



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:09 PM UTC

PDB ID : 1C9I / pdb_00001c9i
Title : PEPTIDE-IN-GROOVE INTERACTIONS LINK TARGET PROTEINS TO
THE B-PROPELLER OF CLATHRIN
Authors : ter Haar, E.; Harrison, S.C.; Kirchhausen, T.
Deposited on : 1999-08-02
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
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

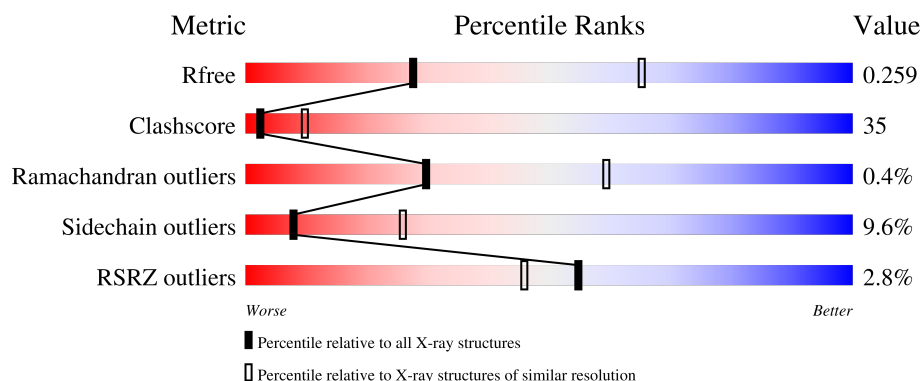
1 Overall quality at a glance

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	359	 3% 51% 40% 8% .
1	B	359	 2% 46% 44% 8% ..
2	C	9	 33% 44% 11% 33% 11%
2	D	9	 22% 11% 44% 22% 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5671 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 CLATHRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2779	1768	478	515	18			
1	B	355	Total	C	N	O	S	0	0	0
			2775	1766	477	514	18			

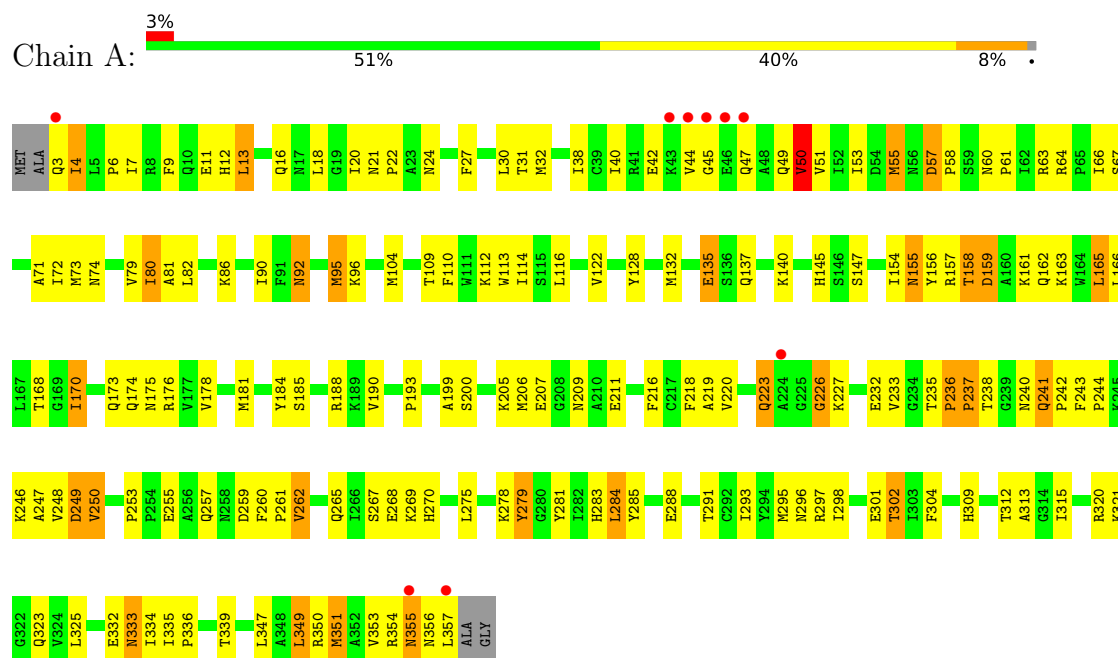
- Molecule 2 is a protein called B-ADAPTIN 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			64	40	9	15			
2	D	7	Total	C	N	O	0	0	0
			53	34	7	12			

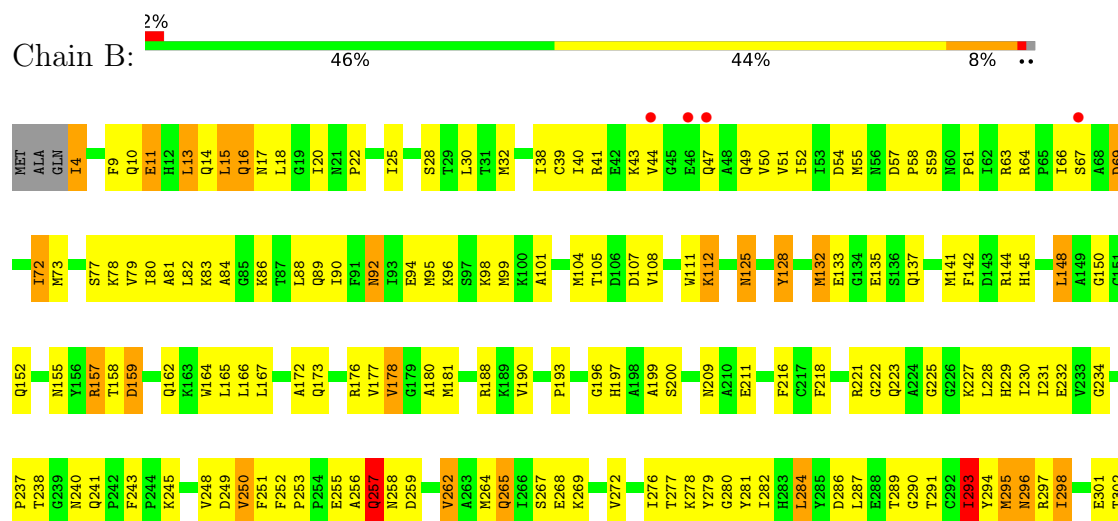
3 Residue-property plots

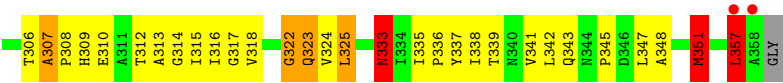
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CLATHRIN



• Molecule 1: CLATHRIN

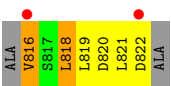




● Molecule 2: B-ADAPTIN 3



● Molecule 2: B-ADAPTIN 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.04Å 131.28Å 79.01Å 90.00° 116.31° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-2.90) 97.2 (30.00-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.72Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.227 , 0.269 0.220 , 0.259	Depositor DCC
R_{free} test set	1515 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5671	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.25% 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	0.86	4/2837 (0.1%)	1.29	24/3847 (0.6%)
1	B	0.88	4/2833 (0.1%)	1.24	25/3842 (0.7%)
2	C	1.65	2/63 (3.2%)	1.71	2/84 (2.4%)
2	D	1.27	0/52	2.47	6/70 (8.6%)
All	All	0.89	10/5785 (0.2%)	1.29	57/7843 (0.7%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	ILE	C-N	11.27	1.47	1.33
1	B	294	TYR	N-CA	9.46	1.58	1.46
2	C	823	ALA	C-OXT	9.16	1.41	1.23
1	A	4	ILE	N-CA	-6.86	1.38	1.46
1	B	298	ILE	N-CA	6.54	1.54	1.46
1	A	95	MET	SD-CE	-6.32	1.63	1.79
1	A	3	GLN	C-N	-6.20	1.23	1.33
2	C	819	LEU	CB-CG	-6.09	1.41	1.53
1	A	74	ASN	N-CA	5.15	1.52	1.45
1	B	351	MET	SD-CE	5.01	1.92	1.79

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	GLN	CA-C-N	-15.12	97.28	122.67
1	A	3	GLN	C-N-CA	-15.12	97.28	122.67
1	B	137	GLN	OE1-CD-NE2	-11.17	111.43	122.60
1	A	241	GLN	OE1-CD-NE2	-10.40	112.20	122.60
1	B	323	GLN	OE1-CD-NE2	-10.07	112.53	122.60
1	A	3	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	B	280	GLY	N-CA-C	8.56	128.08	114.90
1	A	279	TYR	N-CA-C	8.53	122.44	112.72
2	D	816	VAL	CB-CA-C	-8.14	95.92	111.40
2	C	822	ASP	CA-CB-CG	-7.92	104.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	816	VAL	CA-C-N	-7.87	112.15	123.00
2	D	816	VAL	C-N-CA	-7.87	112.15	123.00
1	A	45	GLY	N-CA-C	-7.57	98.44	112.37
1	B	307	ALA	CA-C-N	-7.46	112.30	119.76
1	B	307	ALA	C-N-CA	-7.46	112.30	119.76
1	A	241	GLN	CG-CD-NE2	7.08	127.02	116.40
1	A	236	PRO	O-C-N	6.75	124.42	121.31
1	B	137	GLN	CG-CD-NE2	6.57	126.26	116.40
1	B	323	GLN	CG-CD-NE2	6.53	126.19	116.40
1	B	28	SER	N-CA-C	6.41	120.71	113.02
1	A	3	GLN	CG-CD-NE2	6.37	125.96	116.40
1	A	262	VAL	CB-CA-C	-6.31	104.46	110.70
1	A	57	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	67	SER	N-CA-C	-6.16	102.91	110.61
1	B	150	GLY	N-CA-C	-6.12	106.08	114.64
1	B	294	TYR	N-CA-C	6.09	117.77	108.52
1	B	322	GLY	N-CA-C	-6.07	106.65	114.85
1	B	69	ASP	N-CA-C	-6.05	105.48	112.92
1	A	355	ASN	CA-C-N	6.02	130.94	122.46
1	A	355	ASN	C-N-CA	6.02	130.94	122.46
1	B	241	GLN	N-CA-C	-5.96	101.45	110.39
1	B	132	MET	N-CA-C	-5.94	106.07	113.38
1	B	80	ILE	N-CA-C	5.87	117.21	108.46
1	A	80	ILE	N-CA-C	5.87	116.93	108.48
1	A	50	VAL	CB-CA-C	-5.86	102.46	111.31
1	A	298	ILE	CB-CA-C	-5.83	103.97	111.20
1	A	241	GLN	O-C-N	5.80	126.00	121.88
1	B	159	ASP	N-CA-C	-5.75	102.41	110.35
1	A	159	ASP	N-CA-C	-5.72	102.46	110.35
1	B	125	ASN	N-CA-C	5.70	119.43	111.56
2	C	822	ASP	N-CA-CB	5.63	120.01	110.49
1	A	226	GLY	N-CA-C	5.58	118.85	111.03
1	A	155	ASN	N-CA-C	5.56	116.97	108.52
1	B	67	SER	N-CA-C	-5.44	104.33	112.54
1	A	27	PHE	N-CA-C	5.42	117.89	111.33
1	A	237	PRO	CB-CA-C	5.38	118.40	111.56
1	B	333	ASN	N-CA-C	5.37	120.65	112.54
1	B	13	LEU	N-CA-C	5.33	116.38	108.60
1	B	257	GLN	N-CA-C	-5.23	107.44	113.88
2	D	820	ASP	CA-C-N	-5.23	113.83	121.99
2	D	820	ASP	C-N-CA	-5.23	113.83	121.99
1	B	302	THR	N-CA-C	5.22	117.44	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	GLN	N-CA-C	-5.11	100.41	108.73
1	A	13	LEU	N-CA-C	5.07	116.23	108.42
1	B	357	LEU	CB-CA-C	-5.07	100.34	110.42
2	D	820	ASP	N-CA-C	-5.06	101.51	109.25
1	B	314	GLY	N-CA-C	-5.05	106.73	112.79

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	2779	0	2791	176	0
1	B	2775	0	2788	216	0
2	C	64	0	64	13	0
2	D	53	0	54	17	0
All	All	5671	0	5697	400	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 35.

All (400) 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:148:LEU:HD11	1:B:180:ALA:O	1.29	1.33
2:D:816:VAL:O	2:D:816:VAL:CG2	1.69	1.28
1:B:227:LYS:NZ	1:B:249:ASP:OD1	1.71	1.21
1:B:325:LEU:HD13	1:B:325:LEU:N	1.52	1.19
1:B:64:ARG:HD3	2:D:821:LEU:CD1	1.73	1.16
1:A:270:HIS:HA	1:A:355:ASN:ND2	1.62	1.15
1:B:64:ARG:HD3	2:D:821:LEU:HD12	1.21	1.14
1:B:50:VAL:HG23	1:B:66:ILE:HG12	1.29	1.12
1:B:325:LEU:HD13	1:B:325:LEU:H	0.94	1.10
1:B:325:LEU:N	1:B:325:LEU:CD1	2.10	1.10
1:A:270:HIS:CA	1:A:355:ASN:ND2	2.19	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HG12	1:A:132:MET:HE1	1.41	1.02
1:A:73:MET:CE	1:A:79:VAL:O	2.08	1.02
1:A:270:HIS:C	1:A:355:ASN:ND2	2.18	1.01
1:B:296:ASN:HD22	1:B:297:ARG:N	1.59	0.99
1:A:73:MET:HE2	1:A:79:VAL:O	1.63	0.99
1:B:158:THR:HG22	1:B:159:ASP:O	1.64	0.98
2:C:822:ASP:O	2:C:823:ALA:CB	2.13	0.94
1:B:30:LEU:HD23	1:B:40:ILE:HG13	1.45	0.94
1:B:90:ILE:HG21	1:B:132:MET:HE2	1.50	0.91
1:A:96:LYS:HA	2:C:821:LEU:HD13	1.52	0.91
1:B:92:ASN:HD22	1:B:95:MET:H	1.16	0.90
1:B:64:ARG:CD	2:D:821:LEU:CD1	2.50	0.90
1:A:73:MET:HA	1:A:73:MET:HE3	1.52	0.90
1:A:73:MET:CE	1:A:79:VAL:C	2.47	0.88
1:A:270:HIS:CA	1:A:355:ASN:HD21	1.81	0.88
1:B:16:GLN:NE2	1:B:22:PRO:HG3	1.91	0.86
2:C:822:ASP:O	2:C:823:ALA:HB2	1.75	0.86
1:B:16:GLN:HE22	1:B:22:PRO:HG3	1.40	0.86
1:A:20:ILE:HG12	1:A:40:ILE:HD13	1.56	0.85
1:B:323:GLN:OE1	1:B:325:LEU:HG	1.76	0.85
1:B:144:ARG:NH2	1:B:148:LEU:O	2.09	0.85
1:B:157:ARG:NH1	1:B:200:SER:HB2	1.91	0.85
1:A:7:ILE:HG21	1:A:284:LEU:HD21	1.60	0.84
1:B:73:MET:HE1	1:B:78:LYS:HA	1.58	0.84
1:B:176:ARG:HH12	1:B:222:GLY:HA2	1.42	0.83
1:B:92:ASN:ND2	1:B:95:MET:H	1.76	0.83
1:B:11:GLU:OE1	1:B:323:GLN:HG3	1.79	0.82
1:B:30:LEU:HD21	1:B:38:ILE:CG2	2.08	0.82
1:B:90:ILE:HG13	1:B:132:MET:HE1	1.61	0.82
1:A:90:ILE:HG12	1:A:132:MET:CE	2.10	0.82
1:B:296:ASN:HD22	1:B:297:ARG:H	1.28	0.82
1:A:158:THR:HG21	1:A:162:GLN:HG2	1.62	0.81
1:A:155:ASN:HD21	1:A:157:ARG:HG3	1.45	0.81
1:A:255:GLU:CD	1:A:255:GLU:H	1.88	0.81
1:A:154:ILE:HD13	1:A:170:ILE:HG12	1.61	0.80
1:A:253:PRO:HB2	1:A:255:GLU:OE1	1.82	0.80
1:B:96:LYS:NZ	2:D:822:ASP:OD2	2.15	0.80
1:B:265:GLN:HE21	1:B:308:PRO:N	1.80	0.79
1:A:51:VAL:HG22	1:A:63:ARG:HG2	1.64	0.79
1:A:270:HIS:C	1:A:355:ASN:HD22	1.89	0.78
1:A:73:MET:HE1	1:A:79:VAL:C	2.07	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:CG1	1:A:132:MET:HE1	2.14	0.78
1:B:148:LEU:CD1	1:B:180:ALA:O	2.23	0.78
1:B:284:LEU:HB3	1:B:293:ILE:HG13	1.65	0.78
1:B:166:LEU:HD22	1:B:216:PHE:HE1	1.49	0.77
1:B:323:GLN:HG2	1:B:325:LEU:HD12	1.66	0.77
1:B:72:ILE:HG13	1:B:81:ALA:HB3	1.67	0.77
1:B:284:LEU:HD12	1:B:293:ILE:HD11	1.66	0.77
1:A:161:LYS:HE2	1:A:163:LYS:HZ2	1.49	0.76
1:A:281:TYR:CE2	1:A:297:ARG:HD2	2.20	0.76
1:A:335:ILE:HB	1:A:336:PRO:HD3	1.68	0.76
1:A:270:HIS:C	1:A:355:ASN:HD21	1.90	0.75
1:A:166:LEU:HD22	1:A:216:PHE:HE1	1.52	0.75
1:B:79:VAL:HG13	1:B:99:MET:HE1	1.68	0.74
1:A:6:PRO:HB2	1:A:334:ILE:HD12	1.68	0.74
1:B:181:MET:HE2	1:B:196:GLY:HA3	1.70	0.74
1:B:79:VAL:HG13	1:B:99:MET:CE	2.19	0.73
1:A:20:ILE:HG12	1:A:40:ILE:CD1	2.19	0.72
1:B:335:ILE:HB	1:B:336:PRO:HD3	1.70	0.72
1:A:309:HIS:HD2	1:A:312:THR:HG23	1.54	0.72
1:B:296:ASN:ND2	1:B:297:ARG:H	1.88	0.72
1:B:148:LEU:HD11	1:B:180:ALA:C	2.12	0.71
1:B:296:ASN:ND2	1:B:297:ARG:N	2.37	0.71
1:A:90:ILE:HG21	1:A:132:MET:CE	2.21	0.71
2:D:816:VAL:O	2:D:816:VAL:HG23	0.94	0.70
1:A:158:THR:HG22	1:A:159:ASP:O	1.92	0.70
1:B:16:GLN:HE22	1:B:22:PRO:CG	2.05	0.70
1:B:166:LEU:HD22	1:B:216:PHE:CE1	2.26	0.70
1:B:158:THR:HG23	1:B:162:GLN:HA	1.75	0.69
1:A:166:LEU:HD22	1:A:216:PHE:CE1	2.27	0.68
1:B:79:VAL:CG1	1:B:99:MET:HE1	2.21	0.68
1:B:282:ILE:HG22	1:B:296:ASN:O	1.93	0.68
1:A:57:ASP:N	1:A:58:PRO:CD	2.56	0.68
1:B:312:THR:O	1:B:313:ALA:HB3	1.94	0.67
1:A:7:ILE:HD12	1:A:7:ILE:O	1.94	0.67
1:B:66:ILE:HD12	1:B:66:ILE:C	2.19	0.67
1:B:57:ASP:N	1:B:58:PRO:CD	2.58	0.67
2:C:819:LEU:CD2	2:C:821:LEU:HD21	2.25	0.67
1:A:158:THR:HG21	1:A:162:GLN:CG	2.25	0.66
2:D:822:ASP:OD1	2:D:822:ASP:O	2.14	0.66
1:A:281:TYR:HE2	1:A:297:ARG:HD2	1.59	0.66
1:B:176:ARG:HH12	1:B:222:GLY:CA	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:VAL:HG22	1:B:63:ARG:HG2	1.79	0.65
1:A:57:ASP:N	1:A:58:PRO:HD3	2.11	0.65
1:B:98:LYS:HE2	1:B:101:ALA:HB2	1.77	0.65
1:B:59:SER:C	1:B:61:PRO:HD3	2.22	0.65
1:A:323:GLN:OE1	1:A:325:LEU:HD23	1.96	0.65
1:A:246:LYS:HE2	1:A:288:GLU:O	1.97	0.65
1:B:272:VAL:CG1	1:B:284:LEU:HD22	2.27	0.65
1:A:227:LYS:HA	1:A:249:ASP:HA	1.79	0.65
1:A:92:ASN:CG	1:A:95:MET:HG2	2.22	0.64
1:B:148:LEU:HD12	1:B:180:ALA:CB	2.27	0.64
1:A:13:LEU:HD12	1:A:55:MET:HE1	1.78	0.64
1:A:161:LYS:HE2	1:A:163:LYS:NZ	2.13	0.64
1:A:7:ILE:HG21	1:A:284:LEU:CD2	2.28	0.63
1:A:96:LYS:CA	2:C:821:LEU:HD13	2.27	0.63
1:B:323:GLN:OE1	1:B:325:LEU:CG	2.46	0.63
1:B:293:ILE:C	1:B:293:ILE:HD12	2.22	0.63
1:B:272:VAL:HG12	1:B:284:LEU:HD22	1.80	0.63
1:A:63:ARG:O	1:A:64:ARG:HD3	1.99	0.63
1:A:90:ILE:HG21	1:A:132:MET:HE3	1.79	0.63
1:A:155:ASN:HD21	1:A:157:ARG:CG	2.10	0.62
1:A:255:GLU:CD	1:A:255:GLU:N	2.57	0.62
1:B:4:ILE:HD12	1:B:333:ASN:HB2	1.80	0.62
1:A:174:GLN:NE2	1:A:223:GLN:HE22	1.97	0.62
1:B:64:ARG:CD	2:D:821:LEU:HD11	2.28	0.62
1:A:355:ASN:HB3	1:A:357:LEU:HD11	1.82	0.62
1:B:128:TYR:N	1:B:128:TYR:CD1	2.67	0.62
1:A:267:SER:HB2	1:A:313:ALA:O	1.99	0.62
1:B:145:HIS:CD2	1:B:193:PRO:HG3	2.34	0.62
1:A:18:LEU:HD22	1:A:61:PRO:CG	2.30	0.62
1:B:50:VAL:HG23	1:B:66:ILE:CG1	2.18	0.62
1:A:207:GLU:OE1	1:B:256:ALA:HA	2.00	0.62
1:B:265:GLN:HB2	1:B:315:ILE:HD12	1.80	0.61
1:B:278:LYS:HG2	1:B:279:TYR:CE1	2.34	0.61
1:B:148:LEU:HD12	1:B:180:ALA:HB3	1.81	0.61
1:B:282:ILE:HG21	1:B:298:ILE:CG2	2.30	0.61
1:A:157:ARG:NH1	1:A:200:SER:HB2	2.16	0.61
1:A:232:GLU:HB2	1:A:243:PHE:HB3	1.83	0.61
1:B:90:ILE:HG22	1:B:99:MET:HE3	1.83	0.61
1:A:18:LEU:HD13	1:A:53:ILE:HD13	1.83	0.61
1:B:325:LEU:N	1:B:325:LEU:HD12	2.10	0.60
2:C:822:ASP:O	2:C:823:ALA:HB3	1.97	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLN:NE2	1:A:22:PRO:HG3	2.16	0.60
1:A:188:ARG:O	1:A:190:VAL:HG23	2.01	0.60
2:C:822:ASP:OD1	2:C:822:ASP:C	2.42	0.60
1:A:296:ASN:CG	1:A:297:ARG:H	2.08	0.60
1:B:256:ALA:HB1	1:B:259:ASP:HB3	1.83	0.60
1:B:14:GLN:O	1:B:16:GLN:N	2.35	0.59
1:A:81:ALA:O	1:A:82:LEU:HD23	2.02	0.59
1:A:18:LEU:HD22	1:A:61:PRO:HG2	1.84	0.59
1:A:284:LEU:HB3	1:A:293:ILE:HB	1.85	0.59
1:B:209:ASN:HB3	1:B:240:ASN:ND2	2.18	0.58
1:B:338:ILE:HA	1:B:342:LEU:HD12	1.85	0.58
1:A:50:VAL:HG22	1:A:66:ILE:CG2	2.34	0.58
1:B:4:ILE:HD12	1:B:333:ASN:CB	2.33	0.58
1:A:309:HIS:CD2	1:A:312:THR:HG23	2.37	0.58
1:A:145:HIS:NE2	1:A:193:PRO:HG3	2.18	0.58
1:B:255:GLU:O	1:B:257:GLN:HG3	2.03	0.58
1:B:50:VAL:CG2	1:B:66:ILE:HG12	2.20	0.57
1:B:264:MET:O	1:B:265:GLN:OE1	2.23	0.57
1:B:351:MET:O	1:B:357:LEU:HD12	2.05	0.57
1:A:312:THR:O	1:A:313:ALA:HB3	2.04	0.57
1:A:237:PRO:O	1:A:240:ASN:HB2	2.04	0.56
1:B:32:MET:HE1	1:B:317:GLY:HA2	1.88	0.56
1:B:199:ALA:HB2	1:B:218:PHE:CB	2.34	0.56
1:B:148:LEU:CD1	1:B:180:ALA:CB	2.82	0.56
1:A:114:ILE:HD12	1:A:162:GLN:HE21	1.70	0.56
1:B:89:GLN:HE22	2:D:816:VAL:HG23	1.69	0.56
1:A:51:VAL:CG2	1:A:63:ARG:NH1	2.69	0.56
1:A:155:ASN:ND2	1:A:157:ARG:HG3	2.17	0.56
1:B:83:LYS:NZ	1:B:108:VAL:O	2.27	0.56
1:B:96:LYS:HA	2:D:821:LEU:HD23	1.88	0.56
1:A:353:VAL:O	1:A:356:ASN:ND2	2.38	0.56
1:A:92:ASN:ND2	1:A:95:MET:H	2.03	0.55
1:B:323:GLN:OE1	1:B:325:LEU:CD1	2.54	0.55
1:A:173:GLN:HB2	1:A:178:VAL:HG21	1.87	0.55
1:B:323:GLN:CG	1:B:325:LEU:HD12	2.36	0.55
1:B:90:ILE:HG21	1:B:132:MET:CE	2.31	0.55
1:A:353:VAL:HG21	1:B:177:VAL:HG23	1.88	0.55
1:A:92:ASN:OD1	1:A:95:MET:HE3	2.06	0.55
1:B:44:VAL:HB	1:B:49:GLN:NE2	2.21	0.55
1:B:338:ILE:HG22	1:B:348:ALA:HB2	1.87	0.55
1:B:50:VAL:HG12	1:B:52:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:HG21	1:A:72:ILE:HG22	1.88	0.54
1:A:92:ASN:ND2	1:A:95:MET:HG2	2.22	0.54
1:B:52:ILE:HD12	1:B:52:ILE:N	2.21	0.54
1:B:221:ARG:HH21	1:B:252:PHE:CB	2.19	0.54
1:B:333:ASN:HA	1:B:336:PRO:HD2	1.89	0.54
2:C:819:LEU:HD21	2:C:821:LEU:CD2	2.37	0.54
1:B:173:GLN:HB2	1:B:178:VAL:HG21	1.89	0.54
2:C:819:LEU:HD23	2:C:821:LEU:HD21	1.88	0.54
1:A:96:LYS:HA	2:C:821:LEU:CD1	2.32	0.54
1:B:164:TRP:HZ2	1:B:234:GLY:CA	2.21	0.54
1:A:168:THR:OG1	1:A:181:MET:HG2	2.08	0.54
1:B:158:THR:HG21	1:B:162:GLN:HG3	1.90	0.54
1:B:92:ASN:ND2	1:B:95:MET:N	2.52	0.53
1:A:278:LYS:O	1:A:302:THR:HG22	2.09	0.53
1:A:291:THR:HG21	1:A:347:LEU:HD22	1.90	0.53
1:A:158:THR:HG23	1:A:162:GLN:HA	1.91	0.53
1:A:355:ASN:HB3	1:A:357:LEU:CD1	2.38	0.53
1:B:25:ILE:HG22	1:B:25:ILE:O	2.08	0.53
1:B:251:PHE:CE2	1:B:253:PRO:HD3	2.43	0.53
1:A:86:LYS:HB3	1:A:104:MET:O	2.09	0.53
1:A:335:ILE:HB	1:A:336:PRO:CD	2.38	0.53
1:B:39:CYS:SG	1:B:73:MET:HG2	2.49	0.53
1:B:291:THR:HG21	1:B:347:LEU:HD22	1.89	0.53
1:B:16:GLN:CD	1:B:22:PRO:HG3	2.33	0.53
1:B:57:ASP:H	1:B:58:PRO:HD3	1.74	0.53
1:A:283:HIS:HB3	1:A:285:TYR:CE1	2.43	0.53
1:A:158:THR:CG2	1:A:159:ASP:O	2.56	0.52
1:A:199:ALA:HB2	1:A:218:PHE:CB	2.38	0.52
1:B:148:LEU:CD1	1:B:180:ALA:HB1	2.38	0.52
1:B:164:TRP:O	1:B:165:LEU:HD23	2.09	0.52
1:A:205:LYS:NZ	1:B:257:GLN:NE2	2.57	0.52
1:B:282:ILE:CG2	1:B:298:ILE:CG2	2.87	0.52
1:A:128:TYR:CD2	1:A:140:LYS:HA	2.45	0.52
1:B:265:GLN:HE21	1:B:308:PRO:CD	2.22	0.52
1:B:89:GLN:NE2	2:D:816:VAL:HG23	2.25	0.52
1:B:333:ASN:C	1:B:336:PRO:HD2	2.34	0.52
1:B:157:ARG:HH12	1:B:200:SER:HB2	1.75	0.51
1:A:259:ASP:OD1	1:A:279:TYR:HD1	1.93	0.51
1:B:197:HIS:CD2	1:B:221:ARG:H	2.27	0.51
1:A:333:ASN:O	1:A:334:ILE:C	2.53	0.51
1:B:64:ARG:NE	2:D:821:LEU:HD11	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ILE:HD12	1:B:293:ILE:O	2.11	0.51
1:B:158:THR:HG21	1:B:162:GLN:CG	2.40	0.51
1:B:282:ILE:CG2	1:B:298:ILE:HG23	2.40	0.51
1:B:312:THR:O	1:B:313:ALA:CB	2.57	0.51
1:B:188:ARG:HB2	1:B:190:VAL:HG12	1.92	0.51
1:A:18:LEU:HD21	1:A:58:PRO:O	2.11	0.51
1:A:50:VAL:HG22	1:A:66:ILE:HG21	1.93	0.51
1:B:69:ASP:OD2	1:B:69:ASP:C	2.53	0.51
1:B:54:ASP:O	1:B:58:PRO:HD3	2.11	0.50
1:B:339:THR:O	1:B:343:GLN:HA	2.12	0.50
1:B:57:ASP:N	1:B:58:PRO:HD3	2.26	0.50
1:B:282:ILE:HG21	1:B:298:ILE:HG21	1.93	0.50
2:C:819:LEU:CD2	2:C:821:LEU:CD2	2.89	0.50
1:B:112:LYS:HB2	1:B:112:LYS:NZ	2.26	0.50
1:B:211:GLU:H	1:B:240:ASN:HD21	1.60	0.49
1:B:306:THR:HG22	1:B:317:GLY:HA3	1.94	0.49
1:A:4:ILE:O	1:A:4:ILE:HD12	2.11	0.49
1:A:92:ASN:C	1:A:92:ASN:HD22	2.19	0.49
1:B:250:VAL:CG2	1:B:250:VAL:O	2.60	0.49
1:B:89:GLN:HG2	1:B:98:LYS:HE3	1.94	0.49
1:A:206:MET:HB2	1:A:209:ASN:OD1	2.12	0.49
2:C:819:LEU:HD21	2:C:821:LEU:HD21	1.94	0.49
1:B:267:SER:HB2	1:B:313:ALA:O	2.13	0.49
1:A:30:LEU:C	1:A:30:LEU:HD23	2.38	0.49
1:B:82:LEU:CD1	2:D:819:LEU:HB2	2.43	0.49
1:A:50:VAL:HG13	1:A:66:ILE:HD13	1.93	0.49
1:A:57:ASP:H	1:A:58:PRO:HD3	1.78	0.48
1:A:206:MET:HE1	1:A:242:PRO:O	2.13	0.48
1:B:20:ILE:N	1:B:20:ILE:HD12	2.28	0.48
1:B:83:LYS:HB2	1:B:88:LEU:HD22	1.95	0.48
1:B:255:GLU:H	1:B:255:GLU:CD	2.21	0.48
1:B:30:LEU:CD2	1:B:38:ILE:CG2	2.89	0.48
1:B:49:GLN:OE1	1:B:63:ARG:HD3	2.13	0.48
1:B:92:ASN:HD22	1:B:92:ASN:C	2.22	0.48
1:A:11:GLU:HB2	1:A:323:GLN:HE21	1.78	0.48
1:B:282:ILE:HG22	1:B:298:ILE:HG23	1.96	0.48
1:B:164:TRP:C	1:B:165:LEU:HD23	2.39	0.47
1:B:128:TYR:N	1:B:128:TYR:HD1	2.09	0.47
1:B:145:HIS:NE2	1:B:193:PRO:HG3	2.29	0.47
1:B:221:ARG:HH21	1:B:252:PHE:HB3	1.79	0.47
1:A:50:VAL:HG22	1:A:66:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:CG	1:A:60:ASN:HD22	2.23	0.47
1:A:301:GLU:OE1	1:A:301:GLU:HA	2.14	0.47
1:B:90:ILE:CG2	1:B:99:MET:HE3	2.43	0.47
1:A:92:ASN:HD22	1:A:95:MET:H	1.62	0.47
1:B:197:HIS:HD2	1:B:221:ARG:H	1.61	0.47
2:D:821:LEU:O	2:D:822:ASP:HB2	2.15	0.47
1:A:32:MET:CE	1:A:38:ILE:HD11	2.44	0.47
1:A:12:HIS:N	1:A:12:HIS:CD2	2.81	0.47
1:A:269:LYS:O	1:A:355:ASN:OD1	2.33	0.47
1:B:66:ILE:C	1:B:66:ILE:CD1	2.87	0.47
1:A:32:MET:HE3	1:A:38:ILE:HG12	1.97	0.46
1:A:206:MET:O	1:A:209:ASN:HB2	2.15	0.46
1:B:86:LYS:HG3	1:B:107:ASP:OD1	2.15	0.46
1:B:164:TRP:CZ2	1:B:234:GLY:CA	2.98	0.46
1:A:247:ALA:C	1:A:248:VAL:HG13	2.41	0.46
1:B:72:ILE:HD11	1:B:111:TRP:CD2	2.50	0.46
1:B:262:VAL:HG12	1:B:276:ILE:O	2.16	0.46
1:B:250:VAL:CG2	1:B:252:PHE:HE1	2.29	0.46
1:A:18:LEU:CD1	1:A:53:ILE:HD13	2.44	0.46
1:B:343:GLN:C	1:B:345:PRO:HD3	2.41	0.46
1:B:92:ASN:ND2	1:B:92:ASN:C	2.74	0.46
1:B:255:GLU:CD	1:B:255:GLU:N	2.74	0.46
1:A:30:LEU:HD22	1:A:304:PHE:CE1	2.51	0.46
1:B:286:ASP:OD2	1:B:289:THR:HG23	2.16	0.46
1:B:248:VAL:HG11	1:B:290:GLY:O	2.15	0.45
1:B:230:ILE:HD13	1:B:287:LEU:O	2.16	0.45
1:B:84:ALA:CB	2:D:818:LEU:HD21	2.46	0.45
1:B:347:LEU:O	1:B:351:MET:HG3	2.17	0.45
1:A:174:GLN:O	1:A:175:ASN:HB2	2.16	0.45
1:B:158:THR:CG2	1:B:162:GLN:HA	2.45	0.45
1:A:71:ALA:HA	1:A:82:LEU:HD23	1.98	0.45
1:A:244:PRO:HB2	1:A:246:LYS:NZ	2.31	0.45
1:A:309:HIS:HD2	1:A:312:THR:CG2	2.27	0.45
1:B:232:GLU:HB2	1:B:243:PHE:HB3	1.99	0.45
1:B:338:ILE:HG12	1:B:342:LEU:HD12	1.98	0.45
1:A:205:LYS:HE3	1:A:209:ASN:O	2.17	0.45
1:A:220:VAL:O	1:A:220:VAL:HG13	2.17	0.45
1:A:296:ASN:CG	1:A:297:ARG:N	2.75	0.45
1:A:145:HIS:CE1	1:A:193:PRO:HG3	2.52	0.45
1:B:96:LYS:HG2	2:D:821:LEU:HD23	1.97	0.45
1:B:199:ALA:HB2	1:B:218:PHE:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:GLU:N	1:B:255:GLU:OE2	2.50	0.45
1:A:349:LEU:O	1:A:353:VAL:HG23	2.17	0.45
1:B:50:VAL:HG12	1:B:52:ILE:CD1	2.46	0.45
1:A:158:THR:CG2	1:A:162:GLN:HG2	2.41	0.45
2:D:818:LEU:HD12	2:D:818:LEU:HA	1.86	0.45
1:B:51:VAL:HG21	1:B:63:ARG:CZ	2.46	0.45
1:B:265:GLN:NE2	1:B:308:PRO:HD3	2.31	0.45
1:B:32:MET:CE	1:B:317:GLY:HA2	2.47	0.44
1:B:141:MET:O	1:B:142:PHE:HB3	2.16	0.44
1:A:11:GLU:HB2	1:A:323:GLN:NE2	2.31	0.44
1:A:32:MET:CE	1:A:38:ILE:HG12	2.47	0.44
1:A:73:MET:CE	1:A:73:MET:HA	2.35	0.44
1:A:73:MET:HE3	1:A:79:VAL:O	2.11	0.44
1:A:73:MET:HE1	1:A:80:ILE:N	2.33	0.44
1:A:233:VAL:O	1:A:233:VAL:HG23	2.17	0.44
1:B:148:LEU:HD23	1:B:167:LEU:HG	1.99	0.44
1:A:353:VAL:HG12	1:B:258:ASN:ND2	2.32	0.44
1:B:79:VAL:HG11	1:B:99:MET:HE1	1.99	0.44
1:B:277:THR:HG23	1:B:281:TYR:HB2	1.98	0.44
1:B:309:HIS:HB2	1:B:316:ILE:HB	1.99	0.44
1:B:148:LEU:HD12	1:B:180:ALA:HB1	1.97	0.44
1:A:332:GLU:C	1:A:333:ASN:OD1	2.61	0.44
1:B:237:PRO:O	1:B:238:THR:C	2.61	0.44
1:A:262:VAL:HG11	1:A:278:LYS:HA	1.99	0.43
1:B:221:ARG:NH1	1:B:257:GLN:O	2.47	0.43
1:B:14:GLN:O	1:B:17:ASN:N	2.51	0.43
1:A:116:LEU:HD22	1:A:116:LEU:N	2.33	0.43
1:B:218:PHE:CE1	1:B:229:HIS:HD2	2.36	0.43
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.88	0.43
1:A:244:PRO:O	1:A:246:LYS:HD3	2.18	0.43
1:A:333:ASN:OD1	1:A:333:ASN:N	2.51	0.43
1:B:259:ASP:OD1	1:B:279:TYR:HD1	2.02	0.43
1:A:13:LEU:HD21	1:A:58:PRO:HB3	2.00	0.43
1:A:24:ASN:ND2	1:A:42:GLU:HG2	2.34	0.43
1:B:14:GLN:C	1:B:16:GLN:N	2.77	0.43
1:B:318:VAL:HG22	1:B:324:VAL:HG22	2.00	0.43
1:A:145:HIS:CE1	1:A:147:SER:HG	2.30	0.43
1:A:165:LEU:HD12	1:A:184:TYR:HD2	1.84	0.43
1:B:173:GLN:HB2	1:B:178:VAL:CG2	2.48	0.43
1:B:276:ILE:HA	1:B:281:TYR:O	2.19	0.43
1:B:337:TYR:CE1	1:B:341:VAL:HG11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:CG2	1:A:21:ASN:N	2.82	0.42
1:A:226:GLY:O	1:A:249:ASP:HB3	2.18	0.42
1:A:237:PRO:O	1:A:238:THR:C	2.61	0.42
1:B:41:ARG:HG2	1:B:50:VAL:HG22	2.00	0.42
1:B:157:ARG:HE	1:B:157:ARG:HB3	1.62	0.42
1:B:223:GLN:C	1:B:225:GLY:H	2.26	0.42
1:B:278:LYS:CG	1:B:279:TYR:CE1	3.01	0.42
1:A:73:MET:HE1	1:A:80:ILE:HB	2.01	0.42
1:A:301:GLU:HG3	1:A:321:LYS:HB2	2.01	0.42
1:A:351:MET:HE3	1:A:351:MET:HB2	1.86	0.42
1:A:12:HIS:HE1	1:A:309:HIS:CE1	2.38	0.42
1:B:73:MET:HE3	1:B:73:MET:HB3	1.76	0.42
1:A:250:VAL:HG23	1:A:283:HIS:CE1	2.55	0.42
1:B:18:LEU:HB2	1:B:20:ILE:HD13	2.02	0.42
1:A:82:LEU:HD12	2:C:819:LEU:HB2	2.02	0.42
1:A:219:ALA:CB	1:A:275:LEU:HD11	2.49	0.42
1:A:20:ILE:HD12	1:A:20:ILE:N	2.35	0.42
1:A:278:LYS:HG2	1:A:302:THR:HG22	2.01	0.42
1:B:32:MET:HE1	1:B:317:GLY:CA	2.50	0.42
1:B:77:SER:O	1:B:79:VAL:N	2.45	0.42
1:A:109:THR:N	1:A:122:VAL:O	2.50	0.42
1:B:14:GLN:O	1:B:15:LEU:C	2.62	0.42
1:B:112:LYS:HB2	1:B:112:LYS:HZ2	1.85	0.42
1:A:9:PHE:CD2	1:A:9:PHE:C	2.97	0.42
1:A:166:LEU:HD11	1:A:181:MET:HE3	2.01	0.42
1:A:211:GLU:HB2	1:A:237:PRO:HB2	2.01	0.42
1:B:155:ASN:HD21	1:B:157:ARG:HG2	1.84	0.42
1:B:16:GLN:HE21	1:B:16:GLN:HA	1.84	0.42
1:B:90:ILE:HG22	1:B:99:MET:CE	2.49	0.42
1:B:256:ALA:HB1	1:B:259:ASP:CB	2.47	0.41
1:B:55:MET:C	1:B:58:PRO:HD3	2.44	0.41
1:A:73:MET:CE	1:A:80:ILE:HB	2.50	0.41
1:B:25:ILE:HD13	1:B:322:GLY:HA2	2.02	0.41
1:B:30:LEU:HD21	1:B:38:ILE:HG22	1.94	0.41
1:B:277:THR:CG2	1:B:281:TYR:HB2	2.51	0.41
1:A:265:GLN:HG2	1:A:315:ILE:HD12	2.01	0.41
1:A:110:PHE:CZ	1:A:155:ASN:HA	2.55	0.41
1:A:113:TRP:HH2	1:A:132:MET:HE2	1.86	0.41
1:A:235:THR:HA	1:A:236:PRO:HD3	1.90	0.41
1:B:231:ILE:HG22	1:B:245:LYS:HB2	2.03	0.41
1:A:156:TYR:OH	1:A:165:LEU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASN:HD21	1:A:241:GLN:HB2	1.85	0.41
1:B:13:LEU:HD21	1:B:58:PRO:CB	2.50	0.41
1:B:177:VAL:O	1:B:197:HIS:HE1	2.04	0.41
1:B:295:MET:O	1:B:295:MET:HG3	2.11	0.41
1:A:260:PHE:HB2	1:A:261:PRO:CD	2.51	0.41
1:A:350:ARG:O	1:A:354:ARG:HB3	2.20	0.41
1:A:49:GLN:HA	1:A:66:ILE:HG12	2.03	0.41
1:B:172:ALA:O	1:B:173:GLN:HG2	2.21	0.41
1:B:265:GLN:HE21	1:B:307:ALA:C	2.29	0.41
1:A:135:GLU:H	1:A:135:GLU:HG3	1.39	0.41
1:A:226:GLY:O	1:A:249:ASP:CB	2.69	0.41
1:B:9:PHE:CD1	1:B:10:GLN:N	2.88	0.41
1:A:353:VAL:CG1	1:B:258:ASN:HD22	2.34	0.40
1:B:94:GLU:H	1:B:94:GLU:HG3	1.76	0.40
1:A:71:ALA:C	1:A:72:ILE:HG23	2.47	0.40
1:A:244:PRO:HG2	1:B:301:GLU:OE1	2.21	0.40
1:A:185:SER:OG	1:A:188:ARG:HG2	2.22	0.40
1:A:185:SER:CB	1:A:188:ARG:HG2	2.51	0.40
1:B:351:MET:HE3	1:B:351:MET:HB3	1.89	0.40
1:B:145:HIS:NE2	1:B:193:PRO:CG	2.85	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	353/359 (98%)	321 (91%)	31 (9%)	1 (0%)	36	65
1	B	353/359 (98%)	316 (90%)	36 (10%)	1 (0%)	36	65
2	C	7/9 (78%)	5 (71%)	1 (14%)	1 (14%)	0	0
2	D	5/9 (56%)	5 (100%)	0	0	100	100
All	All	718/736 (98%)	647 (90%)	68 (10%)	3 (0%)	30	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	LEU
1	A	320	ARG
2	C	822	ASP

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	306/307 (100%)	282 (92%)	24 (8%)	11	35
1	B	305/307 (99%)	272 (89%)	33 (11%)	6	21
2	C	7/7 (100%)	5 (71%)	2 (29%)	0	1
2	D	7/7 (100%)	6 (86%)	1 (14%)	3	11
All	All	625/628 (100%)	565 (90%)	60 (10%)	8	26

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	47	GLN
1	A	50	VAL
1	A	55	MET
1	A	92	ASN
1	A	112	LYS
1	A	135	GLU
1	A	137	GLN
1	A	158	THR
1	A	165	LEU
1	A	170	ILE
1	A	176	ARG
1	A	223	GLN
1	A	249	ASP
1	A	250	VAL
1	A	257	GLN
1	A	268	GLU

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Mol	Chain	Res	Type
1	A	284	LEU
1	A	295	MET
1	A	302	THR
1	A	333	ASN
1	A	339	THR
1	A	349	LEU
1	A	351	MET
1	B	4	ILE
1	B	11	GLU
1	B	16	GLN
1	B	43	LYS
1	B	47	GLN
1	B	72	ILE
1	B	92	ASN
1	B	104	MET
1	B	105	THR
1	B	112	LYS
1	B	125	ASN
1	B	128	TYR
1	B	133	GLU
1	B	135	GLU
1	B	148	LEU
1	B	157	ARG
1	B	178	VAL
1	B	228	LEU
1	B	250	VAL
1	B	257	GLN
1	B	262	VAL
1	B	265	GLN
1	B	268	GLU
1	B	269	LYS
1	B	284	LEU
1	B	293	ILE
1	B	295	MET
1	B	296	ASN
1	B	310	GLU
1	B	325	LEU
1	B	333	ASN
1	B	351	MET
1	B	357	LEU
2	C	817	SER
2	C	821	LEU

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Mol	Chain	Res	Type
2	D	818	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	16	GLN
1	A	17	ASN
1	A	24	ASN
1	A	60	ASN
1	A	92	ASN
1	A	137	GLN
1	A	155	ASN
1	A	162	GLN
1	A	203	GLN
1	A	209	ASN
1	A	223	GLN
1	A	309	HIS
1	A	355	ASN
1	A	356	ASN
1	B	16	GLN
1	B	17	ASN
1	B	56	ASN
1	B	92	ASN
1	B	102	HIS
1	B	125	ASN
1	B	152	GLN
1	B	155	ASN
1	B	173	GLN
1	B	175	ASN
1	B	197	HIS
1	B	203	GLN
1	B	229	HIS
1	B	240	ASN
1	B	257	GLN
1	B	258	ASN
1	B	265	GLN
1	B	296	ASN
1	B	309	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	355/359 (98%)	-0.09	9 (2%) 58 48	3, 16, 38, 62	0
1	B	355/359 (98%)	-0.02	6 (1%) 69 61	5, 18, 38, 56	0
2	C	9/9 (100%)	2.24	3 (33%) 1 1	31, 46, 65, 72	0
2	D	7/9 (77%)	2.11	2 (28%) 1 1	47, 55, 67, 80	0
All	All	726/736 (98%)	-0.01	20 (2%) 55 46	3, 18, 41, 80	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	823	ALA	7.3
2	C	822	ASP	4.6
2	D	816	VAL	4.3
1	A	355	ASN	4.1
2	D	822	ASP	3.9
1	B	358	ALA	3.8
1	A	45	GLY	3.4
1	B	357	LEU	3.2
1	A	224	ALA	3.0
2	C	815	ALA	3.0
1	B	44	VAL	2.7
1	B	46	GLU	2.6
1	A	47	GLN	2.6
1	A	43	LYS	2.5
1	A	3	GLN	2.4
1	A	44	VAL	2.3
1	B	47	GLN	2.2
1	A	46	GLU	2.2
1	A	357	LEU	2.1
1	B	67	SER	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.