Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:52 PM GMT

PDB ID	:	1MI1
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

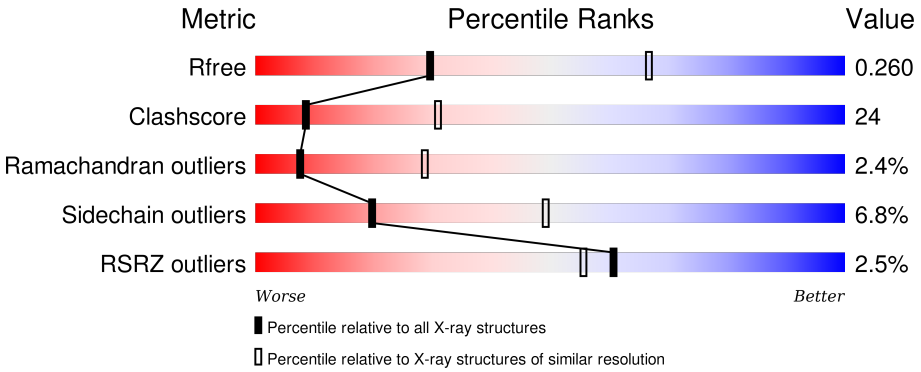
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	3% 54% 41% 5%
1	B	414	2% 53% 38% 6%

2 Entry composition (i)

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:

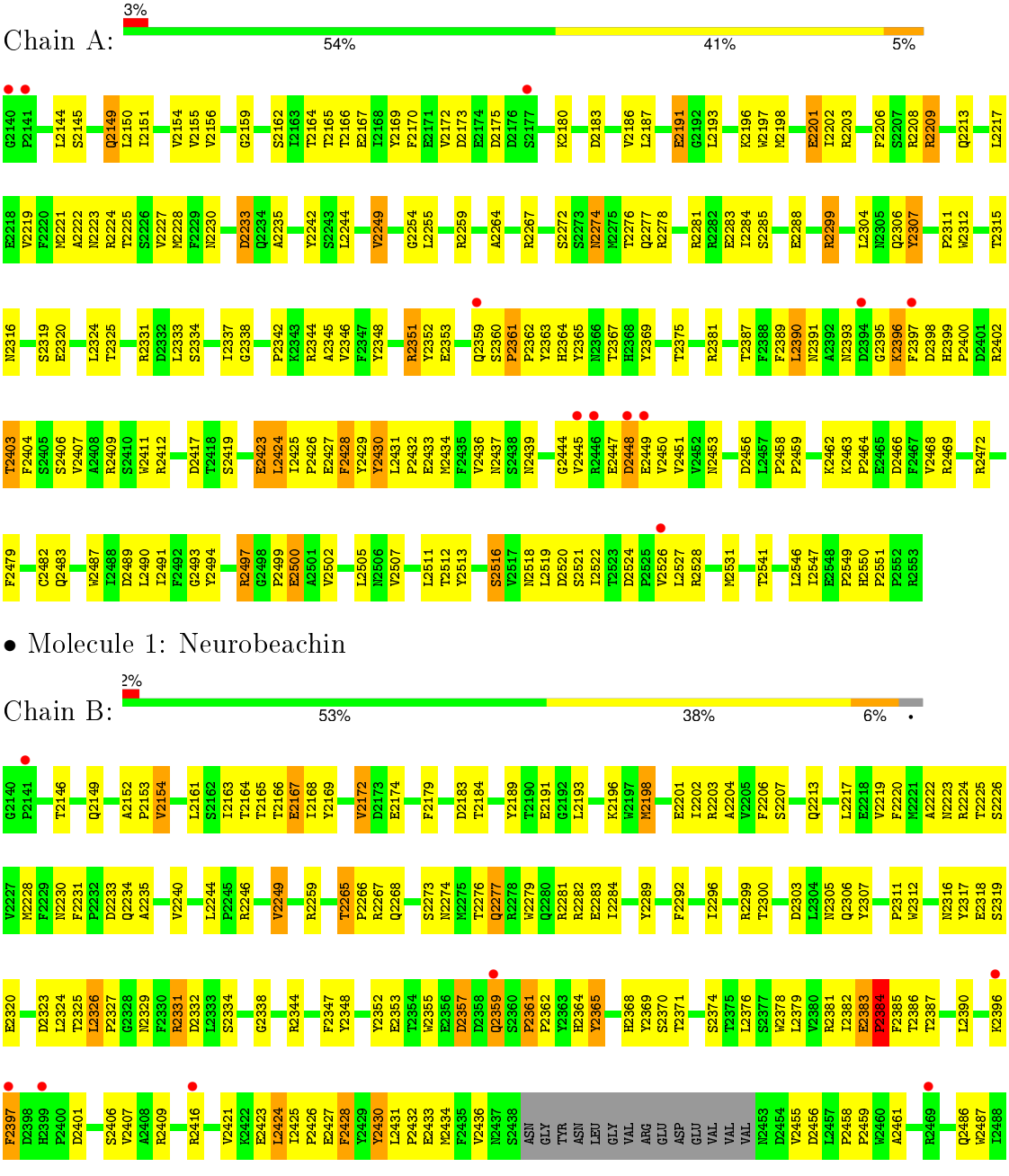
Chain	Residue	Modelled	Actual	Comment	Reference
A	2198	MSE	MET	CLONING ARTIFACT	UNP Q8NFP9
A	2221	MSE	MET	CLONING ARTIFACT	UNP Q8NFP9
A	2228	MSE	MET	CLONING ARTIFACT	UNP Q8NFP9
A	2275	MSE	MET	CLONING ARTIFACT	UNP Q8NFP9
A	2291	MSE	MET	CLONING ARTIFACT	UNP Q8NFP9
A	2434	MSE	MET	CLONING ARTIFACT	UNP Q8NFP9
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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

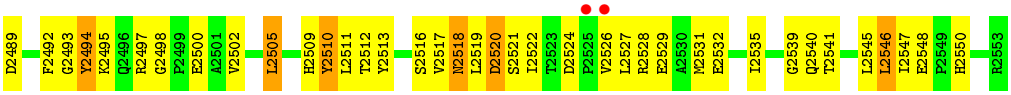
- Molecule 1: Neurobeachin

Chain A:



- Molecule 1: Neurobeachin

Chain B:


D2489
F2492
G2493
V2494
K2495
Q2496
R2497
G2498
P2499
E2500
A2501
V2502
L2505
H2509
Y2510
L2511
T2512
Y2513
S2516
V2517
M2518
L2519
D2520
S2521
I2522
T2523
D2524
P2525
V2526
L2527
R2528
E2529
A2530
M2531
E2532
I2535
G2539
Q2540
T2541
L2545
L2546
I2547
E2548
P2549
H2550
R2553

4 Data and refinement statistics (i)

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 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.71-2.90) 99.0 (29.71-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (4.99%)	DCC
Wilson B-factor (Å^2)	73.4	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.9	EDS
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 40797 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.45	0/3467	0.63	0/4712
1	B	0.45	0/3357	0.62	0/4559
All	All	0.45	0/6824	0.63	0/9271

There are no bond length outliers.

There are no bond angle outliers.

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	3381	0	3286	158	0
1	B	3273	0	3182	159	0
All	All	6654	0	6468	313	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 24.

All (313) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:2546:LEU:HD23	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:A:2316:ASN:HD21	1:A:2319:SER:HB3	1.52	0.73
1:A:2151:ILE:HG21	1:A:2228:MSE:HE2	1.69	0.73
1:B:2497:ARG:HH21	1:B:2513:TYR:HB3	1.54	0.72
1:B:2497:ARG:NH2	1:B:2513:TYR:HB3	2.07	0.70
1:B:2368:HIS:HD2	1:B:2370:SER:H	1.38	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
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:2166:THR:C	1:B:2167:GLU:HG3	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:2281:ARG:HD2	1:A:2283:GLU:OE2	1.99	0.61
1:A:2267:ARG:HH12	1:A:2547:ILE:CD1	2.14	0.61
1:A:2233:ASP:OD2	1:A:2235:ALA:HB3	2.00	0.61
1:A:2333:LEU:HD22	1:A:2487:TRP:HB2	1.82	0.61
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:2172:VAL:HG23	1:A:2193:LEU:O	2.02	0.60
1:B:2494:TYR:CE2	1:B:2495:LYS:HG3	2.37	0.59
1:A:2425:ILE:HG23	1:A:2426:PRO:HD2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2518:ASN:C	1:B:2518:ASN:HD22	2.06	0.58
1:A:2431:LEU:HD23	1:A:2434:MSE:HB2	1.85	0.58
1:A:2423:GLU:HA	1:A:2423:GLU:OE2	2.03	0.58
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:2427:GLU:O	1:A:2429:TYR:N	2.36	0.57
1:B:2277:GLN:H	1:B:2277:GLN:CD	2.07	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: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:2427:GLU:C	1:A:2429:TYR:H	2.09	0.54
1:A:2203:ARG:HH11	1:A:2203:ARG:HG2	1.72	0.54
1:A:2406:SER:HB3	1:A:2409:ARG:CB	2.35	0.54
1:B:2326:LEU:HB3	1:B:2329:ASN:ND2	2.22	0.54
1:B:2249:VAL:O	1:B:2249:VAL:HG13	2.07	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:2331:ARG:HD3	1:B:2332:ASP:C	2.29	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:A:2274:ASN:C	1:A:2274:ASN:HD22	2.12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2154:VAL:HG13	1:B:2154:VAL:O	2.09	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: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:B:2206:PHE:CE2	1:B:2249:VAL:HG22	2.45	0.52
1:A:2254:GLY:HA3	1:A:2274:ASN:OD1	2.09	0.52
1:B:2381:ARG:NH1	1:B:2455:VAL:HG23	2.25	0.51
1:A:2363:TYR:C	1:A:2363:TYR:CD1	2.84	0.51
1:B:2381:ARG:O	1:B:2382:ILE:HG13	2.10	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:2325:THR:O	1:B:2327:PRO:HD3	2.11	0.51
1:A:2462:LYS:HB2	1:A:2466:ASP:OD1	2.11	0.50
1:A:2149:GLN:NE2	1:A:2230:ASN:HD22	2.08	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: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:A:2430:TYR:HA	1:A:2468:VAL:HG11	1.92	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
1:A:2203:ARG:NH1	1:A:2203:ARG:HG2	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:2546:LEU:HD23	1:A:2546:LEU:N	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:2164:THR:HG21	1:B:2167:GLU:CD	2.34	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:2427:GLU:C	1:A:2429:TYR:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2323:ASP:C	1:B:2325:THR:H	2.18	0.47
1:A:2512:THR:CG2	1:A:2541:THR:OG1	2.62	0.47
1:A:2164:THR:OG1	1:A:2165:THR:N	2.46	0.47
1:A:2351:ARG:HH11	1:A:2351:ARG:HG3	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:B:2320:GLU:H	1:B:2320:GLU:CD	2.18	0.47
1:A:2524:ASP:O	1:A:2527:LEU:HB2	2.14	0.47
1:A:2409:ARG:HA	1:A:2412:ARG:HH11	1.79	0.47
1:B:2518:ASN:ND2	1:B:2520:ASP:H	2.13	0.47
1:B:2244:LEU:O	1:B:2259:ARG:NH1	2.47	0.47
1:A:2172:VAL:HG21	1:A:2193:LEU:HB3	1.97	0.47
1:B:2378:TRP:CE3	1:B:2428:PHE:HZ	2.33	0.47
1:A:2424:LEU:O	1:A:2425:ILE:HD12	2.15	0.47
1:A:2276:THR:HB	1:A:2277:GLN:NE2	2.29	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:2466:ASP:HA	1:A:2469:ARG:NH1	2.30	0.46
1:A:2150:LEU:O	1:A:2156:VAL:HA	2.16	0.46
1:B:2401:ASP:HA	1:B:2409:ARG:NH2	2.30	0.46
1:A:2299:ARG:NH2	1:A:2306:GLN:HA	2.30	0.46
1:A:2487:TRP:CZ2	1:A:2491:ILE:HG13	2.51	0.46
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: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:B:2524:ASP:HB3	1:B:2527:LEU:HD12	1.99	0.45
1:B:2378:TRP:HB3	1:B:2434:MSE:HE3	1.98	0.45
1:A:2351:ARG:NH1	1:A:2351:ARG:HG3	2.32	0.45
1:A:2334:SER:O	1:A:2490:LEU:HD11	2.17	0.45
1:A:2166:THR:C	1:A:2167:GLU:HG3	2.37	0.45
1:B:2518:ASN:ND2	1:B:2520:ASP:HB2	2.30	0.45
1:B:2281:ARG:O	1:B:2282:ARG:HB2	2.16	0.45
1:A:2512:THR:CG2	1:A:2541:THR:H	2.30	0.45
1:B:2246:ARG:O	1:B:2246:ARG:HG2	2.15	0.45
1:A:2344:ARG:HG2	1:A:2348:TYR:CE1	2.52	0.45
1:B:2265:THR:HG23	1:B:2266:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2383:GLU:HB3	1:B:2386:THR:N	2.31	0.45
1:A:2151:ILE:HG21	1:A:2228:MSE:CE	2.42	0.45
1:B:2364:HIS:NE2	1:B:2505:LEU:HD22	2.32	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:2338:GLY:HA3	1:B:2365:TYR:HE2	1.82	0.45
1:A:2337:ILE:HA	1:A:2337:ILE:HD13	1.84	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:2512:THR:O	1:B:2512:THR:HG22	2.17	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: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:2432:PRO:HD2	1:B:2433:GLU:OE2	2.18	0.44
1:A:2425:ILE:HG23	1:A:2426:PRO:CD	2.47	0.44
1:B:2299:ARG:HD3	1:B:2306:GLN:O	2.18	0.44
1:B:2231:PHE:CE2	1:B:2240:VAL:HG21	2.53	0.44
1:A:2512:THR:HG23	1:A:2541:THR:H	1.82	0.44
1:B:2365:TYR:CD2	1:B:2421:VAL:HG11	2.52	0.44
1:A:2242:TYR:HA	1:A:2259:ARG:CD	2.47	0.44
1:B:2517:VAL:CG2	1:B:2531:MSE:HE3	2.45	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:2361:PRO:HA	1:B:2362:PRO:HD3	1.86	0.44
1:A:2518:ASN:HD22	1:A:2521:SER:N	2.10	0.44
1:A:2159:GLY:HA3	1:A:2170:PHE:CZ	2.53	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:2524:ASP:OD2	1:A:2526:VAL:HG12	2.18	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:2482:CYS:C	1:A:2483:GLN:HG2	2.39	0.43
1:B:2265:THR:CG2	1:B:2268:GLN:HG3	2.49	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: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:A:2402:ARG:HB3	1:A:2402:ARG:NH1	2.33	0.43
1:A:2172:VAL:HG12	1:A:2173:ASP:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2425:ILE:O	1:B:2426:PRO:C	2.56	0.43
1:B:2365:TYR:N	1:B:2365:TYR:CD1	2.86	0.43
1:B:2334:SER:HA	1:B:2486:GLN:HB3	1.99	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:A:2432:PRO:O	1:A:2433:GLU:C	2.57	0.42
1:B:2528:ARG:O	1:B:2532:GLU:HG3	2.19	0.42
1:A:2472:ARG:HG2	1:A:2472:ARG:HH11	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:B:2164:THR:CG2	1:B:2167:GLU:N	2.79	0.42
1:A:2436:VAL:CG1	1:A:2464:PRO:HG2	2.49	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: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
1:B:2524:ASP:OD1	1:B:2527:LEU:HG	2.19	0.42
1:A:2222:ALA:C	1:A:2224:ARG:H	2.23	0.42
1:A:2499:PRO:O	1:A:2502:VAL:HG13	2.18	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:B:2518:ASN:ND2	1:B:2518:ASN:C	2.73	0.41
1:A:2221:MSE:HB2	1:A:2225:THR:HG22	2.01	0.41
1:A:2191:GLU:OE1	1:A:2191:GLU:N	2.34	0.41
1:B:2505:LEU:HA	1:B:2505:LEU:HD22	1.91	0.41
1:A:2387:THR:HG22	1:A:2391:ASN:ND2	2.34	0.41
1:A:2333:LEU:HD22	1:A:2487:TRP:CB	2.48	0.41
1:B:2303:ASP:C	1:B:2303:ASP:OD1	2.58	0.41
1:B:2368:HIS:HE1	1:B:2541:THR:OG1	2.02	0.41
1:A:2445:VAL:HG12	1:A:2449:GLU:HB3	2.01	0.41
1:B:2277:GLN:H	1:B:2277:GLN:HE21	1.66	0.41
1:B:2265:THR:HG22	1:B:2267:ARG:N	2.35	0.41
1:A:2183:ASP:HB3	1:A:2186:VAL:HG23	2.02	0.41
1:A:2494:TYR:CD2	1:A:2549:PRO:HA	2.55	0.41
1:B:2426:PRO:O	1:B:2427:GLU:C	2.58	0.41
1:A:2424:LEU:HG	1:A:2428:PHE:CG	2.56	0.41
1:A:2320:GLU:HA	1:A:2459:PRO:HB2	2.03	0.41
1:A:2259:ARG:HG2	1:A:2259:ARG:HH11	1.85	0.41
1:A:2522:ILE:HG21	1:A:2528:ARG:N	2.36	0.41
1:B:2376:LEU:HA	1:B:2376:LEU:HD23	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2390:LEU:HA	1:A:2390:LEU:HD12	1.81	0.41
1:B:2518:ASN:ND2	1:B:2521:SER:H	2.18	0.41
1:A:2402:ARG:HH11	1:A:2402:ARG:HB3	1.86	0.41
1:A:2456:ASP:OD1	1:A:2456:ASP:N	2.52	0.41
1:B:2326:LEU:HB3	1:B:2329:ASN:HD22	1.84	0.41
1:B:2191:GLU:H	1:B:2191:GLU:HG2	1.76	0.41
1:B:2219:VAL:O	1:B:2226:SER:HA	2.21	0.41
1:B:2198:MSE:HB3	1:B:2201:GLU:HG2	2.02	0.41
1:B:2433:GLU:O	1:B:2436:VAL:HG22	2.20	0.41
1:A:2518:ASN:HD21	1:A:2520:ASP:HB2	1.86	0.41
1:B:2518:ASN:HD22	1:B:2520:ASP:N	2.19	0.41
1:B:2407:VAL:HG11	1:B:2458:PRO:HD3	2.03	0.41
1:B:2509:HIS:HE1	1:B:2510:TYR:CE2	2.39	0.41
1:A:2360:SER:O	1:A:2361:PRO:C	2.57	0.41
1:A:2144:LEU:C	1:A:2144:LEU:HD23	2.40	0.40
1:B:2202:ILE:O	1:B:2203:ARG:NH1	2.51	0.40
1:A:2315:THR:HG22	1:A:2411:TRP:CZ2	2.56	0.40
1:B:2374:SER:O	1:B:2378:TRP:CD1	2.74	0.40
1:B:2317:TYR:HB3	1:B:2458:PRO:HG3	2.03	0.40
1:B:2213:GLN:NE2	1:B:2519:LEU:H	2.19	0.40
1:A:2162:SER:OG	1:A:2169:TYR:HB2	2.20	0.40
1:B:2283:GLU:O	1:B:2284:ILE:HD12	2.21	0.40
1:A:2512:THR:HG23	1:A:2541:THR:N	2.36	0.40
1:A:2154:VAL:HG23	1:A:2155:VAL:HG23	2.03	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	412/414 (100%)	361 (88%)	42 (10%)	9 (2%)	8 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	396/414 (96%)	351 (89%)	35 (9%)	10 (2%)	7 27
All	All	808/828 (98%)	712 (88%)	77 (10%)	19 (2%)	7 29

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
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 (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	373/365 (102%)	349 (94%)	24 (6%)	22 53
1	B	361/365 (99%)	335 (93%)	26 (7%)	18 46
All	All	734/730 (100%)	684 (93%)	50 (7%)	20 49

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2149	GLN
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	2299	ARG
1	A	2307	TYR
1	A	2331	ARG
1	A	2351	ARG
1	A	2353	GLU
1	A	2359	GLN
1	A	2390	LEU
1	A	2396	LYS
1	A	2403	THR
1	A	2417	ASP
1	A	2423	GLU
1	A	2424	LEU
1	A	2497	ARG
1	A	2500	GLU
1	A	2505	LEU
1	B	2146	THR
1	B	2167	GLU
1	B	2172	VAL
1	B	2198	MSE
1	B	2234	GLN
1	B	2249	VAL
1	B	2265	THR
1	B	2277	GLN
1	B	2300	THR
1	B	2326	LEU
1	B	2331	ARG
1	B	2353	GLU
1	B	2359	GLN
1	B	2365	TYR
1	B	2371	THR
1	B	2383	GLU
1	B	2384	PRO
1	B	2416	ARG
1	B	2424	LEU

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Mol	Chain	Res	Type
1	B	2494	TYR
1	B	2505	LEU
1	B	2510	TYR
1	B	2518	ASN
1	B	2520	ASP
1	B	2529	GLU
1	B	2546	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2149	GLN
1	A	2213	GLN
1	A	2274	ASN
1	A	2277	GLN
1	A	2341	ASN
1	A	2359	GLN
1	A	2483	GLN
1	A	2486	GLN
1	A	2518	ASN
1	B	2149	GLN
1	B	2213	GLN
1	B	2277	GLN
1	B	2316	ASN
1	B	2329	ASN
1	B	2368	HIS
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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 95^{th} 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%)	-0.07	11 (2%) 58 52	35, 57, 83, 106	0
1	B	392/414 (94%)	0.02	9 (2%) 64 59	27, 58, 97, 108	0
All	All	798/828 (96%)	-0.03	20 (2%) 61 55	27, 58, 94, 108	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2359	GLN	4.8
1	B	2397	PHE	4.0
1	A	2449	GLU	3.5
1	A	2445	VAL	3.4
1	A	2448	ASP	3.0
1	B	2359	GLN	3.0
1	A	2446	ARG	3.0
1	B	2399	HIS	2.9
1	A	2526	VAL	2.8
1	A	2177	SER	2.4
1	B	2141	PRO	2.4
1	A	2394	ASP	2.4
1	B	2525	PRO	2.4
1	B	2526	VAL	2.3
1	A	2397	PHE	2.3
1	A	2141	PRO	2.2
1	B	2469	ARG	2.2
1	B	2396	LYS	2.2
1	A	2140	GLY	2.1
1	B	2416	ARG	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.