



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:27 PM UTC

PDB ID : 1T77 / pdb_00001t77
Title : Crystal structure of the PH-BEACH domains of human LRBA/BGL
Authors : Gebauer, D.; Li, J.; Jogl, G.; Shen, Y.; Myszkowski, D.G.; Tong, L.
Deposited on : 2004-05-08
Resolution : 2.40 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

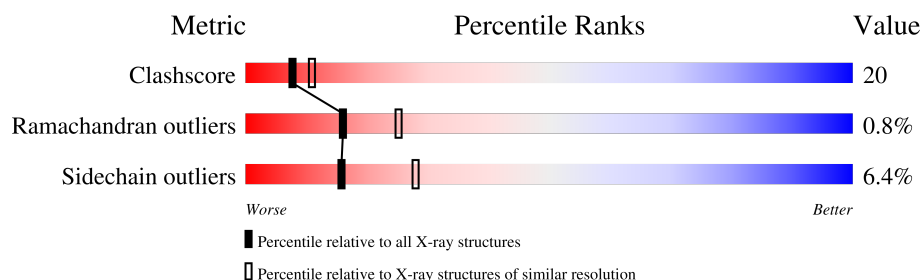
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	414	63% 31% 6%
1	B	414	64% 29% 7%
1	C	414	62% 32% 6%
1	D	414	60% 34% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14010 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 Lipopolysaccharide-responsive and beige-like anchor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3379	2184	565	623	7			
1	B	414	Total	C	N	O	S	0	0	0
			3379	2184	565	623	7			
1	C	414	Total	C	N	O	S	0	0	0
			3379	2184	565	623	7			
1	D	414	Total	C	N	O	S	0	0	0
			3379	2184	565	623	7			

- Molecule 2 is water.

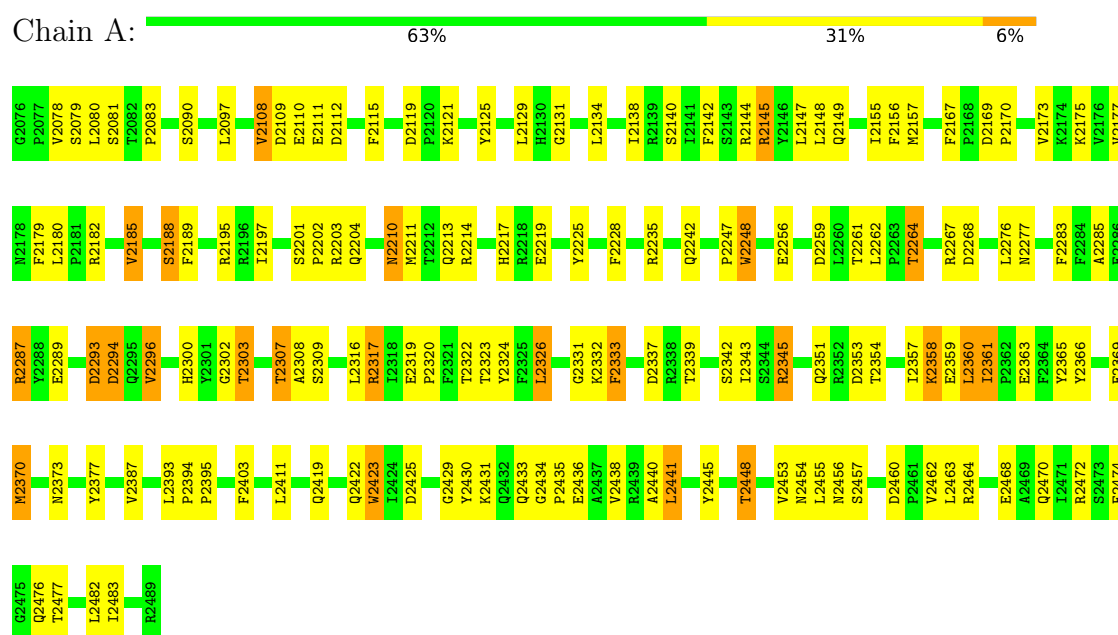
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	130	Total	O	0	0
			130	130		
2	B	113	Total	O	0	0
			113	113		
2	C	125	Total	O	0	0
			125	125		
2	D	126	Total	O	0	0
			126	126		

3 Residue-property plots

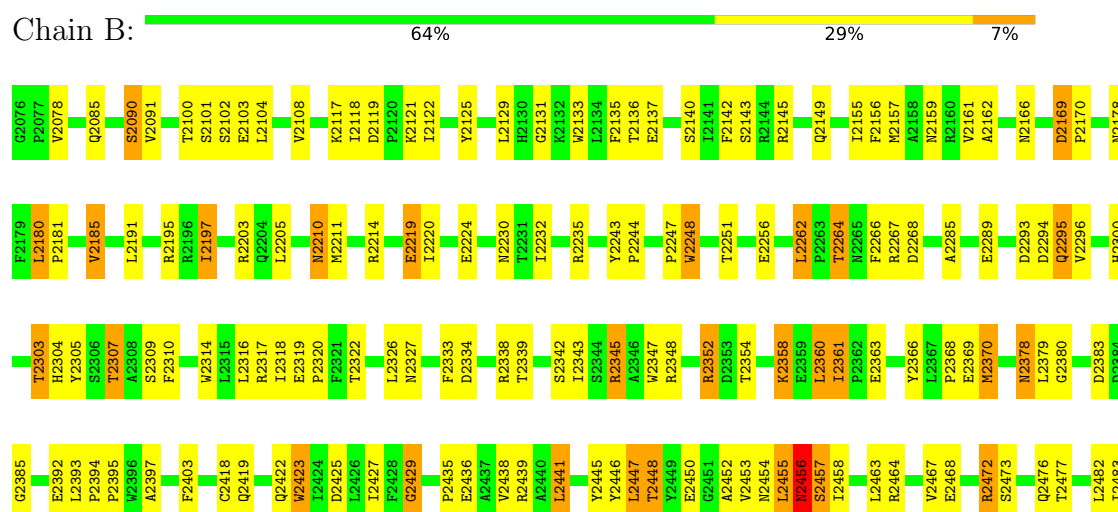
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: Lipopolysaccharide-responsive and beige-like anchor protein



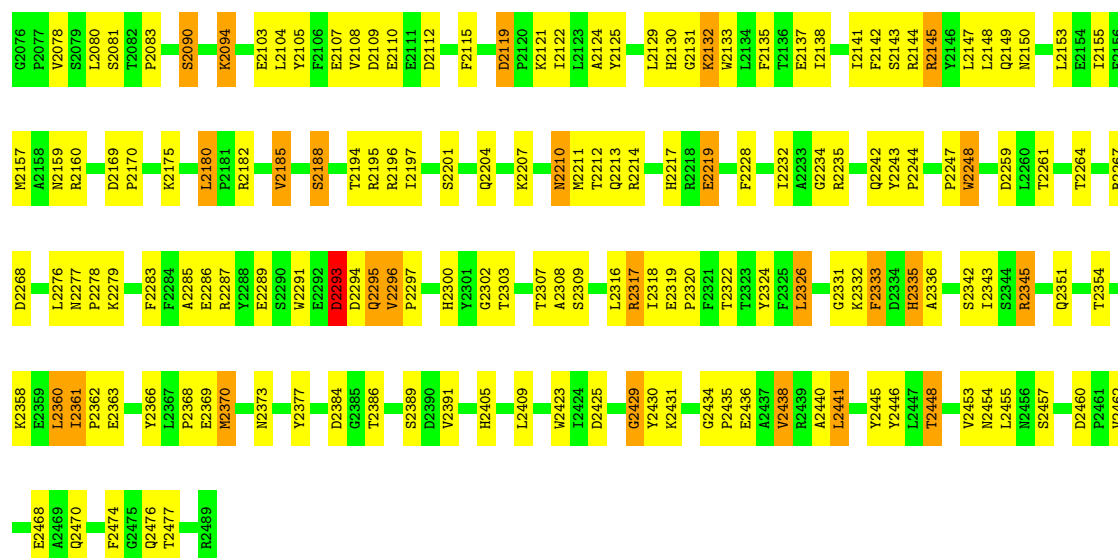
- Molecule 1: Lipopolysaccharide-responsive and beige-like anchor protein



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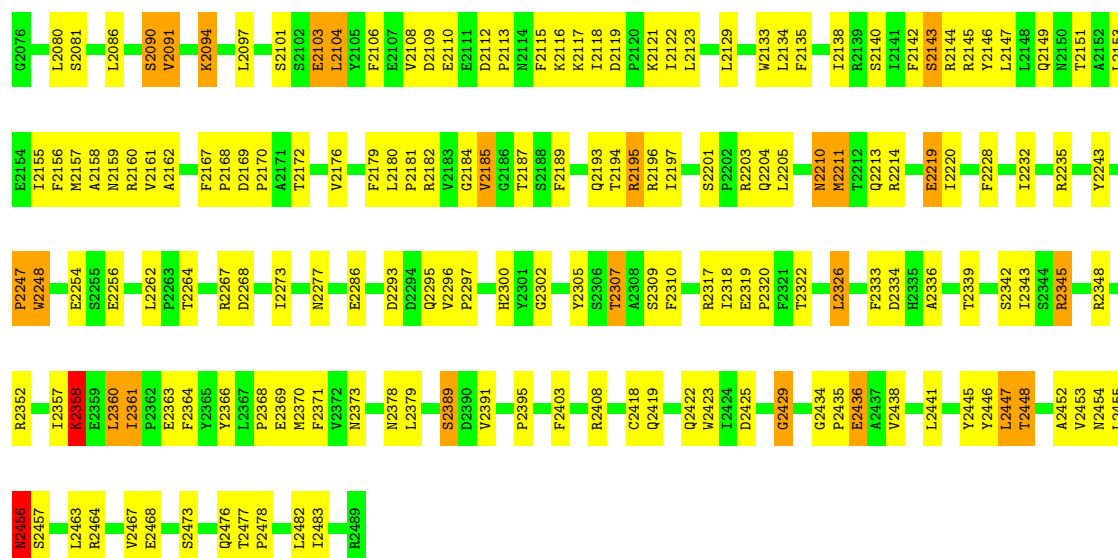
- Molecule 1: Lipopolysaccharide-responsive and beige-like anchor protein

Chain C: 62% 32% 6%



- Molecule 1: Lipopolysaccharide-responsive and beige-like anchor protein

Chain D: 60% 34% 6%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.22Å 102.24Å 131.52Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	88.9 (20.00-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14010	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

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	0.49	1/3477 (0.0%)	0.98	19/4735 (0.4%)
1	B	0.52	4/3477 (0.1%)	1.00	15/4735 (0.3%)
1	C	0.50	1/3477 (0.0%)	0.97	14/4735 (0.3%)
1	D	0.50	1/3477 (0.0%)	1.00	13/4735 (0.3%)
All	All	0.50	7/13908 (0.1%)	0.99	61/18940 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2456	ASN	N-CA	-7.81	1.37	1.46
1	C	2370	MET	SD-CE	-5.97	1.64	1.79
1	B	2456	ASN	CA-C	5.80	1.60	1.52
1	A	2370	MET	SD-CE	-5.39	1.66	1.79
1	B	2370	MET	SD-CE	-5.21	1.66	1.79
1	D	2211	MET	SD-CE	5.16	1.92	1.79
1	B	2455	LEU	C-N	-5.01	1.27	1.33

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2296	VAL	N-CA-C	9.22	115.95	107.56
1	D	2219	GLU	N-CA-C	-8.96	101.78	112.89
1	B	2248	TRP	N-CA-C	-8.41	96.91	110.20
1	D	2248	TRP	N-CA-C	-7.70	98.89	110.28
1	A	2248	TRP	N-CA-C	-7.42	99.30	110.28
1	B	2219	GLU	N-CA-C	-7.26	103.89	112.89
1	C	2429	GLY	N-CA-C	7.02	124.91	112.55
1	C	2219	GLU	N-CA-C	-7.00	104.55	113.23
1	D	2293	ASP	N-CA-C	6.65	119.08	109.71
1	D	2091	VAL	N-CA-C	6.64	116.63	108.53
1	C	2248	TRP	N-CA-C	-6.60	100.51	110.28
1	A	2167	PHE	CA-C-N	6.52	126.02	119.24
1	A	2167	PHE	C-N-CA	6.52	126.02	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2195	ARG	N-CA-C	-6.47	104.32	111.82
1	A	2423	TRP	N-CA-C	-6.46	103.52	111.40
1	A	2188	SER	N-CA-C	6.45	119.12	111.71
1	B	2473	SER	N-CA-C	6.44	121.30	113.38
1	D	2143	SER	N-CA-C	-6.37	101.52	110.50
1	A	2434	GLY	CA-C-N	6.33	127.75	119.84
1	A	2434	GLY	C-N-CA	6.33	127.75	119.84
1	B	2169	ASP	N-CA-C	6.25	113.64	108.07
1	C	2434	GLY	CA-C-N	6.17	126.35	119.32
1	C	2434	GLY	C-N-CA	6.17	126.35	119.32
1	D	2473	SER	N-CA-C	6.08	120.97	113.50
1	B	2293	ASP	N-CA-C	6.00	118.61	109.62
1	A	2294	ASP	N-CA-C	-5.93	104.73	111.14
1	B	2091	VAL	N-CA-C	5.85	115.67	108.53
1	A	2219	GLU	N-CA-C	-5.84	105.65	112.89
1	C	2143	SER	N-CA-C	-5.81	101.68	110.28
1	C	2296	VAL	N-CA-C	5.80	114.27	107.77
1	B	2143	SER	N-CA-C	-5.80	101.70	110.28
1	A	2119	ASP	CA-C-N	5.79	125.47	119.05
1	A	2119	ASP	C-N-CA	5.79	125.47	119.05
1	A	2302	GLY	N-CA-C	-5.78	106.03	115.46
1	D	2456	ASN	CA-CB-CG	-5.74	106.86	112.60
1	D	2429	GLY	N-CA-C	5.62	123.37	112.64
1	A	2287	ARG	N-CA-C	-5.54	105.15	111.07
1	B	2423	TRP	N-CA-C	-5.48	105.39	111.36
1	B	2296	VAL	CA-C-N	5.47	125.41	119.78
1	B	2296	VAL	C-N-CA	5.47	125.41	119.78
1	B	2427	ILE	N-CA-C	5.41	115.67	110.74
1	C	2293	ASP	N-CA-C	5.40	118.26	109.24
1	A	2293	ASP	N-CA-C	5.31	117.97	107.98
1	B	2266	PHE	N-CA-C	5.31	118.14	109.59
1	C	2083	PRO	N-CA-C	-5.29	102.97	111.38
1	C	2302	GLY	N-CA-C	-5.27	106.87	115.46
1	A	2083	PRO	N-CA-C	-5.26	103.02	111.38
1	B	2429	GLY	N-CA-C	5.25	121.78	112.55
1	B	2380	GLY	N-CA-C	5.22	121.30	112.22
1	D	2302	GLY	N-CA-C	-5.20	106.72	115.62
1	C	2188	SER	N-CA-C	5.18	118.69	112.38
1	D	2358	LYS	N-CA-C	5.17	117.39	110.35
1	C	2119	ASP	CA-C-N	5.09	124.58	119.19
1	C	2119	ASP	C-N-CA	5.09	124.58	119.19
1	C	2453	VAL	N-CA-C	5.07	115.05	108.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2131	GLY	N-CA-C	5.07	119.47	112.37
1	B	2456	ASN	CB-CA-C	5.07	118.97	110.92
1	D	2434	GLY	CA-C-N	5.04	125.31	119.47
1	D	2434	GLY	C-N-CA	5.04	125.31	119.47
1	A	2453	VAL	N-CA-C	5.04	115.00	108.35
1	A	2433	GLN	N-CA-C	5.03	116.63	109.14

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	3379	0	3292	129	0
1	B	3379	0	3292	129	0
1	C	3379	0	3292	140	0
1	D	3379	0	3292	138	0
2	A	130	0	0	1	0
2	B	113	0	0	4	0
2	C	125	0	0	4	0
2	D	126	0	0	5	0
All	All	14010	0	13168	534	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (534) 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:C:2138:ILE:HG12	1:C:2157:MET:HE1	1.35	1.07
1:D:2307:THR:HG22	1:D:2310:PHE:H	1.26	1.01
1:A:2138:ILE:HG12	1:A:2157:MET:HE1	1.43	1.01
1:A:2307:THR:HG22	1:A:2309:SER:H	1.27	0.99
1:B:2100:THR:HG23	1:B:2102:SER:H	1.30	0.97
1:C:2307:THR:HG22	1:C:2309:SER:H	1.32	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2307:THR:HG22	1:A:2309:SER:N	1.87	0.88
1:D:2348:ARG:HH11	1:D:2352:ARG:HH22	1.24	0.85
1:A:2285:ALA:O	1:A:2289:GLU:HG2	1.76	0.84
1:C:2157:MET:HE2	1:C:2157:MET:HA	1.59	0.83
1:D:2317:ARG:HG2	1:D:2373:ASN:HA	1.61	0.83
1:A:2470:GLN:HG3	1:A:2474:PHE:CE2	2.14	0.83
1:A:2247:PRO:HB3	1:A:2423:TRP:CE2	2.14	0.82
1:C:2317:ARG:HG2	1:C:2373:ASN:HA	1.60	0.82
1:D:2248:TRP:HA	1:D:2360:LEU:HD22	1.61	0.82
1:D:2080:LEU:HD23	1:D:2081:SER:N	1.96	0.81
1:A:2211:MET:HE1	1:A:2214:ARG:HH21	1.45	0.81
1:C:2210:ASN:C	1:C:2210:ASN:HD22	1.89	0.80
1:B:2435:PRO:O	1:B:2438:VAL:HG22	1.82	0.80
1:B:2307:THR:HG22	1:B:2310:PHE:H	1.45	0.79
1:C:2247:PRO:HB3	1:C:2423:TRP:CE2	2.17	0.79
1:D:2348:ARG:NH1	1:D:2352:ARG:HH22	1.79	0.79
1:A:2460:ASP:OD2	1:A:2462:VAL:HG12	1.83	0.78
1:A:2317:ARG:HG2	1:A:2373:ASN:HA	1.67	0.77
1:C:2285:ALA:O	1:C:2289:GLU:HG2	1.82	0.77
1:C:2155:ILE:HG22	1:C:2157:MET:HE3	1.66	0.76
1:A:2090:SER:HB3	1:A:2324:TYR:CZ	2.21	0.76
1:B:2100:THR:HG21	1:B:2103:GLU:OE1	1.86	0.76
1:C:2363:GLU:HB3	1:C:2370:MET:HE2	1.68	0.76
1:B:2085:GLN:NE2	1:B:2166:ASN:HD22	1.84	0.76
1:B:2211:MET:HE1	1:B:2214:ARG:HH21	1.51	0.75
1:C:2169:ASP:HB2	1:C:2170:PRO:HD2	1.67	0.75
1:C:2119:ASP:OD1	1:C:2121:LYS:HG2	1.85	0.75
1:A:2425:ASP:HA	1:A:2429:GLY:HA3	1.69	0.74
1:B:2285:ALA:O	1:B:2289:GLU:HG2	1.88	0.74
1:A:2431:LYS:HG2	1:A:2436:GLU:HG3	1.70	0.73
1:B:2317:ARG:HG3	1:B:2317:ARG:HH11	1.53	0.73
1:C:2294:ASP:HB3	1:C:2295:GLN:NE2	2.03	0.73
1:C:2110:GLU:HA	1:C:2115:PHE:CD2	2.23	0.73
1:B:2210:ASN:C	1:B:2210:ASN:HD22	1.96	0.73
1:B:2205:LEU:HD13	1:B:2232:ILE:HD12	1.70	0.73
1:C:2194:THR:HG22	1:C:2196:ARG:H	1.53	0.72
1:B:2363:GLU:C	1:B:2370:MET:HE1	2.14	0.72
1:C:2094:LYS:H	1:C:2094:LYS:HZ2	1.36	0.72
1:B:2169:ASP:HB2	1:B:2170:PRO:HD2	1.72	0.72
1:B:2100:THR:HG22	1:B:2103:GLU:O	1.90	0.71
1:D:2456:ASN:OD1	1:D:2456:ASN:N	2.16	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2155:ILE:HG22	1:A:2157:MET:HE3	1.71	0.70
1:A:2307:THR:CG2	1:A:2309:SER:H	2.01	0.70
1:C:2460:ASP:OD2	1:C:2462:VAL:HG12	1.91	0.70
1:D:2326:LEU:HD11	1:D:2333:PHE:CE1	2.27	0.70
1:B:2248:TRP:HA	1:B:2360:LEU:HD22	1.74	0.70
1:D:2348:ARG:HG3	1:D:2352:ARG:NH1	2.07	0.69
1:D:2348:ARG:HH11	1:D:2352:ARG:NH2	1.90	0.69
1:C:2248:TRP:HA	1:C:2360:LEU:HD22	1.74	0.69
1:A:2363:GLU:HB3	1:A:2370:MET:HE2	1.73	0.69
1:A:2454:ASN:O	1:A:2457:SER:HB3	1.93	0.69
1:C:2454:ASN:O	1:C:2457:SER:HB3	1.93	0.69
1:D:2247:PRO:HB3	1:D:2423:TRP:CE2	2.28	0.69
1:A:2445:TYR:O	1:A:2448:THR:HB	1.93	0.69
1:D:2142:PHE:CE2	1:D:2185:VAL:HG22	2.28	0.69
1:A:2157:MET:HE2	1:A:2157:MET:HA	1.74	0.68
1:B:2326:LEU:HD11	1:B:2333:PHE:CE1	2.28	0.68
1:B:2445:TYR:O	1:B:2448:THR:HB	1.93	0.68
1:D:2361:ILE:HG23	1:D:2363:GLU:OE1	1.92	0.68
1:D:2256:GLU:HA	1:D:2395:PRO:HB2	1.76	0.68
1:C:2180:LEU:O	1:C:2195:ARG:NH1	2.26	0.68
1:D:2210:ASN:C	1:D:2210:ASN:HD22	2.01	0.68
1:A:2276:LEU:HB2	1:A:2351:GLN:HE22	1.58	0.68
1:C:2211:MET:HE1	1:C:2214:ARG:HH21	1.59	0.67
1:A:2210:ASN:HD22	1:A:2210:ASN:C	2.01	0.67
1:C:2470:GLN:HG3	1:C:2474:PHE:CE2	2.29	0.67
1:A:2361:ILE:HG23	1:A:2363:GLU:OE1	1.94	0.67
1:D:2142:PHE:O	1:D:2153:LEU:HD12	1.93	0.67
1:B:2361:ILE:HG23	1:B:2363:GLU:OE1	1.95	0.67
1:C:2445:TYR:O	1:C:2448:THR:HB	1.95	0.67
1:D:2445:TYR:O	1:D:2448:THR:HB	1.96	0.66
1:D:2435:PRO:O	1:D:2438:VAL:HG22	1.96	0.66
1:A:2142:PHE:CE2	1:A:2185:VAL:HG22	2.30	0.66
1:A:2435:PRO:O	1:A:2438:VAL:HG22	1.96	0.66
1:C:2331:GLY:C	1:C:2332:LYS:HD2	2.22	0.65
1:D:2342:SER:HB3	1:D:2345:ARG:HB2	1.77	0.65
1:B:2247:PRO:HB3	1:B:2423:TRP:CE2	2.32	0.65
1:A:2180:LEU:O	1:A:2195:ARG:NH1	2.30	0.65
1:C:2182:ARG:HG3	1:C:2195:ARG:HG3	1.77	0.65
1:C:2307:THR:HG22	1:C:2309:SER:N	2.08	0.65
1:D:2455:LEU:HB3	1:D:2464:ARG:NH1	2.12	0.65
1:B:2256:GLU:HA	1:B:2395:PRO:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2343:ILE:HD13	1:A:2403:PHE:CZ	2.33	0.64
1:C:2142:PHE:CE2	1:C:2185:VAL:HG22	2.32	0.64
1:B:2363:GLU:HB3	1:B:2370:MET:CE	2.28	0.64
1:C:2147:LEU:HD13	1:C:2468:GLU:HB2	1.79	0.64
1:A:2110:GLU:HA	1:A:2115:PHE:CD2	2.33	0.64
1:A:2316:LEU:HD21	1:A:2333:PHE:CE1	2.32	0.64
1:D:2097:LEU:HD11	1:D:2104:LEU:HD12	1.80	0.64
1:D:2133:TRP:CD1	1:D:2157:MET:HE3	2.32	0.64
1:D:2211:MET:HE1	1:D:2214:ARG:HH21	1.63	0.63
1:B:2319:GLU:OE2	1:B:2320:PRO:HA	1.99	0.63
1:B:2307:THR:CG2	1:B:2309:SER:HB2	2.27	0.63
1:C:2322:THR:HG21	1:C:2377:TYR:CE1	2.33	0.63
1:D:2454:ASN:O	1:D:2457:SER:HB3	1.99	0.63
1:A:2080:LEU:HD23	1:A:2081:SER:N	2.13	0.62
1:A:2213:GLN:HG2	1:A:2217:HIS:CD2	2.33	0.62
1:B:2348:ARG:O	1:B:2352:ARG:HD3	1.99	0.62
1:B:2342:SER:HB3	1:B:2345:ARG:HB2	1.82	0.62
1:C:2214:ARG:HD2	1:C:2219:GLU:OE1	1.98	0.62
1:D:2103:GLU:HB2	1:D:2133:TRP:O	1.98	0.62
1:B:2145:ARG:HD2	1:B:2450:GLU:OE2	1.99	0.62
1:A:2169:ASP:HB2	1:A:2170:PRO:HD2	1.80	0.62
1:D:2205:LEU:HD13	1:D:2232:ILE:HD12	1.81	0.62
1:A:2448:THR:CG2	1:A:2477:THR:OG1	2.48	0.62
1:B:2343:ILE:HD13	1:B:2403:PHE:CZ	2.35	0.62
1:B:2180:LEU:O	1:B:2195:ARG:NH1	2.25	0.61
1:D:2454:ASN:HB3	1:D:2457:SER:CB	2.31	0.61
1:A:2108:VAL:HG11	1:A:2129:LEU:HD22	1.82	0.61
1:D:2113:PRO:HA	1:D:2116:LYS:HD2	1.83	0.61
1:B:2211:MET:CE	1:B:2214:ARG:HE	2.14	0.61
1:B:2446:TYR:CE1	1:B:2447:LEU:HD13	2.36	0.60
1:C:2316:LEU:C	1:C:2316:LEU:HD23	2.26	0.60
1:D:2425:ASP:HA	1:D:2429:GLY:HA3	1.83	0.60
1:A:2277:ASN:HB3	2:A:10:HOH:O	2.02	0.60
1:A:2210:ASN:C	1:A:2210:ASN:ND2	2.57	0.60
1:B:2262:LEU:HD13	1:B:2264:THR:HG22	1.82	0.60
1:A:2322:THR:HG22	1:A:2326:LEU:CD2	2.31	0.60
1:B:2121:LYS:HE3	1:B:2327:ASN:HB2	1.83	0.60
1:B:2142:PHE:CE2	1:B:2185:VAL:HG22	2.37	0.60
1:D:2334:ASP:HB3	1:D:2339:THR:HG22	1.82	0.60
1:A:2322:THR:HG21	1:A:2377:TYR:CE1	2.35	0.60
1:B:2267:ARG:HD3	1:B:2268:ASP:C	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2094:LYS:H	1:C:2094:LYS:NZ	1.99	0.60
1:D:2343:ILE:HD13	1:D:2403:PHE:CZ	2.36	0.60
1:D:2454:ASN:HB3	1:D:2457:SER:HB2	1.84	0.60
1:C:2201:SER:OG	1:C:2204:GLN:HG3	2.02	0.59
1:B:2100:THR:CG2	1:B:2103:GLU:H	2.15	0.59
1:C:2448:THR:CG2	1:C:2477:THR:OG1	2.51	0.59
1:D:2194:THR:HG22	1:D:2196:ARG:H	1.66	0.59
1:D:2300:HIS:CE1	1:D:2441:LEU:HA	2.37	0.59
1:A:2331:GLY:C	1:A:2332:LYS:HD2	2.27	0.59
1:C:2108:VAL:HG11	1:C:2129:LEU:HD22	1.84	0.59
1:D:2103:GLU:HA	1:D:2135:PHE:CD1	2.38	0.59
1:D:2140:SER:OG	1:D:2156:PHE:HB2	2.03	0.59
1:C:2213:GLN:HG2	1:C:2217:HIS:CD2	2.38	0.59
1:B:2214:ARG:HD2	1:B:2219:GLU:OE1	2.02	0.59
1:B:2300:HIS:CD2	1:B:2441:LEU:HD22	2.38	0.58
1:A:2121:LYS:HD2	1:A:2323:THR:HG23	1.85	0.58
1:B:2307:THR:HG21	1:B:2309:SER:HB2	1.85	0.58
1:C:2138:ILE:HA	1:C:2157:MET:CE	2.33	0.58
1:D:2203:ARG:HH11	1:D:2483:ILE:HG23	1.68	0.58
1:A:2248:TRP:HA	1:A:2360:LEU:HD22	1.85	0.58
1:C:2430:TYR:CE1	1:C:2436:GLU:HG2	2.38	0.58
1:D:2108:VAL:HG11	1:D:2129:LEU:CD2	2.34	0.58
1:A:2080:LEU:HD23	1:A:2080:LEU:C	2.28	0.58
1:A:2155:ILE:HG22	1:A:2157:MET:CE	2.33	0.58
1:D:2307:THR:CG2	1:D:2309:SER:HB2	2.34	0.58
1:B:2108:VAL:HG11	1:B:2129:LEU:HD22	1.86	0.58
1:C:2157:MET:HE2	1:C:2157:MET:CA	2.34	0.58
1:C:2332:LYS:HD2	1:C:2332:LYS:N	2.19	0.58
1:D:2254:GLU:O	1:D:2395:PRO:HG2	2.02	0.58
1:D:2180:LEU:O	1:D:2195:ARG:NH1	2.37	0.57
1:A:2342:SER:HB3	1:A:2345:ARG:HB2	1.85	0.57
1:B:2418:CYS:SG	1:B:2419:GLN:HG2	2.44	0.57
1:D:2419:GLN:OE1	1:D:2422:GLN:NE2	2.38	0.57
1:B:2211:MET:HE1	1:B:2214:ARG:HE	1.68	0.57
1:C:2080:LEU:HD23	1:C:2080:LEU:C	2.30	0.57
1:A:2343:ILE:HD11	1:A:2393:LEU:HD23	1.85	0.57
1:C:2291:TRP:NE1	1:C:2293:ASP:HB2	2.19	0.57
1:D:2185:VAL:O	1:D:2185:VAL:HG13	2.03	0.57
1:B:2317:ARG:HG3	1:B:2317:ARG:NH1	2.18	0.57
1:A:2195:ARG:HG2	1:A:2195:ARG:HH11	1.69	0.56
1:D:2118:ILE:HG21	1:D:2123:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2456:ASN:O	1:B:2458:ILE:N	2.37	0.56
1:C:2276:LEU:HB2	1:C:2351:GLN:HE22	1.71	0.56
1:A:2090:SER:HB3	1:A:2324:TYR:OH	2.06	0.56
1:A:2307:THR:CG2	1:A:2308:ALA:N	2.68	0.56
1:C:2094:LYS:H	1:C:2094:LYS:CE	2.18	0.56
1:D:2363:GLU:C	1:D:2370:MET:HE1	2.30	0.56
1:A:2440:ALA:O	1:A:2441:LEU:HB2	2.03	0.56
1:A:2185:VAL:O	1:A:2185:VAL:HG13	2.05	0.56
1:B:2363:GLU:HB3	1:B:2370:MET:HE2	1.87	0.56
1:B:2140:SER:OG	1:B:2156:PHE:HB2	2.06	0.56
1:C:2307:THR:HG22	1:C:2308:ALA:N	2.21	0.56
1:A:2343:ILE:HD12	1:A:2393:LEU:HA	1.87	0.55
1:C:2228:PHE:CE1	1:C:2232:ILE:HG13	2.42	0.55
1:C:2080:LEU:HD23	1:C:2081:SER:N	2.22	0.55
1:C:2185:VAL:O	1:C:2185:VAL:HG13	2.04	0.55
1:A:2148:LEU:HD21	1:A:2476:GLN:HG2	1.88	0.55
1:A:2322:THR:HG22	1:A:2326:LEU:HD23	1.88	0.55
1:C:2343:ILE:HD12	1:C:2391:VAL:HG12	1.88	0.55
1:D:2094:LYS:HZ3	1:D:2094:LYS:HB2	1.72	0.55
1:D:2307:THR:HG21	1:D:2309:SER:HB2	1.87	0.55
1:C:2431:LYS:HG2	1:C:2436:GLU:HG3	1.87	0.55
1:D:2452:ALA:HB3	2:D:53:HOH:O	2.04	0.55
1:C:2138:ILE:HA	1:C:2157:MET:HE2	1.87	0.55
1:C:2194:THR:HG22	1:C:2195:ARG:N	2.22	0.55
1:A:2316:LEU:C	1:A:2316:LEU:HD23	2.31	0.55
1:A:2235:ARG:HD3	1:A:2242:GLN:O	2.07	0.55
1:B:2394:PRO:HD2	1:B:2397:ALA:HB3	1.89	0.54
1:B:2085:GLN:HE21	1:B:2166:ASN:HD22	1.56	0.54
1:D:2307:THR:HG22	1:D:2310:PHE:N	2.09	0.54
1:B:2090:SER:HB3	1:B:2122:ILE:HG23	1.90	0.54
1:C:2425:ASP:HA	1:C:2429:GLY:HA3	1.89	0.54
1:C:2149:GLN:HE22	1:C:2455:LEU:H	1.54	0.54
1:D:2172:THR:O	1:D:2176:VAL:HG23	2.07	0.54
1:A:2247:PRO:HD3	1:A:2423:TRP:CH2	2.42	0.54
1:A:2262:LEU:HB3	1:A:2264:THR:HG22	1.89	0.54
1:D:2194:THR:HG21	1:D:2196:ARG:NH1	2.23	0.54
1:D:2455:LEU:HB3	1:D:2464:ARG:CZ	2.38	0.54
1:B:2104:LEU:HD21	1:B:2133:TRP:HB2	1.90	0.53
1:A:2430:TYR:CE1	1:A:2436:GLU:HG2	2.43	0.53
1:B:2211:MET:HE1	1:B:2214:ARG:NH2	2.21	0.53
1:B:2425:ASP:HA	1:B:2429:GLY:HA3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2110:GLU:HA	1:D:2115:PHE:CD2	2.43	0.53
1:A:2140:SER:OG	1:A:2156:PHE:HB2	2.09	0.53
1:C:2141:ILE:CG2	1:C:2153:LEU:HD11	2.39	0.53
1:C:2247:PRO:HD3	1:C:2423:TRP:CH2	2.43	0.53
1:C:2322:THR:HG22	1:C:2326:LEU:HD23	1.91	0.52
1:D:2348:ARG:HG3	1:D:2352:ARG:HH12	1.73	0.52
1:B:2104:LEU:H	1:B:2104:LEU:HD23	1.74	0.52
1:B:2133:TRP:CD1	1:B:2157:MET:HE3	2.43	0.52
1:B:2119:ASP:OD1	1:B:2121:LYS:HG2	2.09	0.52
1:D:2108:VAL:HG11	1:D:2129:LEU:HD23	1.90	0.52
1:A:2203:ARG:NH1	1:A:2483:ILE:HG12	2.24	0.52
1:B:2452:ALA:O	1:B:2453:VAL:HG23	2.09	0.52
1:C:2103:GLU:HA	1:C:2135:PHE:CD1	2.45	0.52
1:C:2361:ILE:HG23	1:C:2363:GLU:OE1	2.10	0.52
1:B:2322:THR:O	1:B:2326:LEU:HD13	2.10	0.52
1:C:2342:SER:HB3	1:C:2345:ARG:HB2	1.91	0.52
1:B:2125:TYR:CD2	1:B:2320:PRO:HB3	2.45	0.52
1:B:2452:ALA:HB3	2:B:125:HOH:O	2.10	0.52
1:B:2104:LEU:CD2	1:B:2133:TRP:HB2	2.40	0.52
1:A:2256:GLU:HA	1:A:2395:PRO:HB2	1.92	0.52
1:C:2149:GLN:NE2	1:C:2455:LEU:H	2.07	0.51
1:A:2157:MET:HE2	1:A:2157:MET:CA	2.39	0.51
1:B:2378:ASN:O	1:B:2379:LEU:HB2	2.10	0.51
1:C:2384:ASP:OD2	1:C:2386:THR:OG1	2.29	0.51
1:C:2210:ASN:C	1:C:2210:ASN:ND2	2.58	0.51
1:D:2138:ILE:HG23	1:D:2155:ILE:HG23	1.91	0.51
1:D:2307:THR:HG23	1:D:2309:SER:H	1.74	0.51
1:A:2145:ARG:HE	1:A:2145:ARG:N	2.08	0.51
1:B:2235:ARG:NH2	1:B:2476:GLN:O	2.43	0.51
1:C:2125:TYR:CG	1:C:2320:PRO:HB3	2.45	0.51
1:D:2363:GLU:OE1	1:D:2363:GLU:N	2.41	0.51
1:A:2259:ASP:OD1	1:A:2261:THR:OG1	2.25	0.51
1:A:2287:ARG:HG3	1:A:2287:ARG:HH11	1.76	0.51
1:D:2334:ASP:HB3	1:D:2339:THR:CG2	2.41	0.51
1:C:2094:LYS:HZ2	1:C:2094:LYS:N	2.06	0.51
1:D:2267:ARG:HD3	1:D:2268:ASP:C	2.36	0.51
1:A:2078:VAL:HG23	1:A:2078:VAL:O	2.11	0.51
1:D:2205:LEU:HD13	1:D:2232:ILE:CD1	2.40	0.51
1:B:2307:THR:HG23	1:B:2309:SER:H	1.76	0.50
1:D:2235:ARG:NH2	1:D:2476:GLN:O	2.44	0.50
1:D:2286:GLU:HB3	2:D:472:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2110:GLU:HA	1:C:2115:PHE:HD2	1.74	0.50
1:C:2235:ARG:HD3	1:C:2242:GLN:O	2.12	0.50
1:B:2294:ASP:HB2	1:B:2295:GLN:NE2	2.27	0.50
1:C:2188:SER:O	1:C:2211:MET:HE3	2.11	0.50
1:D:2318:ILE:HG22	1:D:2319:GLU:O	2.12	0.50
1:B:2108:VAL:HG11	1:B:2129:LEU:CD2	2.40	0.50
1:C:2440:ALA:O	1:C:2441:LEU:HB2	2.12	0.50
1:D:2182:ARG:HD2	2:D:368:HOH:O	2.12	0.50
1:A:2343:ILE:HD12	1:A:2394:PRO:HD3	1.92	0.50
1:A:2300:HIS:CD2	1:A:2441:LEU:HD22	2.47	0.50
1:D:2307:THR:HG23	1:D:2309:SER:N	2.27	0.50
1:C:2155:ILE:HG22	1:C:2157:MET:CE	2.38	0.50
1:C:2294:ASP:HB3	1:C:2295:GLN:HE22	1.77	0.50
1:B:2363:GLU:HB3	1:B:2370:MET:HE1	1.94	0.49
1:C:2293:ASP:HB3	1:C:2296:VAL:O	2.12	0.49
1:B:2100:THR:HG23	1:B:2101:SER:N	2.27	0.49
1:C:2080:LEU:HD11	1:C:2175:LYS:HD2	1.94	0.49
1:A:2147:LEU:HD13	1:A:2468:GLU:HB2	1.94	0.49
1:A:2319:GLU:OE2	1:A:2320:PRO:HA	2.13	0.49
1:A:2365:TYR:CE2	1:A:2411:LEU:HB2	2.48	0.49
1:C:2109:ASP:OD1	1:C:2112:ASP:N	2.45	0.49
1:C:2316:LEU:HD23	1:C:2316:LEU:O	2.13	0.49
1:D:2319:GLU:OE2	1:D:2320:PRO:HA	2.13	0.49
1:D:2454:ASN:HD22	1:D:2455:LEU:N	2.10	0.49
1:B:2316:LEU:HD23	1:B:2316:LEU:O	2.13	0.49
1:C:2122:ILE:C	1:C:2124:ALA:N	2.69	0.49
1:B:2334:ASP:OD2	1:B:2338:ARG:HB2	2.13	0.49
1:D:2184:GLY:HA2	1:D:2194:THR:O	2.13	0.49
1:D:2446:TYR:CE1	1:D:2447:LEU:HD13	2.48	0.49
1:B:2078:VAL:O	1:B:2078:VAL:HG23	2.13	0.49
1:B:2145:ARG:HD3	2:B:324:HOH:O	2.13	0.48
1:C:2363:GLU:HB3	1:C:2370:MET:CE	2.42	0.48
1:B:2363:GLU:CB	1:B:2370:MET:HE1	2.43	0.48
1:A:2121:LYS:CD	1:A:2323:THR:HG23	2.43	0.48
1:A:2144:ARG:HA	1:A:2145:ARG:HH21	1.79	0.48
1:B:2100:THR:HG22	1:B:2103:GLU:H	1.79	0.48
1:B:2210:ASN:C	1:B:2210:ASN:ND2	2.64	0.48
1:C:2108:VAL:HG11	1:C:2129:LEU:CD2	2.43	0.48
1:D:2211:MET:CE	1:D:2214:ARG:HE	2.26	0.48
1:A:2456:ASN:HA	1:A:2464:ARG:HH21	1.76	0.48
1:C:2141:ILE:HD13	1:C:2180:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2185:VAL:O	1:C:2185:VAL:CG1	2.62	0.48
1:B:2463:LEU:O	1:B:2467:VAL:HG23	2.13	0.48
1:D:2097:LEU:HD11	1:D:2104:LEU:CD1	2.43	0.48
1:C:2435:PRO:O	1:C:2438:VAL:HG13	2.14	0.48
1:A:2203:ARG:HH12	1:A:2483:ILE:HG12	1.79	0.48
1:D:2158:ALA:C	1:D:2160:ARG:H	2.22	0.48
1:D:2194:THR:HG22	1:D:2195:ARG:N	2.29	0.48
1:B:2159:ASN:OD1	1:B:2161:VAL:HB	2.13	0.48
1:C:2363:GLU:C	1:C:2370:MET:CE	2.87	0.48
1:B:2318:ILE:HG22	1:B:2319:GLU:O	2.13	0.47
1:A:2182:ARG:HG3	1:A:2195:ARG:HG3	1.95	0.47
1:D:2322:THR:O	1:D:2326:LEU:HD13	2.14	0.47
1:D:2464:ARG:NH1	1:D:2468:GLU:OE2	2.47	0.47
1:A:2369:GLU:OE1	1:A:2369:GLU:N	2.28	0.47
1:A:2419:GLN:OE1	1:A:2422:GLN:NE2	2.47	0.47
1:D:2080:LEU:HD12	1:D:2179:PHE:CD1	2.50	0.47
1:A:2090:SER:HB3	1:A:2324:TYR:CE2	2.50	0.47
1:A:2125:TYR:CG	1:A:2320:PRO:HB3	2.49	0.47
1:A:2387:VAL:H	1:B:2178:ASN:HD22	1.62	0.47
1:A:2482:LEU:HD23	1:A:2482:LEU:N	2.30	0.47
1:B:2300:HIS:NE2	1:B:2441:LEU:HD22	2.29	0.47
1:B:2454:ASN:HB3	1:B:2457:SER:HB3	1.96	0.47
1:A:2080:LEU:CD1	1:A:2175:LYS:HG2	2.44	0.47
1:A:2303:THR:HG22	1:A:2357:ILE:HD11	1.97	0.47
1:C:2138:ILE:CG1	1:C:2157:MET:HE1	2.25	0.47
1:D:2118:ILE:HG21	1:D:2123:LEU:CD2	2.45	0.47
1:D:2167:PHE:HB3	1:D:2168:PRO:CD	2.43	0.47
1:A:2267:ARG:HD3	1:A:2268:ASP:C	2.39	0.47
1:D:2210:ASN:C	1:D:2210:ASN:ND2	2.66	0.47
1:B:2456:ASN:C	1:B:2458:ILE:H	2.23	0.46
1:A:2079:SER:HB3	1:A:2179:PHE:HE2	1.80	0.46
1:A:2357:ILE:C	1:A:2357:ILE:HD12	2.40	0.46
1:A:2431:LYS:HG2	1:A:2436:GLU:CG	2.42	0.46
1:D:2091:VAL:HG11	1:D:2118:ILE:HD12	1.97	0.46
1:D:2368:PRO:HG2	1:D:2369:GLU:OE1	2.14	0.46
1:B:2230:ASN:OD1	1:B:2244:PRO:HA	2.15	0.46
1:D:2453:VAL:HG12	1:D:2454:ASN:N	2.29	0.46
1:C:2277:ASN:HB3	2:C:41:HOH:O	2.15	0.46
1:A:2316:LEU:HD23	1:A:2316:LEU:O	2.14	0.46
1:B:2316:LEU:HD21	1:B:2333:PHE:CE1	2.51	0.46
1:A:2189:PHE:HA	1:A:2211:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2142:PHE:CZ	1:B:2185:VAL:HG22	2.50	0.46
1:C:2307:THR:CG2	1:C:2308:ALA:N	2.79	0.46
1:C:2470:GLN:HG3	1:C:2474:PHE:CD2	2.51	0.46
1:B:2203:ARG:NH1	1:B:2483:ILE:HG23	2.31	0.46
1:A:2173:VAL:O	1:A:2177:VAL:HG23	2.15	0.46
1:A:2307:THR:HG22	1:A:2308:ALA:N	2.30	0.46
1:B:2104:LEU:HD23	1:B:2133:TRP:O	2.16	0.46
1:B:2464:ARG:HG2	1:B:2464:ARG:HH11	1.81	0.46
1:A:2121:LYS:CE	1:A:2323:THR:HG23	2.47	0.45
1:A:2373:ASN:OD1	1:A:2373:ASN:O	2.35	0.45
1:B:2210:ASN:HD22	1:B:2211:MET:N	2.13	0.45
1:C:2122:ILE:C	1:C:2124:ALA:H	2.25	0.45
1:C:2295:GLN:NE2	1:C:2295:GLN:N	2.64	0.45
1:A:2108:VAL:HG11	1:A:2129:LEU:CD2	2.46	0.45
1:B:2185:VAL:O	1:B:2185:VAL:HG13	2.16	0.45
1:D:2379:LEU:HD12	1:D:2389:SER:HA	1.99	0.45
1:D:2463:LEU:O	1:D:2467:VAL:HG23	2.16	0.45
1:A:2454:ASN:C	1:A:2454:ASN:HD22	2.24	0.45
1:B:2419:GLN:OE1	1:B:2422:GLN:NE2	2.49	0.45
1:C:2277:ASN:C	1:C:2277:ASN:OD1	2.59	0.45
1:C:2318:ILE:HG22	1:C:2319:GLU:O	2.17	0.45
1:A:2454:ASN:C	1:A:2454:ASN:ND2	2.73	0.45
1:B:2361:ILE:HG23	1:B:2363:GLU:H	1.82	0.45
1:D:2343:ILE:HD13	1:D:2403:PHE:CE1	2.52	0.45
1:A:2148:LEU:CD2	1:A:2476:GLN:HG2	2.46	0.45
1:B:2303:THR:CG2	1:B:2304:HIS:N	2.79	0.45
1:B:2393:LEU:HB3	1:B:2394:PRO:CD	2.46	0.45
1:B:2345:ARG:NH2	1:B:2392:GLU:OE2	2.43	0.44
1:D:2357:ILE:C	1:D:2357:ILE:HD12	2.42	0.44
1:D:2454:ASN:HB3	1:D:2457:SER:HB3	1.99	0.44
1:A:2293:ASP:HB2	1:A:2296:VAL:O	2.18	0.44
1:B:2448:THR:HG23	1:B:2477:THR:OG1	2.17	0.44
1:B:2456:ASN:C	1:B:2458:ILE:N	2.76	0.44
1:D:2228:PHE:CE1	1:D:2232:ILE:HG13	2.51	0.44
1:D:2370:MET:HE3	1:D:2371:PHE:CE1	2.52	0.44
1:C:2291:TRP:HE1	1:C:2293:ASP:HB2	1.80	0.44
1:D:2086:LEU:HB2	1:D:2106:PHE:CE2	2.52	0.44
1:A:2201:SER:OG	1:A:2204:GLN:HG3	2.18	0.44
1:A:2247:PRO:HB3	1:A:2423:TRP:NE1	2.32	0.44
1:A:2267:ARG:HD3	1:A:2267:ARG:C	2.43	0.44
1:B:2100:THR:HG21	1:B:2103:GLU:CD	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2454:ASN:HD22	1:B:2455:LEU:N	2.16	0.44
1:D:2155:ILE:N	1:D:2155:ILE:HD12	2.33	0.44
1:A:2125:TYR:CD2	1:A:2320:PRO:HB3	2.52	0.44
1:A:2210:ASN:HD22	1:A:2211:MET:N	2.16	0.44
1:C:2145:ARG:HG3	1:C:2150:ASN:HA	1.98	0.44
1:D:2119:ASP:OD1	1:D:2121:LYS:HG2	2.18	0.44
1:D:2189:PHE:HA	1:D:2211:MET:HE3	1.98	0.44
1:D:2371:PHE:HA	1:D:2391:VAL:CG2	2.48	0.44
1:D:2436:GLU:HA	1:D:2436:GLU:OE1	2.17	0.44
1:B:2203:ARG:NH1	1:B:2483:ILE:CG2	2.81	0.44
1:C:2247:PRO:HD3	1:C:2423:TRP:CZ3	2.52	0.44
1:C:2322:THR:HG22	1:C:2326:LEU:CD2	2.48	0.44
1:C:2454:ASN:C	1:C:2454:ASN:ND2	2.75	0.44
1:A:2342:SER:CB	1:A:2345:ARG:HB2	2.48	0.44
1:A:2456:ASN:HA	1:A:2464:ARG:NH2	2.32	0.44
1:B:2307:THR:HG22	1:B:2310:PHE:N	2.23	0.44
1:B:2383:ASP:C	1:B:2385:GLY:N	2.74	0.44
1:B:2472:ARG:HG2	1:B:2472:ARG:HH11	1.83	0.44
1:C:2131:GLY:HA3	1:C:2133:TRP:CH2	2.53	0.44
1:D:2453:VAL:CG1	1:D:2454:ASN:N	2.81	0.44
1:C:2094:LYS:H	1:C:2094:LYS:HE3	1.83	0.44
1:D:2108:VAL:HG11	1:D:2129:LEU:HD22	1.99	0.44
1:D:2214:ARG:HD2	1:D:2219:GLU:OE1	2.18	0.44
1:C:2267:ARG:C	1:C:2267:ARG:HD3	2.43	0.43
1:D:2151:THR:HG22	1:D:2170:PRO:HD3	2.00	0.43
1:D:2408:ARG:HG2	1:D:2408:ARG:HH11	1.83	0.43
1:A:2283:PHE:CD2	1:A:2283:PHE:C	2.96	0.43
1:B:2145:ARG:HA	1:B:2149:GLN:O	2.17	0.43
1:B:2334:ASP:HB3	1:B:2339:THR:CG2	2.48	0.43
1:D:2159:ASN:CG	1:D:2161:VAL:HG23	2.42	0.43
1:D:2305:TYR:HA	1:D:2358:LYS:HA	2.00	0.43
1:D:2446:TYR:CE2	1:D:2447:LEU:HD22	2.53	0.43
1:C:2210:ASN:O	1:C:2214:ARG:HG3	2.18	0.43
1:A:2387:VAL:H	1:B:2178:ASN:ND2	2.16	0.43
1:B:2482:LEU:N	1:B:2482:LEU:HD23	2.32	0.43
1:C:2080:LEU:CD1	1:C:2175:LYS:HD2	2.48	0.43
1:C:2144:ARG:NH1	1:C:2234:GLY:HA2	2.33	0.43
1:D:2161:VAL:HG12	1:D:2162:ALA:N	2.32	0.43
1:B:2104:LEU:HD23	1:B:2104:LEU:N	2.33	0.43
1:B:2243:TYR:HD2	1:B:2361:ILE:HD11	1.83	0.43
1:D:2235:ARG:HD3	1:D:2243:TYR:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2273:ILE:HG23	2:D:249:HOH:O	2.17	0.43
1:A:2185:VAL:O	1:A:2185:VAL:CG1	2.63	0.43
1:B:2220:ILE:HG23	1:B:2224:GLU:HB3	2.01	0.43
1:A:2353:ASP:OD2	1:A:2353:ASP:C	2.61	0.43
1:B:2232:ILE:HD13	1:B:2232:ILE:HA	1.71	0.43
1:C:2368:PRO:HG2	1:C:2369:GLU:OE1	2.18	0.43
1:B:2339:THR:HG22	2:B:258:HOH:O	2.18	0.43
1:C:2105:TYR:HB2	1:C:2131:GLY:O	2.18	0.43
1:D:2094:LYS:H	1:D:2094:LYS:HZ2	1.65	0.43
1:C:2244:PRO:HB2	1:C:2362:PRO:HG2	2.00	0.43
1:C:2335:HIS:O	1:C:2336:ALA:C	2.62	0.43
1:D:2169:ASP:HB2	1:D:2170:PRO:HD2	2.00	0.43
1:D:2418:CYS:SG	1:D:2419:GLN:HG2	2.59	0.43
1:A:2468:GLU:O	1:A:2472:ARG:HB2	2.19	0.42
1:C:2300:HIS:CE1	1:C:2441:LEU:HA	2.54	0.42
1:B:2314:TRP:CZ2	1:B:2358:LYS:HD3	2.54	0.42
1:C:2300:HIS:CD2	1:C:2441:LEU:HD22	2.55	0.42
1:C:2322:THR:HG21	1:C:2377:TYR:HE1	1.80	0.42
1:A:2363:GLU:C	1:A:2370:MET:CE	2.92	0.42
1:B:2267:ARG:HD3	1:B:2267:ARG:C	2.43	0.42
1:C:2090:SER:HA	1:C:2324:TYR:CE1	2.54	0.42
1:C:2107:GLU:OE2	1:C:2130:HIS:HA	2.19	0.42
1:C:2283:PHE:HE2	1:C:2287:ARG:NH2	2.17	0.42
1:C:2326:LEU:HD21	1:C:2333:PHE:CZ	2.54	0.42
1:A:2149:GLN:NE2	1:A:2455:LEU:H	2.18	0.42
1:B:2464:ARG:O	1:B:2468:GLU:HG3	2.19	0.42
1:D:2248:TRP:CD2	1:D:2360:LEU:HD13	2.54	0.42
1:C:2212:THR:HB	2:C:449:HOH:O	2.19	0.42
1:D:2117:LYS:O	1:D:2118:ILE:C	2.62	0.42
1:D:2197:ILE:HD13	1:D:2197:ILE:HA	1.93	0.42
1:B:2197:ILE:HD13	1:B:2197:ILE:HA	1.85	0.42
1:C:2110:GLU:HA	1:C:2115:PHE:CE2	2.54	0.42
1:C:2259:ASP:OD1	1:C:2261:THR:OG1	2.35	0.42
1:D:2201:SER:OG	1:D:2204:GLN:HG3	2.20	0.42
1:B:2185:VAL:HG11	1:B:2191:LEU:HD12	2.02	0.42
1:B:2251:THR:HG22	1:B:2347:TRP:CZ2	2.55	0.42
1:C:2103:GLU:OE1	1:C:2132:LYS:HE2	2.20	0.42
1:C:2430:TYR:CD1	1:C:2436:GLU:HG2	2.55	0.42
1:B:2211:MET:HE1	1:B:2214:ARG:NE	2.34	0.42
1:D:2319:GLU:OE2	1:D:2319:GLU:HA	2.20	0.42
1:D:2448:THR:HG23	1:D:2477:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2211:MET:HE1	1:A:2214:ARG:NH2	2.25	0.42
1:A:2462:VAL:HG13	1:A:2463:LEU:N	2.35	0.42
1:B:2476:GLN:HG3	2:B:167:HOH:O	2.20	0.42
1:A:2188:SER:O	1:A:2211:MET:HE3	2.20	0.42
1:A:2287:ARG:HG3	1:A:2287:ARG:NH1	2.35	0.42
1:C:2210:ASN:HD22	1:C:2211:MET:N	2.18	0.42
1:C:2235:ARG:HD3	1:C:2243:TYR:O	2.19	0.42
1:D:2211:MET:HE1	1:D:2214:ARG:HE	1.85	0.42
1:D:2277:ASN:HB3	2:D:5:HOH:O	2.20	0.42
1:C:2104:LEU:HD23	1:C:2133:TRP:HB2	2.03	0.41
1:D:2378:ASN:O	1:D:2379:LEU:HB2	2.20	0.41
1:A:2097:LEU:HD23	1:A:2097:LEU:C	2.45	0.41
1:A:2235:ARG:NH2	1:A:2476:GLN:O	2.50	0.41
1:B:2205:LEU:HD13	1:B:2232:ILE:CD1	2.45	0.41
1:C:2267:ARG:HD3	1:C:2268:ASP:C	2.45	0.41
1:C:2405:HIS:O	1:C:2409:LEU:HG	2.20	0.41
1:C:2454:ASN:C	1:C:2454:ASN:HD22	2.26	0.41
1:A:2213:GLN:HG2	1:A:2217:HIS:NE2	2.34	0.41
1:B:2117:LYS:O	1:B:2118:ILE:C	2.63	0.41
1:C:2295:GLN:N	1:C:2295:GLN:HE21	2.18	0.41
1:D:2135:PHE:CD2	1:D:2181:PRO:HG3	2.54	0.41
1:A:2293:ASP:O	1:A:2293:ASP:CG	2.63	0.41
1:B:2464:ARG:HG2	1:B:2464:ARG:NH1	2.36	0.41
1:D:2477:THR:HA	1:D:2478:PRO:HD3	1.91	0.41
1:A:2460:ASP:CG	1:A:2462:VAL:HG12	2.45	0.41
1:B:2363:GLU:OE1	1:B:2363:GLU:N	2.44	0.41
1:C:2137:GLU:HG3	2:C:130:HOH:O	2.20	0.41
1:D:2103:GLU:HB3	1:D:2134:LEU:HA	2.01	0.41
1:B:2368:PRO:HG2	1:B:2369:GLU:OE1	2.20	0.41
1:C:2090:SER:HA	1:C:2324:TYR:CZ	2.56	0.41
1:C:2248:TRP:CE2	1:C:2360:LEU:HD13	2.55	0.41
1:D:2232:ILE:HD13	1:D:2232:ILE:HA	1.80	0.41
1:D:2296:VAL:HA	1:D:2297:PRO:HD3	1.94	0.41
1:C:2277:ASN:HA	1:C:2278:PRO:HD2	1.87	0.41
1:D:2203:ARG:NH1	1:D:2483:ILE:HG23	2.33	0.41
1:D:2429:GLY:HA2	1:D:2482:LEU:CD2	2.51	0.41
1:A:2322:THR:HG21	1:A:2377:TYR:HE1	1.82	0.41
1:A:2343:ILE:HD13	1:A:2403:PHE:CE1	2.56	0.41
1:B:2464:ARG:NH1	1:B:2468:GLU:OE2	2.54	0.41
1:C:2316:LEU:HD21	1:C:2333:PHE:CE1	2.56	0.41
1:D:2248:TRP:CE2	1:D:2360:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2080:LEU:HD11	1:A:2175:LYS:HG2	2.03	0.41
1:B:2305:TYR:HA	1:B:2358:LYS:HA	2.03	0.41
1:B:2307:THR:CG2	1:B:2309:SER:N	2.84	0.41
1:C:2135:PHE:HB2	2:C:202:HOH:O	2.21	0.41
1:C:2159:ASN:O	1:C:2160:ARG:HB2	2.21	0.41
1:D:2080:LEU:HD23	1:D:2080:LEU:C	2.45	0.41
1:D:2118:ILE:HG22	1:D:2123:LEU:HG	2.03	0.41
1:D:2214:ARG:NH2	1:D:2220:ILE:HD11	2.35	0.41
1:D:2146:TYR:CE2	1:D:2147:LEU:HG	2.56	0.41
1:D:2187:THR:HG22	1:D:2193:GLN:CD	2.46	0.41
1:A:2109:ASP:OD1	1:A:2112:ASP:N	2.54	0.40
1:A:2358:LYS:HG2	1:A:2359:GLU:O	2.21	0.40
1:C:2326:LEU:HD12	1:C:2331:GLY:O	2.20	0.40
1:D:2109:ASP:OD1	1:D:2112:ASP:N	2.54	0.40
1:D:2364:PHE:N	1:D:2370:MET:HE1	2.36	0.40
1:A:2145:ARG:HA	1:A:2149:GLN:O	2.21	0.40
1:B:2135:PHE:CD2	1:B:2181:PRO:HG3	2.57	0.40
1:C:2078:VAL:O	1:C:2078:VAL:HG23	2.21	0.40
1:C:2448:THR:HG23	1:C:2477:THR:OG1	2.21	0.40
1:D:2113:PRO:HA	1:D:2116:LYS:CD	2.50	0.40
1:D:2454:ASN:HD22	1:D:2454:ASN:C	2.29	0.40
1:A:2225:TYR:O	1:A:2228:PHE:HB3	2.20	0.40
1:B:2155:ILE:O	1:B:2162:ALA:HA	2.22	0.40
1:C:2235:ARG:NH2	1:C:2476:GLN:O	2.54	0.40
1:C:2297:PRO:HD2	1:C:2446:TYR:CD2	2.56	0.40
1:D:2143:SER:O	1:D:2144:ARG:HG2	2.21	0.40
1:D:2145:ARG:HA	1:D:2149:GLN:O	2.21	0.40
1:A:2145:ARG:HH12	1:A:2202:PRO:HG2	1.87	0.40
1:B:2131:GLY:HA3	1:B:2133:TRP:CH2	2.57	0.40
1:C:2142:PHE:CZ	1:C:2185:VAL:HG22	2.55	0.40
1:C:2148:LEU:H	1:C:2476:GLN:NE2	2.19	0.40
1:C:2322:THR:HG21	1:C:2377:TYR:CD1	2.57	0.40
1:A:2365:TYR:CD2	1:A:2411:LEU:HD22	2.56	0.40
1:B:2316:LEU:HD23	1:B:2316:LEU:C	2.46	0.40
1:C:2104:LEU:CD2	1:C:2133:TRP:HB2	2.51	0.40
1:C:2194:THR:CG2	1:C:2195:ARG:N	2.84	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%)	392 (95%)	18 (4%)	2 (0%)	24	37
1	B	412/414 (100%)	389 (94%)	19 (5%)	4 (1%)	12	20
1	C	412/414 (100%)	390 (95%)	19 (5%)	3 (1%)	18	28
1	D	412/414 (100%)	386 (94%)	22 (5%)	4 (1%)	12	20
All	All	1648/1656 (100%)	1557 (94%)	78 (5%)	13 (1%)	16	25

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2366	TYR
1	B	2457	SER
1	C	2333	PHE
1	B	2366	TYR
1	C	2366	TYR
1	D	2090	SER
1	B	2378	ASN
1	D	2336	ALA
1	B	2136	THR
1	D	2389	SER
1	A	2333	PHE
1	C	2389	SER
1	D	2366	TYR

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	371/371 (100%)	349 (94%)	22 (6%)	18	31
1	B	371/371 (100%)	347 (94%)	24 (6%)	15	27
1	C	371/371 (100%)	345 (93%)	26 (7%)	14	24
1	D	371/371 (100%)	348 (94%)	23 (6%)	16	29
All	All	1484/1484 (100%)	1389 (94%)	95 (6%)	16	28

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2108	VAL
1	A	2111	GLU
1	A	2134	LEU
1	A	2145	ARG
1	A	2185	VAL
1	A	2197	ILE
1	A	2210	ASN
1	A	2264	THR
1	A	2294	ASP
1	A	2303	THR
1	A	2307	THR
1	A	2317	ARG
1	A	2326	LEU
1	A	2337	ASP
1	A	2339	THR
1	A	2345	ARG
1	A	2354	THR
1	A	2358	LYS
1	A	2360	LEU
1	A	2361	ILE
1	A	2441	LEU
1	A	2448	THR
1	B	2090	SER
1	B	2137	GLU
1	B	2180	LEU
1	B	2185	VAL
1	B	2197	ILE
1	B	2210	ASN
1	B	2262	LEU
1	B	2264	THR
1	B	2295	GLN
1	B	2303	THR
1	B	2307	THR

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Mol	Chain	Res	Type
1	B	2345	ARG
1	B	2352	ARG
1	B	2354	THR
1	B	2358	LYS
1	B	2360	LEU
1	B	2361	ILE
1	B	2436	GLU
1	B	2439	ARG
1	B	2441	LEU
1	B	2447	LEU
1	B	2448	THR
1	B	2456	ASN
1	B	2472	ARG
1	C	2090	SER
1	C	2094	LYS
1	C	2132	LYS
1	C	2145	ARG
1	C	2180	LEU
1	C	2185	VAL
1	C	2197	ILE
1	C	2207	LYS
1	C	2210	ASN
1	C	2264	THR
1	C	2279	LYS
1	C	2286	GLU
1	C	2293	ASP
1	C	2295	GLN
1	C	2303	THR
1	C	2317	ARG
1	C	2326	LEU
1	C	2335	HIS
1	C	2345	ARG
1	C	2354	THR
1	C	2358	LYS
1	C	2360	LEU
1	C	2361	ILE
1	C	2438	VAL
1	C	2441	LEU
1	C	2448	THR
1	D	2090	SER
1	D	2094	LYS
1	D	2101	SER

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Mol	Chain	Res	Type
1	D	2103	GLU
1	D	2104	LEU
1	D	2122	ILE
1	D	2185	VAL
1	D	2210	ASN
1	D	2213	GLN
1	D	2247	PRO
1	D	2262	LEU
1	D	2264	THR
1	D	2295	GLN
1	D	2307	THR
1	D	2326	LEU
1	D	2345	ARG
1	D	2358	LYS
1	D	2360	LEU
1	D	2361	ILE
1	D	2436	GLU
1	D	2447	LEU
1	D	2448	THR
1	D	2456	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2085	GLN
1	A	2149	GLN
1	A	2166	ASN
1	A	2210	ASN
1	A	2217	HIS
1	A	2295	GLN
1	A	2351	GLN
1	A	2405	HIS
1	A	2422	GLN
1	A	2454	ASN
1	B	2085	GLN
1	B	2210	ASN
1	B	2295	GLN
1	B	2327	ASN
1	B	2405	HIS
1	B	2419	GLN
1	B	2422	GLN
1	B	2454	ASN

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Mol	Chain	Res	Type
1	B	2470	GLN
1	B	2476	GLN
1	C	2085	GLN
1	C	2149	GLN
1	C	2166	ASN
1	C	2210	ASN
1	C	2295	GLN
1	C	2351	GLN
1	C	2405	HIS
1	C	2432	GLN
1	C	2433	GLN
1	C	2454	ASN
1	C	2476	GLN
1	D	2085	GLN
1	D	2114	ASN
1	D	2210	ASN
1	D	2295	GLN
1	D	2405	HIS
1	D	2432	GLN
1	D	2433	GLN
1	D	2454	ASN
1	D	2470	GLN
1	D	2476	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.