



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:59 AM UTC

PDB ID : 1MI1 / pdb_00001mi1
Title : Crystal Structure of the PH-BEACH Domain of Human Neurobeachin
Authors : Jogl, G.; Shen, Y.; Gebauer, D.; Li, J.; Wiegmann, K.; Kashkar, H.; Kroenke, M.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2002-08-21
Resolution : 2.90 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
Mogul : 2022.3.0, CSD as543be (2022)
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

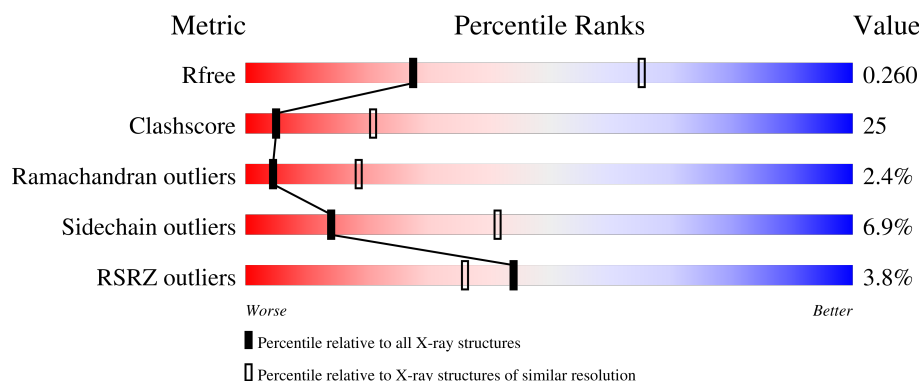
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	414	
1	B	414	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6654 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 Neurobeachin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	Se	0	0	0
			3381	2168	571	633	1	8			
1	B	400	Total	C	N	O	S	Se	0	0	0
			3273	2101	552	611	1	8			

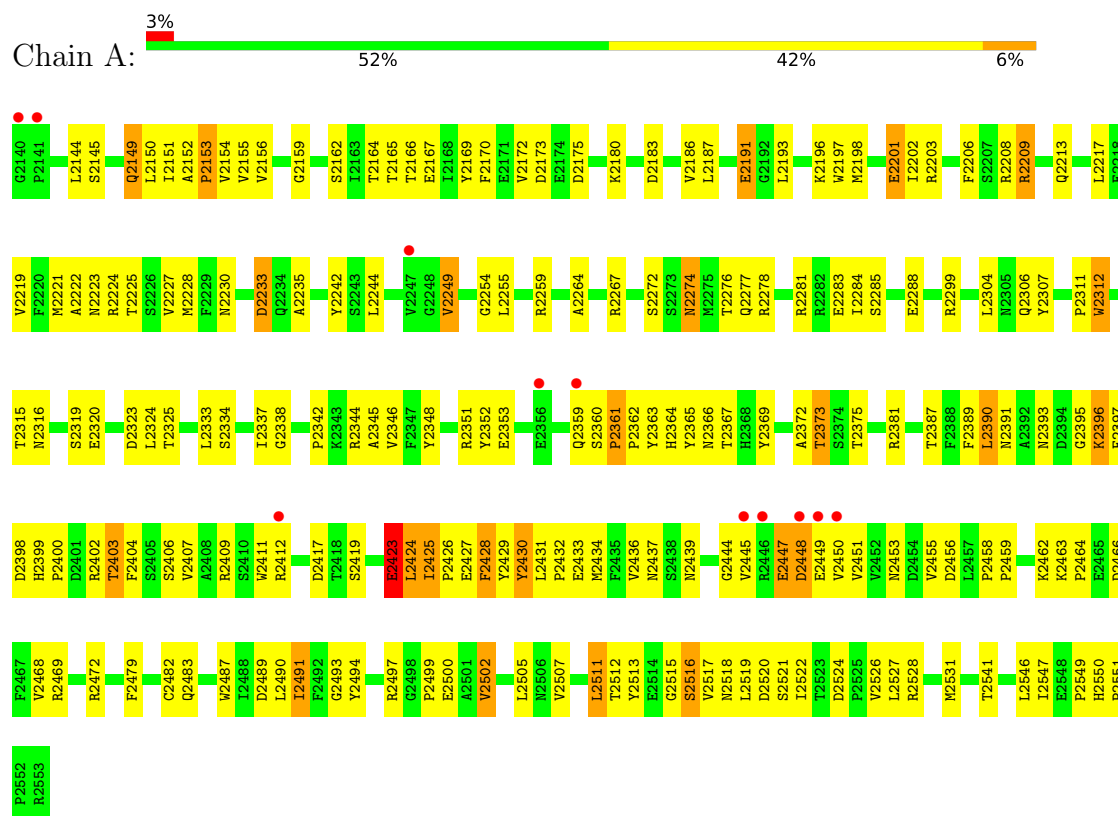
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2198	MSE	MET	cloning artifact	UNP Q8NFP9
A	2221	MSE	MET	cloning artifact	UNP Q8NFP9
A	2228	MSE	MET	cloning artifact	UNP Q8NFP9
A	2275	MSE	MET	cloning artifact	UNP Q8NFP9
A	2291	MSE	MET	cloning artifact	UNP Q8NFP9
A	2434	MSE	MET	cloning artifact	UNP Q8NFP9
A	2473	MSE	MET	cloning artifact	UNP Q8NFP9
A	2531	MSE	MET	cloning artifact	UNP Q8NFP9
B	2198	MSE	MET	cloning artifact	UNP Q8NFP9
B	2221	MSE	MET	cloning artifact	UNP Q8NFP9
B	2228	MSE	MET	cloning artifact	UNP Q8NFP9
B	2275	MSE	MET	cloning artifact	UNP Q8NFP9
B	2291	MSE	MET	cloning artifact	UNP Q8NFP9
B	2434	MSE	MET	cloning artifact	UNP Q8NFP9
B	2473	MSE	MET	cloning artifact	UNP Q8NFP9
B	2531	MSE	MET	cloning artifact	UNP Q8NFP9

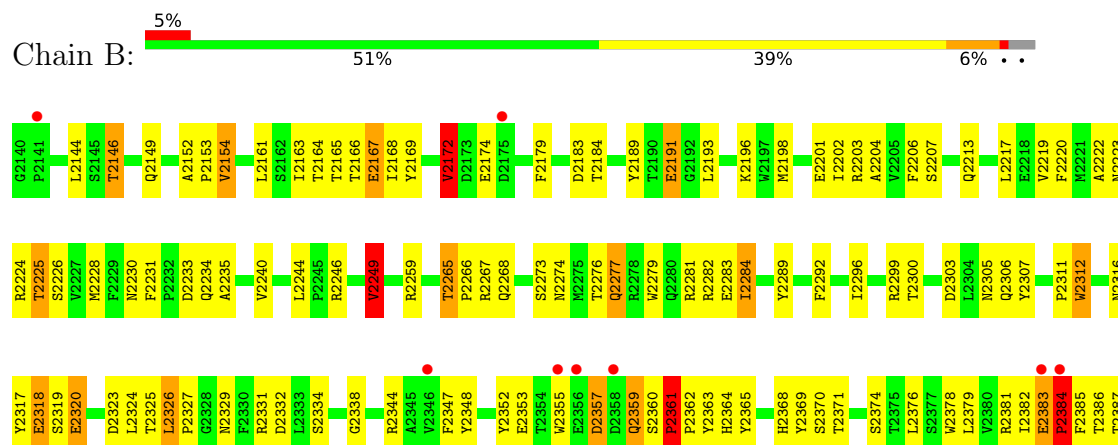
3 Residue-property plots [i](#)

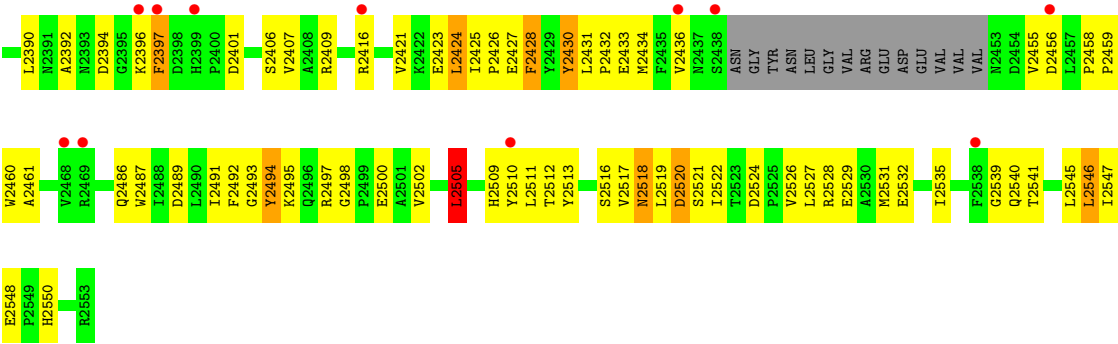
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Neurobeachin





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	179.91Å 179.91Å 98.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.71 – 2.90 29.71 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.71-2.90) 99.0 (29.71-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.264 0.227 , 0.260	Depositor DCC
R_{free} test set	1995 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6654	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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	0.53	0/3467	0.96	6/4712 (0.1%)
1	B	0.53	0/3357	0.95	8/4559 (0.2%)
All	All	0.53	0/6824	0.96	14/9271 (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	2312	TRP	N-CA-C	-8.13	98.25	110.28
1	A	2447	GLU	N-CA-C	-6.66	105.68	113.88
1	B	2312	TRP	N-CA-C	-6.44	100.74	110.28
1	B	2491	ILE	N-CA-C	6.13	117.68	111.00
1	A	2366	ASN	N-CA-C	-5.93	105.69	113.17
1	A	2491	ILE	N-CA-C	5.80	117.73	111.58
1	B	2249	VAL	N-CA-C	-5.78	107.11	112.43
1	B	2172	VAL	CB-CA-C	-5.54	104.10	111.13
1	B	2359	GLN	N-CA-C	-5.48	104.46	113.50
1	B	2146	THR	N-CA-C	5.47	115.17	108.11
1	B	2491	ILE	CB-CA-C	-5.47	104.91	112.24
1	A	2423	GLU	N-CA-C	-5.40	101.55	109.81
1	A	2455	VAL	N-CA-C	-5.35	102.68	109.58
1	B	2505	LEU	N-CA-C	-5.23	104.92	111.92

There are no chirality outliers.

There are no planarity outliers.

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	3381	0	3286	164	0
1	B	3273	0	3182	167	0
All	All	6654	0	6468	327	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 25.

All (327) 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:2164:THR:HG23	1:B:2166:THR:H	1.32	0.94
1:A:2209:ARG:HB2	1:A:2209:ARG:HH11	1.31	0.93
1:B:2165:THR:HG23	1:B:2166:THR:HG23	1.53	0.90
1:B:2204:ALA:HB3	1:B:2220:PHE:HB2	1.55	0.89
1:A:2494:TYR:HE1	1:A:2500:GLU:HG2	1.37	0.88
1:A:2164:THR:HG23	1:A:2166:THR:H	1.40	0.85
1:B:2382:ILE:O	1:B:2385:PHE:HB2	1.78	0.84
1:B:2311:PRO:HB3	1:B:2487:TRP:CE2	2.13	0.83
1:A:2489:ASP:HA	1:A:2493:GLY:HA3	1.60	0.83
1:A:2437:ASN:HD21	1:B:2224:ARG:NH2	1.77	0.81
1:A:2524:ASP:HB3	1:A:2527:LEU:HD12	1.63	0.79
1:A:2406:SER:HB3	1:A:2409:ARG:HB3	1.63	0.79
1:B:2489:ASP:HA	1:B:2493:GLY:HA3	1.64	0.78
1:B:2277:GLN:H	1:B:2277:GLN:NE2	1.82	0.77
1:B:2265:THR:HB	1:B:2268:GLN:HG3	1.66	0.77
1:B:2149:GLN:NE2	1:B:2230:ASN:HD22	1.84	0.76
1:B:2546:LEU:HD23	1:B:2546:LEU:N	2.01	0.75
1:B:2546:LEU:HD23	1:B:2546:LEU:H	1.52	0.74
1:A:2494:TYR:CE1	1:A:2500:GLU:HG2	2.21	0.73
1:B:2166:THR:C	1:B:2167:GLU:HG3	2.12	0.73
1:A:2151:ILE:HG21	1:A:2228:MSE:HE2	1.69	0.73
1:A:2316:ASN:HD21	1:A:2319:SER:HB3	1.52	0.73
1:B:2497:ARG:HH21	1:B:2513:TYR:HB3	1.54	0.72
1:B:2368:HIS:HD2	1:B:2370:SER:H	1.38	0.70
1:B:2497:ARG:NH2	1:B:2513:TYR:HB3	2.07	0.70
1:A:2451:VAL:HG21	1:B:2224:ARG:HE	1.55	0.70
1:B:2406:SER:HB3	1:B:2456:ASP:HB2	1.74	0.70
1:A:2267:ARG:HH12	1:A:2547:ILE:HD13	1.55	0.70
1:A:2407:VAL:HG11	1:A:2458:PRO:HD3	1.73	0.69
1:A:2399:HIS:ND1	1:A:2400:PRO:HD2	2.07	0.69
1:A:2518:ASN:HD22	1:A:2521:SER:H	1.40	0.69
1:A:2369:TYR:HB2	1:A:2423:GLU:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2396:LYS:HE3	1:A:2449:GLU:HG3	1.75	0.69
1:B:2518:ASN:HD21	1:B:2520:ASP:HB2	1.58	0.69
1:B:2161:LEU:HD21	1:B:2163:ILE:HD11	1.75	0.69
1:A:2144:LEU:HD23	1:A:2145:SER:N	2.08	0.69
1:A:2202:ILE:HD12	1:A:2219:VAL:HG11	1.74	0.68
1:A:2406:SER:HA	1:A:2456:ASP:OD1	1.93	0.68
1:B:2316:ASN:HD21	1:B:2319:SER:HB3	1.58	0.68
1:A:2311:PRO:HB3	1:A:2487:TRP:CE2	2.29	0.68
1:B:2164:THR:CG2	1:B:2167:GLU:H	2.06	0.68
1:A:2451:VAL:HG21	1:B:2224:ARG:NE	2.08	0.67
1:A:2172:VAL:HG21	1:A:2193:LEU:HD22	1.76	0.67
1:A:2398:ASP:HB3	1:A:2403:THR:HG23	1.75	0.67
1:A:2197:TRP:HB3	1:A:2221:MSE:CE	2.25	0.67
1:B:2164:THR:HG21	1:B:2167:GLU:OE1	1.95	0.66
1:A:2447:GLU:HG3	1:A:2448:ASP:OD1	1.96	0.66
1:B:2517:VAL:HG21	1:B:2531:MSE:HE3	1.77	0.66
1:B:2265:THR:HG22	1:B:2268:GLN:H	1.59	0.66
1:A:2304:LEU:HD22	1:A:2375:THR:HG21	1.78	0.66
1:A:2206:PHE:CZ	1:A:2249:VAL:HG22	2.31	0.66
1:B:2369:TYR:HB2	1:B:2423:GLU:HB2	1.79	0.65
1:A:2209:ARG:HB2	1:A:2209:ARG:NH1	2.09	0.65
1:B:2511:LEU:HA	1:B:2516:SER:OG	1.97	0.65
1:B:2431:LEU:HD23	1:B:2434:MSE:HB2	1.80	0.64
1:B:2172:VAL:HG11	1:B:2193:LEU:HD22	1.79	0.64
1:B:2164:THR:HG23	1:B:2165:THR:N	2.13	0.64
1:A:2175:ASP:O	1:A:2180:LYS:HE3	1.96	0.64
1:A:2284:ILE:HG23	1:A:2288:GLU:HB2	1.78	0.64
1:A:2299:ARG:HD3	1:A:2307:TYR:O	1.98	0.64
1:A:2285:SER:OG	1:A:2288:GLU:HG3	1.98	0.63
1:B:2430:TYR:O	1:B:2432:PRO:HD3	1.99	0.63
1:B:2383:GLU:CG	1:B:2386:THR:HB	2.27	0.63
1:B:2518:ASN:C	1:B:2518:ASN:HD22	2.06	0.63
1:A:2482:CYS:O	1:A:2483:GLN:HG2	1.99	0.63
1:B:2524:ASP:OD2	1:B:2526:VAL:HG12	1.99	0.62
1:A:2396:LYS:HG3	1:A:2450:VAL:HG22	1.80	0.62
1:A:2381:ARG:NH2	1:A:2404:PHE:O	2.29	0.62
1:B:2277:GLN:H	1:B:2277:GLN:CD	2.07	0.62
1:A:2281:ARG:HD2	1:A:2283:GLU:OE2	1.99	0.61
1:A:2233:ASP:OD2	1:A:2235:ALA:HB3	2.00	0.61
1:A:2267:ARG:HH12	1:A:2547:ILE:CD1	2.14	0.61
1:A:2333:LEU:HD22	1:A:2487:TRP:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2437:ASN:HD21	1:B:2224:ARG:HH21	1.48	0.61
1:B:2383:GLU:HA	1:B:2385:PHE:N	2.16	0.61
1:A:2164:THR:CG2	1:A:2167:GLU:H	2.13	0.60
1:B:2149:GLN:NE2	1:B:2230:ASN:ND2	2.50	0.60
1:A:2427:GLU:C	1:A:2429:TYR:H	2.09	0.60
1:A:2172:VAL:HG23	1:A:2193:LEU:O	2.02	0.60
1:A:2425:ILE:HG23	1:A:2426:PRO:HD2	1.85	0.59
1:B:2494:TYR:CE2	1:B:2495:LYS:HG3	2.37	0.59
1:B:2305:ASN:HB3	1:B:2540:GLN:HE21	1.65	0.59
1:B:2299:ARG:HD3	1:B:2307:TYR:O	2.03	0.59
1:A:2342:PRO:O	1:A:2346:VAL:HG23	2.02	0.59
1:A:2267:ARG:NH1	1:A:2547:ILE:HD13	2.18	0.58
1:B:2164:THR:HG22	1:B:2167:GLU:O	2.03	0.58
1:B:2379:LEU:HD21	1:B:2427:GLU:HG2	1.85	0.58
1:A:2431:LEU:HD23	1:A:2434:MSE:HB2	1.85	0.58
1:B:2331:ARG:HD3	1:B:2332:ASP:C	2.29	0.58
1:A:2274:ASN:C	1:A:2274:ASN:HD22	2.12	0.58
1:A:2423:GLU:HA	1:A:2423:GLU:OE2	2.03	0.58
1:A:2427:GLU:O	1:A:2429:TYR:N	2.36	0.57
1:B:2383:GLU:HB3	1:B:2387:THR:H	1.68	0.57
1:B:2546:LEU:N	1:B:2546:LEU:CD2	2.66	0.57
1:A:2197:TRP:HB3	1:A:2221:MSE:HE1	1.87	0.57
1:A:2206:PHE:HB3	1:A:2208:ARG:NH1	2.19	0.57
1:A:2511:LEU:HA	1:A:2516:SER:OG	2.05	0.56
1:A:2312:TRP:HA	1:A:2424:LEU:HD22	1.87	0.56
1:B:2281:ARG:HD2	1:B:2283:GLU:OE2	2.05	0.56
1:A:2206:PHE:O	1:A:2217:LEU:HD12	2.06	0.56
1:B:2344:ARG:O	1:B:2347:PHE:HB3	2.06	0.56
1:A:2363:TYR:CD1	1:A:2363:TYR:C	2.84	0.56
1:A:2513:TYR:O	1:A:2516:SER:HB2	2.05	0.56
1:A:2316:ASN:HD21	1:A:2319:SER:CB	2.18	0.55
1:A:2201:GLU:HB3	1:A:2221:MSE:HE3	1.88	0.55
1:A:2164:THR:HG23	1:A:2167:GLU:H	1.71	0.55
1:A:2407:VAL:HG12	1:A:2456:ASP:O	2.07	0.55
1:B:2265:THR:CB	1:B:2268:GLN:HG3	2.35	0.55
1:A:2396:LYS:HG3	1:A:2450:VAL:CG2	2.36	0.55
1:B:2183:ASP:OD2	1:B:2184:THR:N	2.39	0.55
1:B:2289:TYR:OH	1:B:2550:HIS:HE1	1.90	0.55
1:B:2368:HIS:CD2	1:B:2370:SER:H	2.22	0.54
1:A:2203:ARG:HG2	1:A:2203:ARG:HH11	1.72	0.54
1:A:2406:SER:HB3	1:A:2409:ARG:CB	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2326:LEU:HB3	1:B:2329:ASN:ND2	2.22	0.54
1:A:2463:LYS:O	1:A:2466:ASP:HB2	2.07	0.54
1:B:2276:THR:O	1:B:2279:TRP:HB3	2.08	0.54
1:B:2203:ARG:HG3	1:B:2222:ALA:HA	1.90	0.54
1:B:2312:TRP:CE2	1:B:2424:LEU:HD13	2.42	0.54
1:B:2249:VAL:HG13	1:B:2249:VAL:O	2.07	0.53
1:A:2367:THR:HG21	1:A:2419:SER:O	2.08	0.53
1:B:2383:GLU:HG2	1:B:2386:THR:HB	1.89	0.53
1:B:2164:THR:HG21	1:B:2167:GLU:CD	2.34	0.53
1:B:2517:VAL:HG11	1:B:2535:ILE:HD11	1.90	0.53
1:A:2524:ASP:HB3	1:A:2527:LEU:CD1	2.35	0.53
1:A:2427:GLU:C	1:A:2429:TYR:N	2.67	0.52
1:B:2428:PHE:CE1	1:B:2434:MSE:HE1	2.45	0.52
1:A:2428:PHE:CE1	1:A:2434:MSE:HE1	2.44	0.52
1:B:2323:ASP:C	1:B:2325:THR:H	2.18	0.52
1:A:2164:THR:HG21	1:A:2167:GLU:OE1	2.10	0.52
1:B:2396:LYS:HG3	1:B:2397:PHE:H	1.73	0.52
1:B:2240:VAL:O	1:B:2244:LEU:HD13	2.10	0.52
1:B:2320:GLU:H	1:B:2320:GLU:CD	2.18	0.52
1:A:2274:ASN:ND2	1:A:2278:ARG:HE	2.08	0.52
1:B:2492:PHE:HB3	1:B:2545:LEU:HG	1.92	0.52
1:A:2254:GLY:HA3	1:A:2274:ASN:OD1	2.09	0.52
1:B:2206:PHE:CE2	1:B:2249:VAL:HG22	2.45	0.52
1:B:2154:VAL:HG13	1:B:2154:VAL:O	2.09	0.51
1:B:2381:ARG:NH1	1:B:2455:VAL:HG23	2.25	0.51
1:A:2255:LEU:HD23	1:A:2272:SER:O	2.10	0.51
1:B:2273:SER:OG	1:B:2274:ASN:N	2.43	0.51
1:B:2381:ARG:O	1:B:2382:ILE:HG13	2.10	0.51
1:B:2325:THR:O	1:B:2327:PRO:HD3	2.11	0.51
1:A:2149:GLN:NE2	1:A:2230:ASN:HD22	2.08	0.50
1:A:2462:LYS:HB2	1:A:2466:ASP:OD1	2.11	0.50
1:A:2395:GLY:O	1:A:2396:LYS:HD2	2.11	0.50
1:A:2381:ARG:NH1	1:A:2453:ASN:O	2.43	0.50
1:A:2430:TYR:HA	1:A:2468:VAL:HG11	1.92	0.50
1:B:2164:THR:HG23	1:B:2165:THR:H	1.77	0.50
1:B:2319:SER:O	1:B:2459:PRO:HB2	2.11	0.50
1:B:2164:THR:HG23	1:B:2167:GLU:H	1.74	0.50
1:A:2187:LEU:HD22	1:A:2193:LEU:HD11	1.93	0.50
1:A:2352:TYR:CE1	1:A:2362:PRO:HB2	2.47	0.50
1:B:2318:GLU:O	1:B:2459:PRO:HG2	2.12	0.49
1:B:2390:LEU:HD22	1:B:2396:LYS:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2203:ARG:HG2	1:A:2203:ARG:NH1	2.27	0.49
1:A:2213:GLN:NE2	1:A:2519:LEU:H	2.11	0.49
1:B:2406:SER:CB	1:B:2456:ASP:HB2	2.42	0.49
1:B:2518:ASN:HD21	1:B:2520:ASP:CB	2.24	0.49
1:A:2166:THR:C	1:A:2167:GLU:HG3	2.37	0.49
1:A:2546:LEU:N	1:A:2546:LEU:HD23	2.27	0.49
1:B:2424:LEU:HG	1:B:2428:PHE:CG	2.48	0.49
1:A:2364:HIS:ND1	1:A:2507:VAL:HB	2.27	0.49
1:A:2197:TRP:HB3	1:A:2221:MSE:HE2	1.94	0.48
1:B:2513:TYR:O	1:B:2516:SER:HB2	2.14	0.48
1:A:2223:ASN:OD1	1:A:2225:THR:HG22	2.13	0.48
1:B:2460:TRP:H	1:B:2460:TRP:CD1	2.29	0.48
1:A:2482:CYS:C	1:A:2483:GLN:HG2	2.39	0.48
1:B:2381:ARG:HD2	1:B:2436:VAL:O	2.14	0.48
1:B:2352:TYR:CE1	1:B:2362:PRO:HB2	2.47	0.48
1:B:2379:LEU:HD23	1:B:2434:MSE:HG3	1.96	0.48
1:A:2512:THR:CG2	1:A:2541:THR:OG1	2.62	0.47
1:B:2425:ILE:O	1:B:2426:PRO:C	2.56	0.47
1:A:2432:PRO:O	1:A:2433:GLU:C	2.57	0.47
1:A:2164:THR:OG1	1:A:2165:THR:N	2.46	0.47
1:A:2351:ARG:HG3	1:A:2351:ARG:HH11	1.79	0.47
1:B:2338:GLY:HA3	1:B:2365:TYR:CE2	2.49	0.47
1:A:2249:VAL:HG11	1:A:2255:LEU:HD12	1.96	0.47
1:A:2409:ARG:HA	1:A:2412:ARG:HH11	1.79	0.47
1:A:2524:ASP:O	1:A:2527:LEU:HB2	2.14	0.47
1:B:2244:LEU:O	1:B:2259:ARG:NH1	2.47	0.47
1:B:2518:ASN:ND2	1:B:2520:ASP:H	2.13	0.47
1:A:2172:VAL:HG21	1:A:2193:LEU:HB3	1.97	0.47
1:A:2222:ALA:C	1:A:2224:ARG:H	2.23	0.47
1:A:2276:THR:HB	1:A:2277:GLN:NE2	2.29	0.47
1:A:2424:LEU:O	1:A:2425:ILE:HD12	2.15	0.47
1:B:2303:ASP:C	1:B:2303:ASP:OD1	2.58	0.47
1:B:2378:TRP:CE3	1:B:2428:PHE:HZ	2.33	0.47
1:A:2430:TYR:HA	1:A:2468:VAL:CG1	2.45	0.46
1:B:2364:HIS:HB2	1:B:2365:TYR:CE1	2.49	0.46
1:B:2164:THR:HG22	1:B:2167:GLU:H	1.79	0.46
1:A:2150:LEU:O	1:A:2156:VAL:HA	2.16	0.46
1:A:2466:ASP:HA	1:A:2469:ARG:NH1	2.30	0.46
1:A:2299:ARG:NH2	1:A:2306:GLN:HA	2.30	0.46
1:B:2401:ASP:HA	1:B:2409:ARG:NH2	2.30	0.46
1:A:2487:TRP:CZ2	1:A:2491:ILE:HG13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2497:ARG:HH21	1:A:2513:TYR:HB3	1.81	0.46
1:B:2206:PHE:CD2	1:B:2249:VAL:HG22	2.51	0.46
1:B:2207:SER:HA	1:B:2217:LEU:HD12	1.98	0.46
1:B:2189:TYR:HB2	1:B:2384:PRO:HG3	1.98	0.46
1:B:2426:PRO:O	1:B:2427:GLU:C	2.58	0.46
1:B:2169:TYR:CE2	1:B:2196:LYS:HG3	2.51	0.46
1:B:2344:ARG:HG2	1:B:2348:TYR:CE1	2.50	0.46
1:B:2152:ALA:HB1	1:B:2153:PRO:HD2	1.98	0.45
1:A:2144:LEU:HD23	1:A:2144:LEU:C	2.40	0.45
1:A:2360:SER:O	1:A:2361:PRO:C	2.57	0.45
1:B:2524:ASP:HB3	1:B:2527:LEU:HD12	1.99	0.45
1:A:2334:SER:O	1:A:2490:LEU:HD11	2.17	0.45
1:A:2351:ARG:HG3	1:A:2351:ARG:NH1	2.32	0.45
1:B:2378:TRP:HB3	1:B:2434:MSE:HE3	1.98	0.45
1:A:2344:ARG:HG2	1:A:2348:TYR:CE1	2.52	0.45
1:A:2512:THR:CG2	1:A:2541:THR:H	2.30	0.45
1:B:2281:ARG:O	1:B:2282:ARG:HB2	2.16	0.45
1:B:2518:ASN:ND2	1:B:2520:ASP:HB2	2.30	0.45
1:B:2265:THR:HG23	1:B:2266:PRO:HD2	1.99	0.45
1:A:2151:ILE:HG21	1:A:2228:MSE:CE	2.42	0.45
1:A:2389:PHE:O	1:A:2393:ASN:HB2	2.16	0.45
1:B:2292:PHE:CZ	1:B:2296:ILE:HD13	2.52	0.45
1:B:2364:HIS:NE2	1:B:2505:LEU:HD22	2.32	0.45
1:B:2383:GLU:HB3	1:B:2386:THR:N	2.31	0.45
1:A:2337:ILE:HD13	1:A:2337:ILE:HA	1.84	0.45
1:B:2338:GLY:HA3	1:B:2365:TYR:HE2	1.82	0.45
1:B:2498:GLY:O	1:B:2502:VAL:HG23	2.17	0.45
1:B:2265:THR:HB	1:B:2268:GLN:CG	2.41	0.45
1:B:2406:SER:OG	1:B:2409:ARG:HB2	2.17	0.45
1:B:2458:PRO:HD2	1:B:2461:ALA:HB3	1.99	0.45
1:B:2512:THR:O	1:B:2512:THR:HG22	2.17	0.45
1:B:2144:LEU:HD23	1:B:2144:LEU:C	2.41	0.44
1:B:2512:THR:HG22	1:B:2541:THR:OG1	2.17	0.44
1:B:2174:GLU:HA	1:B:2179:PHE:CD2	2.52	0.44
1:B:2512:THR:HG23	1:B:2539:GLY:O	2.18	0.44
1:B:2246:ARG:HG2	1:B:2246:ARG:O	2.15	0.44
1:B:2432:PRO:HD2	1:B:2433:GLU:OE2	2.18	0.44
1:A:2242:TYR:HA	1:A:2259:ARG:CD	2.47	0.44
1:A:2425:ILE:HG23	1:A:2426:PRO:CD	2.47	0.44
1:A:2512:THR:HG23	1:A:2541:THR:H	1.82	0.44
1:B:2231:PHE:CE2	1:B:2240:VAL:HG21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2299:ARG:HD3	1:B:2306:GLN:O	2.18	0.44
1:B:2365:TYR:CD2	1:B:2421:VAL:HG11	2.52	0.44
1:A:2499:PRO:O	1:A:2502:VAL:CG1	2.66	0.44
1:B:2357:ASP:OD1	1:B:2359:GLN:HB3	2.18	0.44
1:B:2517:VAL:CG2	1:B:2531:MSE:HE3	2.45	0.44
1:B:2361:PRO:HA	1:B:2362:PRO:HD3	1.86	0.44
1:B:2363:TYR:CD1	1:B:2363:TYR:C	2.96	0.44
1:A:2159:GLY:HA3	1:A:2170:PHE:CZ	2.53	0.44
1:A:2518:ASN:HD22	1:A:2521:SER:N	2.10	0.44
1:B:2547:ILE:HG13	1:B:2548:GLU:OE2	2.18	0.44
1:A:2167:GLU:HB2	1:A:2169:TYR:CE1	2.53	0.43
1:A:2312:TRP:HA	1:A:2424:LEU:CD2	2.48	0.43
1:A:2338:GLY:HA3	1:A:2365:TYR:CE2	2.53	0.43
1:A:2524:ASP:OD2	1:A:2526:VAL:HG12	2.18	0.43
1:B:2217:LEU:O	1:B:2228:MSE:HG3	2.18	0.43
1:B:2223:ASN:OD1	1:B:2225:THR:HB	2.17	0.43
1:B:2265:THR:CG2	1:B:2268:GLN:HG3	2.49	0.43
1:B:2495:LYS:HG2	1:B:2500:GLU:HG3	2.00	0.43
1:A:2550:HIS:HA	1:A:2551:PRO:HD3	1.84	0.43
1:B:2360:SER:O	1:B:2361:PRO:C	2.61	0.43
1:A:2402:ARG:NH1	1:A:2402:ARG:HB3	2.33	0.43
1:A:2172:VAL:HG12	1:A:2173:ASP:N	2.34	0.43
1:B:2334:SER:HA	1:B:2486:GLN:HB3	1.99	0.43
1:B:2365:TYR:CD1	1:B:2365:TYR:N	2.86	0.43
1:A:2203:ARG:HG3	1:A:2222:ALA:HA	2.01	0.42
1:B:2168:ILE:HD11	1:B:2244:LEU:HG	2.01	0.42
1:B:2331:ARG:HD3	1:B:2331:ARG:C	2.44	0.42
1:B:2528:ARG:O	1:B:2532:GLU:HG3	2.19	0.42
1:A:2472:ARG:HH11	1:A:2472:ARG:HG2	1.84	0.42
1:A:2437:ASN:OD1	1:A:2439:ASN:HB2	2.18	0.42
1:A:2528:ARG:O	1:A:2531:MSE:HB3	2.19	0.42
1:A:2436:VAL:CG1	1:A:2464:PRO:HG2	2.49	0.42
1:B:2164:THR:CG2	1:B:2167:GLU:N	2.79	0.42
1:A:2515:GLY:O	1:A:2516:SER:C	2.62	0.42
1:B:2383:GLU:CB	1:B:2384:PRO:C	2.92	0.42
1:B:2392:ALA:C	1:B:2394:ASP:H	2.27	0.42
1:A:2342:PRO:HA	1:A:2345:ALA:HB3	2.01	0.42
1:B:2233:ASP:OD2	1:B:2235:ALA:HB3	2.20	0.42
1:B:2433:GLU:H	1:B:2433:GLU:CD	2.27	0.42
1:A:2325:THR:HA	1:A:2479:PHE:HE2	1.85	0.42
1:A:2197:TRP:CD1	1:A:2197:TRP:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2499:PRO:O	1:A:2502:VAL:HG13	2.18	0.42
1:B:2524:ASP:OD1	1:B:2527:LEU:HG	2.19	0.42
1:A:2167:GLU:OE2	1:A:2196:LYS:HE3	2.20	0.42
1:A:2197:TRP:CH2	1:A:2227:VAL:HB	2.55	0.42
1:B:2364:HIS:HB2	1:B:2365:TYR:CD1	2.55	0.42
1:A:2191:GLU:OE1	1:A:2191:GLU:N	2.34	0.41
1:A:2221:MSE:HB2	1:A:2225:THR:HG22	2.01	0.41
1:A:2387:THR:HG22	1:A:2391:ASN:ND2	2.34	0.41
1:B:2505:LEU:HD22	1:B:2505:LEU:HA	1.91	0.41
1:A:2183:ASP:OD2	1:A:2183:ASP:C	2.63	0.41
1:A:2274:ASN:C	1:A:2274:ASN:ND2	2.77	0.41
1:A:2333:LEU:HD22	1:A:2487:TRP:CB	2.48	0.41
1:A:2445:VAL:HG12	1:A:2449:GLU:HB3	2.01	0.41
1:B:2368:HIS:HE1	1:B:2541:THR:OG1	2.02	0.41
1:A:2183:ASP:HB3	1:A:2186:VAL:HG23	2.02	0.41
1:B:2265:THR:HG22	1:B:2267:ARG:N	2.35	0.41
1:B:2277:GLN:H	1:B:2277:GLN:HE21	1.66	0.41
1:A:2320:GLU:HA	1:A:2459:PRO:HB2	2.03	0.41
1:A:2424:LEU:HG	1:A:2428:PHE:CG	2.56	0.41
1:A:2494:TYR:CD2	1:A:2549:PRO:HA	2.55	0.41
1:A:2259:ARG:HH11	1:A:2259:ARG:HG2	1.85	0.41
1:A:2390:LEU:HD12	1:A:2390:LEU:HA	1.81	0.41
1:A:2522:ILE:HG21	1:A:2528:ARG:N	2.36	0.41
1:B:2376:LEU:HD23	1:B:2376:LEU:HA	1.93	0.41
1:A:2402:ARG:HB3	1:A:2402:ARG:HH11	1.86	0.41
1:B:2518:ASN:ND2	1:B:2521:SER:H	2.18	0.41
1:A:2372:ALA:O	1:A:2373:THR:C	2.63	0.41
1:A:2456:ASP:OD1	1:A:2456:ASP:N	2.52	0.41
1:B:2191:GLU:H	1:B:2191:GLU:HG2	1.76	0.41
1:B:2198:MSE:HB3	1:B:2201:GLU:HG2	2.02	0.41
1:B:2219:VAL:O	1:B:2226:SER:HA	2.21	0.41
1:B:2326:LEU:HB3	1:B:2329:ASN:HD22	1.84	0.41
1:A:2518:ASN:HD21	1:A:2520:ASP:HB2	1.86	0.41
1:B:2407:VAL:HG11	1:B:2458:PRO:HD3	2.03	0.41
1:B:2433:GLU:O	1:B:2436:VAL:HG22	2.20	0.41
1:B:2509:HIS:HE1	1:B:2510:TYR:CE2	2.39	0.41
1:B:2518:ASN:HD22	1:B:2520:ASP:N	2.19	0.41
1:A:2315:THR:HG22	1:A:2411:TRP:CZ2	2.56	0.40
1:B:2202:ILE:O	1:B:2203:ARG:NH1	2.51	0.40
1:B:2213:GLN:NE2	1:B:2519:LEU:H	2.19	0.40
1:B:2317:TYR:HB3	1:B:2458:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2374:SER:O	1:B:2378:TRP:CD1	2.74	0.40
1:B:2518:ASN:C	1:B:2518:ASN:ND2	2.73	0.40
1:A:2152:ALA:O	1:A:2153:PRO:C	2.65	0.40
1:A:2162:SER:OG	1:A:2169:TYR:HB2	2.20	0.40
1:A:2512:THR:HG23	1:A:2541:THR:N	2.36	0.40
1:B:2283:GLU:O	1:B:2284:ILE:HD12	2.21	0.40
1:A:2154:VAL:HG23	1:A:2155:VAL:HG23	2.03	0.40
1:A:2323:ASP:C	1:A:2325:THR:H	2.29	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	412/414 (100%)	361 (88%)	42 (10%)	9 (2%)	5	20
1	B	396/414 (96%)	351 (89%)	35 (9%)	10 (2%)	4	17
All	All	808/828 (98%)	712 (88%)	77 (10%)	19 (2%)	4	18

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2448	ASP
1	B	2384	PRO
1	B	2397	PHE
1	A	2264	ALA
1	A	2397	PHE
1	A	2428	PHE
1	A	2444	GLY
1	B	2154	VAL
1	A	2430	TYR
1	B	2357	ASP

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Mol	Chain	Res	Type
1	B	2361	PRO
1	B	2428	PHE
1	B	2430	TYR
1	B	2522	ILE
1	A	2324	LEU
1	B	2355	TRP
1	A	2516	SER
1	B	2324	LEU
1	A	2361	PRO

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	373/365 (102%)	349 (94%)	24 (6%)	16	44
1	B	361/365 (99%)	334 (92%)	27 (8%)	12	37
All	All	734/730 (100%)	683 (93%)	51 (7%)	14	41

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2149	GLN
1	A	2153	PRO
1	A	2191	GLU
1	A	2198	MSE
1	A	2201	GLU
1	A	2209	ARG
1	A	2233	ASP
1	A	2244	LEU
1	A	2249	VAL
1	A	2274	ASN
1	A	2353	GLU
1	A	2359	GLN
1	A	2373	THR
1	A	2390	LEU

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Mol	Chain	Res	Type
1	A	2396	LYS
1	A	2403	THR
1	A	2417	ASP
1	A	2423	GLU
1	A	2424	LEU
1	A	2425	ILE
1	A	2502	VAL
1	A	2505	LEU
1	A	2511	LEU
1	A	2517	VAL
1	B	2146	THR
1	B	2167	GLU
1	B	2172	VAL
1	B	2191	GLU
1	B	2225	THR
1	B	2234	GLN
1	B	2249	VAL
1	B	2265	THR
1	B	2277	GLN
1	B	2284	ILE
1	B	2300	THR
1	B	2318	GLU
1	B	2320	GLU
1	B	2326	LEU
1	B	2353	GLU
1	B	2361	PRO
1	B	2371	THR
1	B	2383	GLU
1	B	2384	PRO
1	B	2416	ARG
1	B	2424	LEU
1	B	2494	TYR
1	B	2505	LEU
1	B	2518	ASN
1	B	2520	ASP
1	B	2529	GLU
1	B	2546	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2213	GLN

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Mol	Chain	Res	Type
1	A	2230	ASN
1	A	2274	ASN
1	A	2277	GLN
1	A	2341	ASN
1	A	2359	GLN
1	A	2415	GLN
1	A	2483	GLN
1	A	2486	GLN
1	A	2518	ASN
1	A	2534	GLN
1	A	2540	GLN
1	B	2149	GLN
1	B	2213	GLN
1	B	2277	GLN
1	B	2316	ASN
1	B	2368	HIS
1	B	2486	GLN
1	B	2496	GLN
1	B	2506	ASN
1	B	2518	ASN
1	B	2540	GLN
1	B	2550	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	406/414 (98%)	0.11	11 (2%) 56 47	35, 57, 83, 106	0
1	B	392/414 (94%)	0.27	19 (4%) 35 28	27, 58, 97, 108	0
All	All	798/828 (96%)	0.19	30 (3%) 44 36	27, 58, 94, 108	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2445	VAL	4.2
1	B	2469	ARG	3.9
1	A	2446	ARG	3.7
1	A	2359	GLN	3.7
1	B	2438	SER	3.6
1	B	2397	PHE	3.6
1	A	2450	VAL	3.2
1	A	2449	GLU	3.2
1	B	2384	PRO	3.0
1	A	2141	PRO	2.9
1	A	2448	ASP	2.8
1	B	2356	GLU	2.5
1	B	2436	VAL	2.4
1	A	2140	GLY	2.4
1	A	2247	VAL	2.4
1	B	2383	GLU	2.4
1	B	2416	ARG	2.3
1	B	2538	PHE	2.3
1	B	2468	VAL	2.3
1	B	2358	ASP	2.2
1	B	2456	ASP	2.2
1	B	2346	VAL	2.2
1	B	2141	PRO	2.2
1	A	2356	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2510	TYR	2.2
1	B	2399	HIS	2.1
1	B	2355	TRP	2.1
1	A	2412	ARG	2.1
1	B	2396	LYS	2.0
1	B	2175	ASP	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.