5
1	B	655	ASP	5.3
1	B	612	PHE	5.3
1	B	640	VAL	5.2
1	B	678	SER	5.1
1	B	649	ARG	5.0
1	B	656	PHE	5.0
1	B	637	ASP	4.8
1	B	648	GLY	4.7
1	B	643	TRP	4.7
1	B	672	LEU	4.7
1	B	617	ASP	4.7
1	B	450	VAL	4.6
1	B	628	GLY	4.6
1	B	651	LEU	4.5
1	B	671	TRP	4.5
1	B	514	HIS	4.4
1	B	639	THR	4.4
1	B	448	PHE	4.4
1	B	459	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	435	TYR	4.2
1	B	676	MET	4.2
1	B	636	LEU	4.2
1	B	692	TYR	4.2
1	B	684	LEU	4.1
1	A	434	ASP	4.1
1	B	659	GLN	4.0
1	B	690	ASP	4.0
1	B	445	ALA	4.0
1	B	638	ASN	4.0
1	B	458	PRO	3.9
1	A	626	ASN	3.9
1	B	660	ILE	3.9
1	B	616	THR	3.9
1	B	642	SER	3.9
1	B	532	TYR	3.8
1	B	681	VAL	3.8
1	A	516	GLY	3.8
1	B	614	GLY	3.8
1	B	657	THR	3.8
1	B	674	VAL	3.8
1	B	635	GLY	3.7
1	A	565	ARG	3.7
1	B	685	HIS	3.7
1	B	669	GLY	3.7
1	B	647	GLU	3.7
1	B	449	HIS	3.7
1	A	559	LEU	3.6
1	A	514	HIS	3.6
1	B	663	LEU	3.6
1	B	543	CYS	3.6
1	B	653	GLN	3.6
1	A	566	ILE	3.6
1	B	564	PRO	3.5
1	A	456	MET	3.5
1	B	541	ASP	3.5
1	A	457	GLN	3.5
1	A	686	VAL	3.5
1	A	646	ARG	3.5
1	B	634	GLY	3.5
1	A	515	PRO	3.4
1	B	666	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	641	ARG	3.4
1	B	646	ARG	3.4
1	A	610	ARG	3.4
1	B	435	TYR	3.3
1	B	654	HIS	3.3
1	A	558	ASP	3.3
1	B	551	ALA	3.3
1	A	564	PRO	3.3
1	B	571	THR	3.2
1	B	644	ASP	3.1
1	B	670	GLU	3.1
1	B	566	ILE	3.1
1	B	618	GLY	3.1
1	B	743	LEU	3.1
1	B	652	GLN	3.1
1	B	682	GLU	3.1
1	B	560	ALA	3.1
1	B	694	LEU	3.0
1	B	704	LEU	3.0
1	A	560	ALA	3.0
1	B	539	LEU	3.0
1	A	543	CYS	3.0
1	B	572	SER	3.0
1	B	573	SER	3.0
1	A	542	GLY	3.0
1	B	609	VAL	2.9
1	B	574	ALA	2.9
1	B	632	TRP	2.9
1	B	680	ASN	2.9
1	B	615	HIS	2.9
1	B	679	SER	2.9
1	B	505	GLY	2.9
1	B	565	ARG	2.9
1	A	627	ASP	2.9
1	A	604	HIS	2.8
1	A	689	PRO	2.8
1	B	575	PRO	2.8
1	A	648	GLY	2.8
1	B	462	PRO	2.8
1	B	608	LEU	2.8
1	A	687	ASN	2.7
1	B	540	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	627	ASP	2.7
1	A	451	THR	2.7
1	B	434	ASP	2.7
1	B	527	LEU	2.7
1	B	691	LYS	2.7
1	A	526	CYS	2.7
1	B	605	ASN	2.7
1	B	530	ASP	2.7
1	B	633	THR	2.6
1	B	675	GLY	2.6
1	B	665	TYR	2.6
1	B	456	MET	2.6
1	B	461	PHE	2.6
1	A	608	LEU	2.6
1	B	593	CYS	2.6
1	B	620	SER	2.6
1	B	673	ALA	2.6
1	A	645	LEU	2.6
1	B	645	LEU	2.6
1	A	605	ASN	2.6
1	A	453	ASP	2.5
1	B	457	GLN	2.5
1	B	587	LYS	2.5
1	B	570	LEU	2.5
1	B	693	GLN	2.5
1	B	664	GLY	2.5
1	B	559	LEU	2.5
1	B	465	ALA	2.5
1	B	526	CYS	2.4
1	A	628	GLY	2.4
1	B	667	PRO	2.4
1	B	552	SER	2.4
1	B	661	PHE	2.4
1	B	597	ASN	2.4
1	B	658	SER	2.4
1	A	611	GLN	2.4
1	B	650	GLN	2.3
1	A	625	SER	2.3
1	A	528	ASN	2.3
1	B	688	LYS	2.3
1	B	568	ALA	2.3
1	B	631	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	622	ILE	2.3
1	A	529	ARG	2.3
1	B	553	THR	2.3
1	A	536	CYS	2.3
1	B	531	ASN	2.3
1	A	467	ILE	2.3
1	B	460	PRO	2.2
1	B	610	ARG	2.2
1	B	603	LEU	2.2
1	B	598	ILE	2.2
1	A	455	GLN	2.2
1	B	581	ALA	2.2
1	B	536	CYS	2.2
1	A	532	TYR	2.2
1	B	629	THR	2.2
1	B	668	THR	2.2
1	B	447	SER	2.2
1	B	513	SER	2.2
1	A	541	ASP	2.1
1	B	626	ASN	2.1
1	B	556	ILE	2.1
1	A	685	HIS	2.1
1	B	621	CYS	2.1
1	A	569	GLU	2.1
1	A	647	GLU	2.1
1	B	444	PRO	2.1
1	B	624	ILE	2.1
1	B	619	ALA	2.1
1	A	450	VAL	2.1
1	B	700	CYS	2.1
1	B	467	ILE	2.1
1	A	517	ASN	2.0
1	B	497	ARG	2.0
1	A	496	THR	2.0
1	B	695	HIS	2.0
1	B	557	TRP	2.0
1	B	512	ILE	2.0
1	B	518	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	1003	1/1	0.93	0.25	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.