



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:17 AM UTC

PDB ID : 2RIN / pdb_00002rin
Title : ABC-transporter choline binding protein in complex with acetylcholine
Authors : Oswald, C.; Smits, S.H.J.; Hoeing, M.; Sohn-Boeser, L.; Le Rudulier, D.; Schmitt, L.; Bremer, E.
Deposited on : 2007-10-12
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

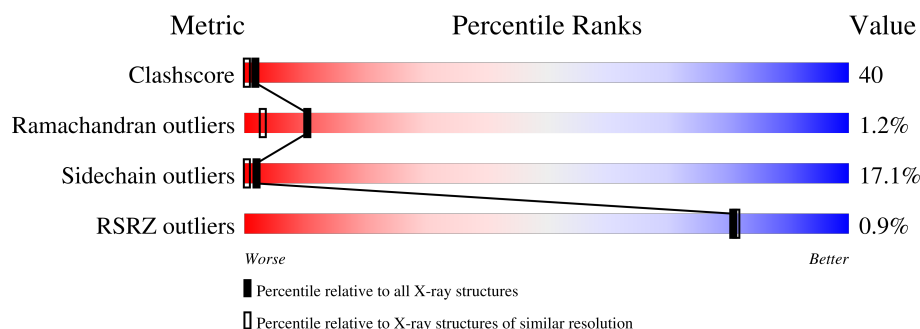
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	298	% 33% 49% 13% ..
1	B	298	35% 45% 15% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACH	A	1	-	-	X	-
2	ACH	B	1	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4616 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.

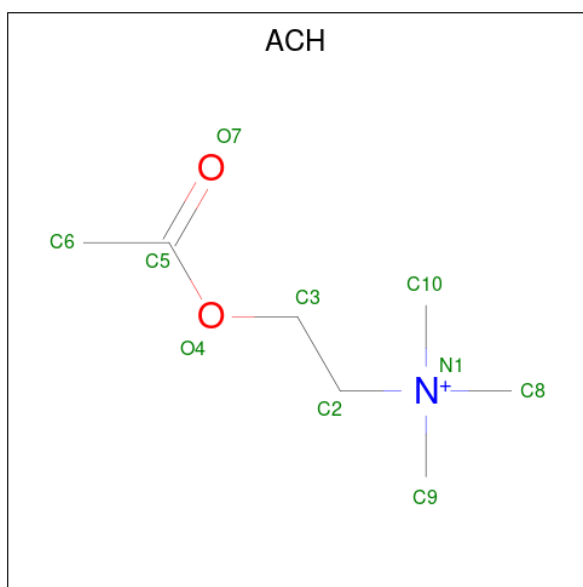
- Molecule 1 is a protein called PUTATIVE GLYCINE BETAIN-BINDING ABC TRANSPORTER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2180	1373	357	441	9			
1	B	288	Total	C	N	O	S	0	0	0
			2180	1373	357	441	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	ASP	GLY	engineered mutation	UNP Q92N37
A	319	GLU	-	expression tag	UNP Q92N37
A	320	HIS	-	expression tag	UNP Q92N37
A	321	HIS	-	expression tag	UNP Q92N37
A	322	HIS	-	expression tag	UNP Q92N37
A	323	HIS	-	expression tag	UNP Q92N37
A	324	HIS	-	expression tag	UNP Q92N37
A	325	HIS	-	expression tag	UNP Q92N37
B	251	ASP	GLY	engineered mutation	UNP Q92N37
B	319	GLU	-	expression tag	UNP Q92N37
B	320	HIS	-	expression tag	UNP Q92N37
B	321	HIS	-	expression tag	UNP Q92N37
B	322	HIS	-	expression tag	UNP Q92N37
B	323	HIS	-	expression tag	UNP Q92N37
B	324	HIS	-	expression tag	UNP Q92N37
B	325	HIS	-	expression tag	UNP Q92N37

- Molecule 2 is ACETYLCHOLINE (CCD ID: ACH) (formula: C₇H₁₆NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	7	1	2		
2	B	1	Total	C	N	O	0	0
			10	7	1	2		

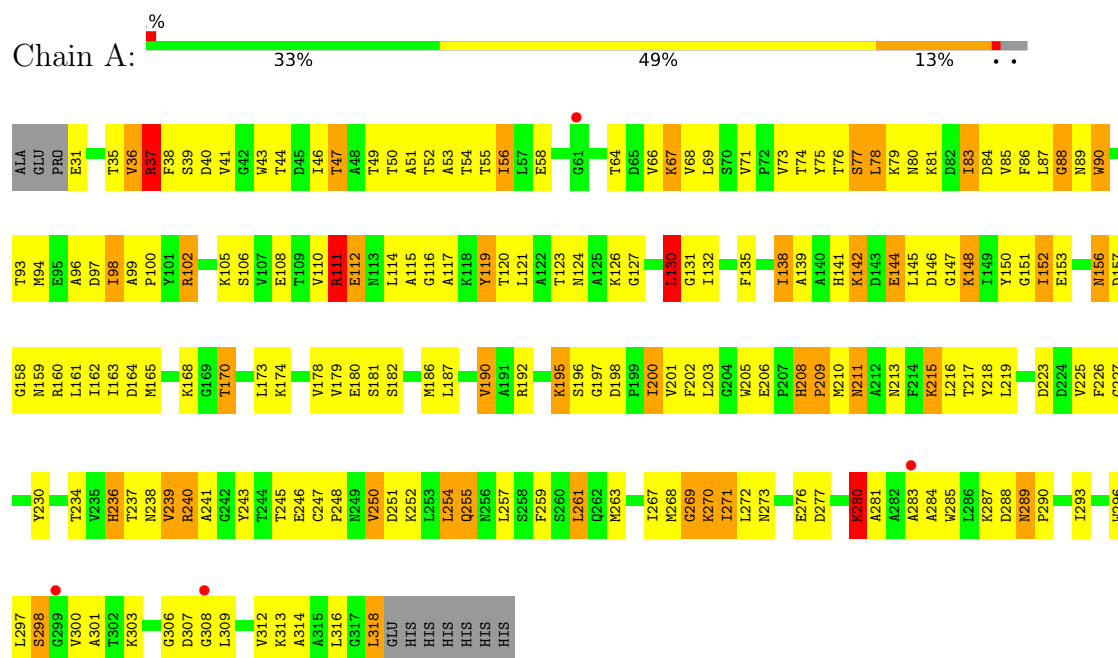
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	0	0
			120	120		
3	B	116	Total	O	0	0
			116	116		

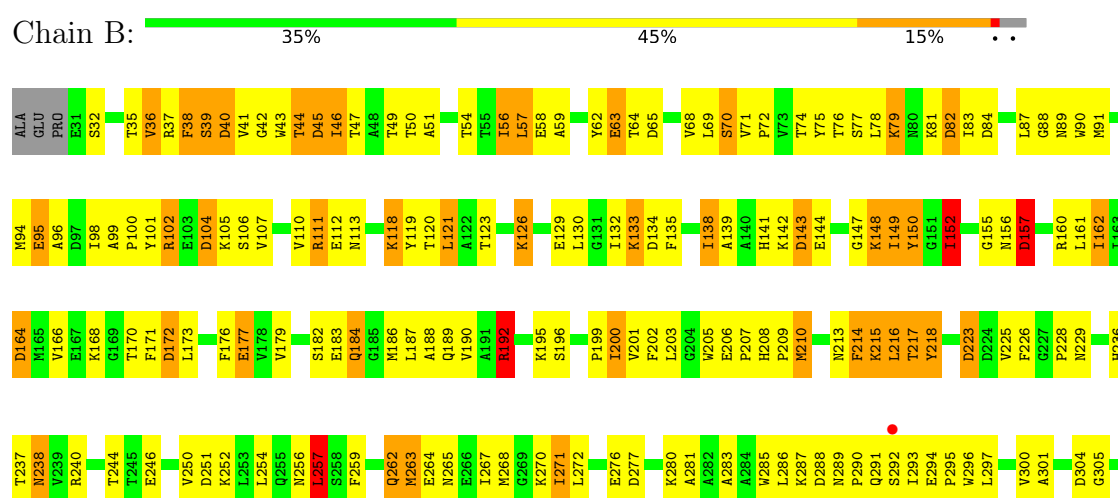
3 Residue-property plots

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: PUTATIVE GLYCINE BETAIN-BINDING ABC TRANSPORTER PROTEIN



• Molecule 1: PUTATIVE GLYCINE BETAIN-BINDING ABC TRANSPORTER PROTEIN



L309	L318
A310	GLU
A311	HIS
V312	HIS
K313	HIS
A314	HIS
	HIS
	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	31.20Å 212.70Å 42.80Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	89.3 (20.00-1.80) 89.3 (20.00-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.33 (at 1.80Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.154 , 0.210 0.143 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	4.5	Xtriage
Anisotropy	0.923	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 132.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.097 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4616	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.48	0/2221	1.81	64/3015 (2.1%)
1	B	0.49	0/2221	1.76	48/3015 (1.6%)
All	All	0.49	0/4442	1.79	112/6030 (1.9%)

There are no bond length outliers.

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	LYS	CA-C-N	11.43	138.11	123.14
1	A	148	LYS	C-N-CA	11.43	138.11	123.14
1	B	138	ILE	CA-C-N	9.43	133.30	120.38
1	B	138	ILE	C-N-CA	9.43	133.30	120.38
1	B	104	ASP	CA-CB-CG	9.10	121.70	112.60
1	A	280	LYS	CA-C-N	8.58	131.78	120.28
1	A	280	LYS	C-N-CA	8.58	131.78	120.28
1	A	86	PHE	CA-CB-CG	8.39	122.19	113.80
1	A	190	VAL	O-C-N	7.78	129.42	121.87
1	B	229	ASN	CA-C-N	7.74	133.35	122.36
1	B	229	ASN	C-N-CA	7.74	133.35	122.36
1	B	304	ASP	CA-C-N	7.52	134.87	120.66
1	B	304	ASP	C-N-CA	7.52	134.87	120.66
1	B	40	ASP	CA-CB-CG	7.43	120.03	112.60
1	A	192	ARG	CA-C-N	7.33	130.43	120.38
1	A	192	ARG	C-N-CA	7.33	130.43	120.38
1	B	157	ASP	O-C-N	7.20	129.75	122.12
1	A	156	ASN	CA-CB-CG	-7.14	105.46	112.60
1	A	58	GLU	CA-C-N	7.07	129.75	120.28
1	A	58	GLU	C-N-CA	7.07	129.75	120.28
1	A	112	GLU	O-C-N	-6.95	115.14	123.13
1	A	200	ILE	CA-C-N	6.73	132.54	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ILE	C-N-CA	6.73	132.54	122.98
1	A	280	LYS	O-C-N	6.73	129.36	122.09
1	A	215	LYS	CA-C-N	6.72	131.67	122.19
1	A	215	LYS	C-N-CA	6.72	131.67	122.19
1	B	38	PHE	CA-CB-CG	6.69	120.49	113.80
1	A	52	THR	O-C-N	6.66	129.22	122.03
1	B	172	ASP	O-C-N	-6.56	115.26	122.67
1	B	150	TYR	CA-C-N	6.54	128.75	122.27
1	B	150	TYR	C-N-CA	6.54	128.75	122.27
1	A	271	ILE	CA-C-N	6.50	129.52	120.29
1	A	271	ILE	C-N-CA	6.50	129.52	120.29
1	A	119	TYR	O-C-N	-6.48	115.58	123.36
1	A	182	SER	CA-C-O	-6.37	114.13	121.26
1	A	218	TYR	O-C-N	-6.20	115.25	122.87
1	B	49	THR	CA-C-N	-6.18	110.02	120.58
1	B	49	THR	C-N-CA	-6.18	110.02	120.58
1	A	289	ASN	CA-C-N	6.14	126.04	119.28
1	A	289	ASN	C-N-CA	6.14	126.04	119.28
1	A	190	VAL	CA-C-N	6.05	128.66	120.44
1	A	190	VAL	C-N-CA	6.05	128.66	120.44
1	A	208	HIS	CA-CB-CG	-6.05	107.75	113.80
1	B	32	SER	CA-C-N	6.04	132.32	122.65
1	B	32	SER	C-N-CA	6.04	132.32	122.65
1	A	37	ARG	CA-C-N	6.03	132.89	122.64
1	A	37	ARG	C-N-CA	6.03	132.89	122.64
1	B	44	THR	O-C-N	5.95	128.43	122.12
1	B	229	ASN	CA-CB-CG	5.95	118.55	112.60
1	A	71	VAL	O-C-N	5.89	124.19	120.42
1	B	218	TYR	CA-C-N	-5.89	113.38	122.09
1	B	218	TYR	C-N-CA	-5.89	113.38	122.09
1	A	52	THR	CA-C-N	5.75	132.52	121.54
1	A	52	THR	C-N-CA	5.75	132.52	121.54
1	A	88	GLY	CA-C-N	-5.71	115.42	122.84
1	A	88	GLY	C-N-CA	-5.71	115.42	122.84
1	A	96	ALA	CA-C-N	5.68	128.21	120.54
1	A	96	ALA	C-N-CA	5.68	128.21	120.54
1	A	76	THR	CA-C-N	5.67	129.32	120.82
1	A	76	THR	C-N-CA	5.67	129.32	120.82
1	A	112	GLU	CA-C-O	5.63	126.73	120.43
1	A	211	ASN	CA-CB-CG	-5.61	106.99	112.60
1	B	45	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	102	ARG	CA-C-N	5.57	128.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ARG	C-N-CA	5.57	128.31	120.28
1	B	79	LYS	O-C-N	5.55	127.80	122.03
1	B	270	LYS	CA-C-N	5.55	129.40	120.30
1	B	270	LYS	C-N-CA	5.55	129.40	120.30
1	B	263	MET	O-C-N	5.54	127.78	122.07
1	B	210	MET	CA-C-N	5.53	128.45	120.38
1	B	210	MET	C-N-CA	5.53	128.45	120.38
1	A	269	GLY	CA-C-N	5.50	127.65	120.28
1	A	269	GLY	C-N-CA	5.50	127.65	120.28
1	B	121	LEU	O-C-N	5.50	129.69	122.93
1	B	262	GLN	O-C-N	5.48	127.93	122.12
1	A	170	THR	CA-C-N	5.46	130.12	122.36
1	A	170	THR	C-N-CA	5.46	130.12	122.36
1	A	119	TYR	CA-C-N	-5.42	113.10	122.10
1	A	119	TYR	C-N-CA	-5.42	113.10	122.10
1	B	65	ASP	CA-CB-CG	-5.36	107.25	112.60
1	B	121	LEU	CA-C-N	5.35	131.80	122.81
1	B	121	LEU	C-N-CA	5.35	131.80	122.81
1	B	177	GLU	CA-C-O	5.32	126.70	120.80
1	A	119	TYR	CA-C-O	5.32	126.20	119.98
1	A	138	ILE	CA-C-N	5.30	131.66	121.54
1	A	138	ILE	C-N-CA	5.30	131.66	121.54
1	B	172	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	90	TRP	O-C-N	5.30	129.26	123.22
1	A	130	LEU	CA-C-O	5.28	126.11	120.24
1	B	82	ASP	CA-C-N	-5.27	115.44	122.77
1	B	82	ASP	C-N-CA	-5.27	115.44	122.77
1	B	42	GLY	CA-C-O	5.27	124.65	118.96
1	B	310	ALA	CA-C-N	5.26	129.50	120.72
1	B	310	ALA	C-N-CA	5.26	129.50	120.72
1	A	43	TRP	O-C-N	-5.21	116.30	122.65
1	A	307	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	192	ARG	CD-NE-CZ	-5.19	117.14	124.40
1	A	307	ASP	CA-C-N	5.16	125.82	119.99
1	A	307	ASP	C-N-CA	5.16	125.82	119.99
1	B	81	LYS	CA-C-N	5.15	127.45	120.44
1	B	81	LYS	C-N-CA	5.15	127.45	120.44
1	B	262	GLN	CA-C-O	-5.15	115.07	120.63
1	B	36	VAL	CA-C-N	-5.10	115.68	122.72
1	B	36	VAL	C-N-CA	-5.10	115.68	122.72
1	A	314	ALA	CA-C-N	5.10	127.42	120.54
1	A	314	ALA	C-N-CA	5.10	127.42	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ALA	CA-C-O	5.08	126.34	120.90
1	A	97	ASP	CA-CB-CG	-5.07	107.53	112.60
1	A	182	SER	CA-CB-OG	5.05	121.20	111.10
1	A	236	HIS	CA-C-O	5.04	126.90	121.06
1	B	238	ASN	CA-CB-CG	5.04	117.64	112.60
1	B	70	SER	CA-C-O	-5.01	116.28	121.99

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	2180	0	2125	165	0
1	B	2180	0	2125	179	0
2	A	10	0	16	13	0
2	B	10	0	16	9	0
3	A	120	0	0	11	0
3	B	116	0	0	22	0
All	All	4616	0	4282	347	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 40.

All (347) 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:90:TRP:HB2	1:B:94:MET:HE3	1.53	0.90
1:A:114:LEU:HD11	1:A:261:LEU:HD23	1.54	0.89
1:B:98:ILE:HG23	1:B:102:ARG:HD3	1.56	0.85
1:A:132:ILE:HG22	1:A:219:LEU:HD21	1.57	0.82
1:B:99:ALA:HA	1:B:102:ARG:HE	1.42	0.82
1:A:277:ASP:HB3	1:A:280:LYS:HB2	1.61	0.81
1:A:44:THR:HG21	1:A:272:LEU:HG	1.63	0.81
1:A:293:ILE:HG21	1:A:312:VAL:HG11	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LYS:HA	1:A:318:LEU:HD21	1.63	0.79
1:A:126:LYS:O	1:A:130:LEU:HD13	1.83	0.79
1:A:187:LEU:HA	1:A:190:VAL:HG23	1.65	0.79
1:A:267:ILE:HG22	1:A:271:ILE:HD11	1.66	0.77
1:B:287:LYS:HA	1:B:318:LEU:HD23	1.67	0.77
1:B:170:THR:O	1:B:173:LEU:HD12	1.84	0.77
1:B:138:ILE:HG21	1:B:149:ILE:HD11	1.67	0.76
1:B:290:PRO:HB3	1:B:318:LEU:HD22	1.67	0.76
1:A:141:HIS:O	1:A:144:GLU:HG2	1.86	0.75
1:B:166:VAL:HG13	1:B:173:LEU:O	1.87	0.75
1:B:72:PRO:O	1:B:76:THR:HG23	1.86	0.75
1:A:85:VAL:HG22	1:A:239:VAL:HG23	1.68	0.74
1:B:50:THR:O	1:B:54:THR:HG23	1.86	0.74
1:A:135:PHE:O	1:A:138:ILE:HD12	1.88	0.74
1:B:45:ASP:N	1:B:268:MET:HE3	2.03	0.73
1:A:251:ASP:HA	1:A:254:LEU:HD12	1.71	0.73
1:B:207:PRO:HA	3:B:418:HOH:O	1.88	0.73
1:A:83:ILE:O	1:A:240:ARG:HD3	1.88	0.73
1:B:188:ALA:O	1:B:192:ARG:HG3	1.88	0.73
1:B:99:ALA:HA	1:B:102:ARG:NE	2.03	0.72
1:B:277:ASP:HB3	1:B:280:LYS:HE3	1.71	0.72
1:A:163:ILE:HG13	1:A:178:VAL:HG21	1.72	0.71
1:A:159:ASN:O	1:A:163:ILE:HD12	1.90	0.71
1:A:269:GLY:O	1:A:273:ASN:HB2	1.91	0.71
1:B:44:THR:HG22	1:B:268:MET:HG2	1.73	0.70
1:B:271:ILE:HG22	1:B:272:LEU:HG	1.71	0.70
1:A:205:TRP:NE1	2:A:1:ACH:H91	2.06	0.70
1:A:267:ILE:O	1:A:271:ILE:HG13	1.93	0.69
1:B:39:SER:OG	1:B:69:LEU:HD12	1.93	0.69
1:B:101:TYR:HB3	1:B:106:SER:OG	1.93	0.68
1:A:157:ASP:OD1	2:A:1:ACH:H63	1.94	0.68
1:B:166:VAL:HG11	1:B:176:PHE:O	1.93	0.68
1:A:298:SER:HA	3:A:398:HOH:O	1.94	0.67
1:A:50:THR:O	1:A:54:THR:HG23	1.95	0.66
1:B:121:LEU:HD21	1:B:162:ILE:HD13	1.78	0.66
1:B:267:ILE:HG22	1:B:271:ILE:HD12	1.76	0.66
1:A:146:ASP:O	1:A:148:LYS:HG3	1.94	0.66
1:B:202:PHE:CE1	1:B:216:LEU:HD22	2.31	0.65
1:B:218:TYR:HB2	3:B:388:HOH:O	1.97	0.65
1:A:217:THR:HG22	3:A:436:HOH:O	1.97	0.64
1:A:68:VAL:HG22	3:A:385:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ALA:O	1:B:287:LYS:HG3	1.98	0.64
1:B:44:THR:HG23	1:B:271:ILE:HG21	1.79	0.64
1:B:202:PHE:HE1	1:B:216:LEU:HD22	1.63	0.64
1:B:192:ARG:HG2	3:B:395:HOH:O	1.98	0.64
1:B:208:HIS:ND1	1:B:210:MET:HG2	2.12	0.64
1:A:67:LYS:HD3	3:A:428:HOH:O	1.98	0.63
1:B:119:TYR:CE1	1:B:203:LEU:HD22	2.34	0.63
1:A:268:MET:HA	1:A:271:ILE:HD12	1.80	0.63
1:A:165:MET:HA	1:A:170:THR:HB	1.80	0.63
1:A:73:VAL:O	1:A:77:SER:HB2	1.98	0.63
1:A:116:GLY:HA3	3:A:399:HOH:O	1.98	0.63
1:B:300:VAL:HG13	3:B:429:HOH:O	1.99	0.63
1:B:72:PRO:HD3	1:B:155:GLY:O	1.98	0.62
1:A:119:TYR:CE2	2:A:1:ACH:H62	2.34	0.62
1:A:239:VAL:HG13	1:A:240:ARG:O	2.00	0.62
1:B:256:ASN:HB3	1:B:295:PRO:O	2.00	0.61
1:A:90:TRP:CG	2:A:1:ACH:H32	2.35	0.61
1:B:264:GLU:O	1:B:268:MET:HG3	2.01	0.61
1:B:267:ILE:HG23	1:B:281:ALA:HB1	1.82	0.60
1:A:209:PRO:HD2	1:A:268:MET:HE2	1.84	0.60
2:B:1:ACH:O7	2:B:1:ACH:H22	1.99	0.60
1:A:81:LYS:HE2	3:A:401:HOH:O	2.01	0.59
1:A:124:ASN:ND2	1:A:200:ILE:HG22	2.17	0.59
1:A:156:ASN:HB3	1:A:159:ASN:HB2	1.84	0.59
1:B:309:LEU:HB3	3:B:357:HOH:O	2.01	0.59
1:B:205:TRP:CD2	2:B:1:ACH:H81	2.37	0.59
1:A:37:ARG:HG3	1:A:84:ASP:OD2	2.03	0.58
1:A:164:ASP:O	1:A:168:LYS:HG3	2.03	0.58
1:A:77:SER:HB3	1:A:83:ILE:HG23	1.84	0.58
1:B:96:ALA:HB3	1:B:160:ARG:NH1	2.18	0.58
1:B:35:THR:HA	1:B:63:GLU:O	2.02	0.58
1:A:120:THR:HG23	1:A:121:LEU:O	2.03	0.58
1:A:127:GLY:CA	1:A:132:ILE:HD12	2.33	0.58
1:A:210:MET:HA	1:A:213:ASN:HB2	1.85	0.58
1:B:252:LYS:HB3	3:B:429:HOH:O	2.03	0.57
1:A:40:ASP:OD1	1:A:46:ILE:HG23	2.05	0.57
1:A:35:THR:HB	3:A:430:HOH:O	2.03	0.57
1:B:111:ARG:HD3	1:B:112:GLU:O	2.04	0.57
1:B:101:TYR:HA	1:B:104:ASP:OD1	2.04	0.57
1:A:170:THR:O	1:A:173:LEU:HB2	2.05	0.57
1:B:119:TYR:CE2	2:B:1:ACH:H61	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:HD13	1:A:88:GLY:HA3	1.86	0.56
1:B:205:TRP:CE3	2:B:1:ACH:H81	2.41	0.56
1:A:98:ILE:HD12	1:A:98:ILE:O	2.06	0.56
1:A:80:ASN:O	1:A:81:LYS:HB2	2.04	0.56
1:B:138:ILE:CG2	1:B:149:ILE:HD11	2.36	0.56
1:A:84:ASP:HA	1:A:240:ARG:HG2	1.88	0.56
1:A:257:LEU:HD11	1:A:259:PHE:CZ	2.41	0.56
1:A:162:ILE:HG22	1:A:178:VAL:HG22	1.87	0.55
1:A:145:LEU:HD21	1:A:201:VAL:HG23	1.89	0.55
1:A:165:MET:HG2	1:A:170:THR:HG21	1.87	0.55
1:B:91:MET:HE1	1:B:95:GLU:HG2	1.88	0.55
1:B:150:TYR:CE1	1:B:200:ILE:HD11	2.42	0.55
1:A:156:ASN:OD1	2:A:1:ACH:H61	2.08	0.54
1:A:110:VAL:O	1:A:111:ARG:HB3	2.06	0.54
1:B:118:LYS:HG2	1:B:206:GLU:HG3	1.89	0.54
1:A:132:ILE:HG22	1:A:219:LEU:CD2	2.34	0.54
1:A:293:ILE:HA	1:A:296:TRP:CE3	2.43	0.54
1:B:314:ALA:HB1	3:B:380:HOH:O	2.08	0.54
1:A:111:ARG:HB2	3:A:429:HOH:O	2.08	0.54
1:B:171:PHE:HB2	1:B:173:LEU:CD1	2.37	0.54
1:A:141:HIS:HB3	1:A:144:GLU:HG3	1.89	0.53
1:A:145:LEU:CD2	1:A:201:VAL:HG23	2.38	0.53
1:A:77:SER:HB3	1:A:83:ILE:CG2	2.38	0.53
1:A:301:ALA:HB1	1:A:306:GLY:O	2.08	0.53
1:A:75:TYR:CE2	1:A:98:ILE:HD13	2.43	0.53
1:A:150:TYR:CE2	1:A:179:VAL:HG11	2.44	0.53
1:B:189:GLN:HA	1:B:192:ARG:HE	1.74	0.53
1:A:89:ASN:HB2	1:A:238:ASN:HD21	1.74	0.53
1:A:276:GLU:HB3	1:A:281:ALA:HB2	1.90	0.53
1:B:78:LEU:HG	1:B:83:ILE:HG13	1.91	0.53
1:B:74:THR:O	1:B:83:ILE:HD11	2.09	0.53
1:A:257:LEU:HA	1:A:296:TRP:CD1	2.43	0.52
1:B:170:THR:HG22	1:B:171:PHE:CD1	2.44	0.52
1:B:68:VAL:HG23	1:B:68:VAL:O	2.10	0.52
1:B:214:PHE:C	1:B:215:LYS:HD3	2.35	0.52
1:B:205:TRP:NE1	2:B:1:ACH:H91	2.24	0.52
1:B:152:ILE:HG22	1:B:182:SER:O	2.09	0.52
1:A:119:TYR:CZ	2:A:1:ACH:H62	2.45	0.52
1:A:293:ILE:HG21	1:A:312:VAL:CG1	2.36	0.52
1:A:293:ILE:O	1:A:297:LEU:HG	2.09	0.52
1:A:49:THR:HB	1:A:259:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TRP:CD2	2:A:1:ACH:H32	2.45	0.51
1:B:132:ILE:O	1:B:132:ILE:HG22	2.10	0.51
1:A:68:VAL:O	1:A:68:VAL:HG23	2.10	0.51
1:A:157:ASP:CG	2:A:1:ACH:H63	2.35	0.51
1:B:126:LYS:HB2	3:B:327:HOH:O	2.09	0.51
1:B:157:ASP:O	1:B:161:LEU:HG	2.11	0.51
1:A:112:GLU:OE2	1:A:115:ALA:HB2	2.10	0.51
1:B:95:GLU:O	1:B:99:ALA:HB2	2.10	0.51
1:B:263:MET:HE1	1:B:296:TRP:CH2	2.46	0.51
1:B:78:LEU:CD2	1:B:83:ILE:HG13	2.41	0.51
1:B:130:LEU:HD12	1:B:199:PRO:CG	2.41	0.51
1:B:200:ILE:HD12	3:B:319:HOH:O	2.11	0.51
1:B:149:ILE:HG13	1:B:201:VAL:HB	1.93	0.51
1:B:190:VAL:HA	1:B:200:ILE:HG21	1.91	0.51
1:A:208:HIS:HA	1:A:268:MET:HE1	1.93	0.51
1:B:149:ILE:HD12	1:B:176:PHE:CD2	2.46	0.51
1:B:208:HIS:N	1:B:265:ASN:HD21	2.09	0.51
1:B:300:VAL:HG22	3:B:429:HOH:O	2.11	0.51
1:A:84:ASP:HA	1:A:240:ARG:HD3	1.94	0.50
1:B:77:SER:O	1:B:82:ASP:HB2	2.11	0.50
1:A:270:LYS:HB3	1:A:276:GLU:OE1	2.10	0.50
1:A:84:ASP:HB3	1:A:243:TYR:CE1	2.47	0.50
1:B:250:VAL:O	1:B:254:LEU:HG	2.12	0.50
1:B:200:ILE:HG23	1:B:202:PHE:CD2	2.47	0.50
1:A:38:PHE:CE1	1:A:54:THR:HG22	2.47	0.50
1:A:99:ALA:HB3	1:A:100:PRO:HD3	1.92	0.50
1:B:129:GLU:OE2	1:B:130:LEU:HD21	2.12	0.50
1:B:118:LYS:HD2	1:B:218:TYR:CD2	2.47	0.50
1:B:113:ASN:HB2	1:B:259:PHE:CD1	2.47	0.49
1:A:309:LEU:HD11	1:A:313:LYS:HE3	1.94	0.49
1:B:56:ILE:O	1:B:59:ALA:HB3	2.11	0.49
1:B:148:LYS:HD2	1:B:150:TYR:OH	2.12	0.49
1:B:240:ARG:HH22	1:B:246:GLU:CD	2.19	0.49
1:A:41:VAL:HG22	1:A:69:LEU:O	2.13	0.49
1:A:108:GLU:OE2	1:A:241:ALA:HA	2.13	0.49
1:B:160:ARG:O	1:B:164:ASP:OD1	2.30	0.49
1:B:215:LYS:HD3	1:B:215:LYS:N	2.27	0.49
1:B:69:LEU:HA	3:B:323:HOH:O	2.12	0.49
1:B:290:PRO:CB	1:B:318:LEU:HD22	2.39	0.49
1:A:117:ALA:HB1	1:A:206:GLU:O	2.13	0.48
1:B:71:VAL:HB	1:B:72:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:HIS:HB3	1:A:144:GLU:CG	2.43	0.48
1:A:290:PRO:HB3	1:A:318:LEU:CD1	2.44	0.48
1:B:46:ILE:O	1:B:46:ILE:HD12	2.13	0.48
1:B:78:LEU:HD23	1:B:83:ILE:HG13	1.94	0.48
1:B:244:THR:HG22	1:B:251:ASP:OD1	2.12	0.48
3:A:407:HOH:O	1:B:143:ASP:HA	2.13	0.48
1:B:184:GLN:H	1:B:184:GLN:NE2	2.10	0.48
1:A:151:GLY:O	1:A:186:MET:HB2	2.14	0.48
1:A:288:ASP:C	1:A:290:PRO:HD3	2.38	0.48
1:A:123:THR:HG23	1:A:124:ASN:O	2.13	0.48
1:A:259:PHE:HD2	1:A:263:MET:SD	2.37	0.48
1:B:228:PRO:HD2	3:B:340:HOH:O	2.13	0.48
1:A:110:VAL:HB	1:A:237:THR:HB	1.95	0.48
1:B:57:LEU:O	1:B:62:TYR:HB2	2.13	0.48
1:B:297:LEU:CD1	1:B:312:VAL:HG21	2.43	0.48
1:A:283:ALA:O	1:A:287:LYS:HG3	2.14	0.48
1:A:309:LEU:HG	1:A:313:LYS:HD2	1.95	0.48
1:B:287:LYS:O	1:B:290:PRO:HD3	2.14	0.48
1:B:297:LEU:HA	1:B:300:VAL:HG21	1.96	0.47
1:B:58:GLU:OE2	1:B:64:THR:OG1	2.30	0.47
1:A:39:SER:HA	1:A:67:LYS:O	2.13	0.47
1:A:79:LYS:HD2	1:A:106:SER:CB	2.44	0.47
1:B:133:LYS:HD3	1:B:217:THR:HG21	1.95	0.47
1:A:89:ASN:HD22	1:A:236:HIS:HB2	1.80	0.47
1:A:209:PRO:CD	1:A:268:MET:HE2	2.45	0.47
1:A:246:GLU:C	1:A:248:PRO:HD3	2.39	0.47
1:A:285:TRP:O	1:A:288:ASP:HB3	2.14	0.47
1:B:90:TRP:O	1:B:94:MET:HB2	2.13	0.47
1:A:205:TRP:CE2	2:A:1:ACH:H91	2.50	0.47
1:B:37:ARG:HB2	1:B:84:ASP:OD2	2.15	0.47
1:B:99:ALA:HA	1:B:102:ARG:CD	2.45	0.47
1:B:263:MET:HE1	1:B:296:TRP:HH2	1.80	0.47
1:A:121:LEU:HD21	1:A:162:ILE:CD1	2.45	0.47
1:A:270:LYS:O	1:A:276:GLU:HB2	2.15	0.47
1:B:100:PRO:HB2	3:B:427:HOH:O	2.14	0.47
1:B:257:LEU:HD11	3:B:405:HOH:O	2.15	0.47
2:A:1:ACH:H103	2:A:1:ACH:H31	1.41	0.46
1:B:89:ASN:HB3	1:B:236:HIS:HB2	1.96	0.46
1:A:150:TYR:O	1:A:202:PHE:HA	2.15	0.46
1:A:84:ASP:O	1:A:240:ARG:HG2	2.16	0.46
1:B:135:PHE:O	1:B:138:ILE:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ARG:H	1:B:84:ASP:HB2	1.79	0.46
1:B:123:THR:O	1:B:217:THR:N	2.49	0.46
1:A:234:THR:OG1	1:A:236:HIS:HE1	1.98	0.46
1:B:150:TYR:CE2	1:B:189:GLN:HG2	2.50	0.46
1:A:247:CYS:HB3	1:A:250:VAL:CG2	2.45	0.46
1:A:309:LEU:HD21	1:A:313:LYS:NZ	2.31	0.46
1:A:209:PRO:C	1:A:213:ASN:HD22	2.22	0.46
1:A:243:TYR:CE2	1:A:247:CYS:HB2	2.51	0.46
1:A:263:MET:HG3	1:A:285:TRP:CH2	2.51	0.46
1:B:78:LEU:HB3	1:B:107:VAL:HG12	1.98	0.46
1:B:171:PHE:HB2	1:B:173:LEU:HD11	1.98	0.46
1:A:54:THR:HB	1:A:64:THR:HG21	1.97	0.45
1:B:208:HIS:CG	1:B:210:MET:HG2	2.51	0.45
1:A:318:LEU:N	1:A:318:LEU:HD23	2.31	0.45
1:B:119:TYR:CZ	1:B:203:LEU:HD22	2.50	0.45
1:B:139:ALA:HB2	1:B:172:ASP:O	2.16	0.45
1:A:153:GLU:O	1:A:156:ASN:HB2	2.16	0.45
1:A:293:ILE:HG22	1:A:297:LEU:HD11	1.97	0.45
1:B:43:TRP:CD2	2:B:1:ACH:H21	2.52	0.45
1:B:56:ILE:O	1:B:59:ALA:N	2.50	0.45
1:B:267:ILE:CG2	1:B:271:ILE:HD12	2.46	0.45
1:A:161:LEU:O	1:A:165:MET:HG3	2.16	0.45
1:B:141:HIS:HA	3:B:329:HOH:O	2.17	0.45
1:B:164:ASP:OD1	1:B:164:ASP:N	2.49	0.45
1:B:268:MET:O	1:B:272:LEU:N	2.50	0.45
1:A:284:ALA:O	1:A:288:ASP:HB2	2.17	0.45
1:A:84:ASP:HA	1:A:240:ARG:CD	2.47	0.45
1:A:142:LYS:HG2	1:A:147:GLY:HA2	1.99	0.45
1:A:246:GLU:O	1:A:248:PRO:HD3	2.16	0.45
1:B:36:VAL:HG21	1:B:57:LEU:HD22	1.99	0.45
1:B:110:VAL:HG13	3:B:360:HOH:O	2.17	0.45
1:B:171:PHE:HB2	1:B:173:LEU:HD12	1.99	0.45
2:A:1:ACH:O7	2:A:1:ACH:H22	2.16	0.45
1:A:206:GLU:HG2	1:A:211:ASN:ND2	2.32	0.45
1:A:255:GLN:NE2	3:A:372:HOH:O	2.50	0.45
1:A:285:TRP:O	1:A:289:ASN:N	2.50	0.45
1:B:39:SER:HB2	1:B:83:ILE:HD13	1.98	0.44
1:B:120:THR:HA	1:B:226:PHE:CD2	2.52	0.44
1:B:291:GLN:NE2	1:B:294:GLU:OE2	2.50	0.44
1:A:257:LEU:HD11	1:A:259:PHE:CE2	2.52	0.44
1:B:288:ASP:HB3	3:B:408:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:TRP:HB2	1:B:46:ILE:HG22	2.00	0.44
1:B:141:HIS:ND1	1:B:144:GLU:OE1	2.49	0.44
1:B:189:GLN:OE1	1:B:192:ARG:NE	2.49	0.44
1:B:297:LEU:CD1	1:B:312:VAL:HG11	2.46	0.44
1:A:239:VAL:CG1	1:A:243:TYR:HB3	2.47	0.44
1:A:300:VAL:O	1:A:308:GLY:HA3	2.17	0.44
1:B:223:ASP:OD2	1:B:223:ASP:N	2.50	0.44
1:A:156:ASN:OD1	1:A:158:GLY:N	2.50	0.44
1:A:159:ASN:ND2	1:A:180:GLU:HG2	2.32	0.44
1:B:89:ASN:ND2	1:B:238:ASN:OD1	2.50	0.44
1:B:209:PRO:HB3	3:B:404:HOH:O	2.17	0.44
1:B:90:TRP:H	1:B:94:MET:HE3	1.83	0.44
1:B:205:TRP:CD1	2:B:1:ACH:H91	2.52	0.44
1:B:205:TRP:CZ3	1:B:210:MET:HE1	2.53	0.43
1:A:53:ALA:O	1:A:56:ILE:HB	2.18	0.43
1:A:163:ILE:HG13	1:A:178:VAL:CG2	2.46	0.43
1:B:75:TYR:HB3	1:B:101:TYR:CE1	2.53	0.43
1:B:76:THR:O	1:B:79:LYS:HB3	2.18	0.43
1:B:252:LYS:HD2	1:B:252:LYS:O	2.19	0.43
1:A:150:TYR:HA	1:A:179:VAL:HB	2.00	0.43
1:A:90:TRP:O	1:A:94:MET:HB2	2.18	0.43
1:B:43:TRP:CE3	2:B:1:ACH:H32	2.54	0.43
1:B:186:MET:HE1	1:B:205:TRP:CZ3	2.54	0.43
1:A:131:GLY:HA3	3:A:365:HOH:O	2.18	0.43
1:A:157:ASP:OD1	1:A:157:ASP:N	2.50	0.43
1:B:88:GLY:O	1:B:94:MET:HE1	2.18	0.43
1:B:147:GLY:HA3	3:B:339:HOH:O	2.18	0.43
1:B:189:GLN:HA	1:B:192:ARG:NE	2.32	0.43
1:A:196:SER:OG	1:A:198:ASP:OD2	2.30	0.43
1:B:102:ARG:NH2	3:B:400:HOH:O	2.52	0.43
1:A:252:LYS:HA	1:A:252:LYS:HD2	1.76	0.43
1:B:130:LEU:HD12	1:B:199:PRO:HG3	2.00	0.43
1:B:213:ASN:HD22	1:B:213:ASN:HA	1.58	0.43
1:B:40:ASP:OD1	1:B:46:ILE:HG23	2.19	0.43
1:B:41:VAL:HG21	1:B:43:TRP:CH2	2.54	0.43
1:B:126:LYS:O	1:B:129:GLU:HB3	2.19	0.43
1:B:289:ASN:O	1:B:292:SER:OG	2.29	0.43
1:A:153:GLU:O	1:A:153:GLU:HG2	2.19	0.42
1:A:271:ILE:HG23	1:A:276:GLU:O	2.19	0.42
1:B:285:TRP:HA	3:B:408:HOH:O	2.19	0.42
1:A:151:GLY:HA2	1:A:203:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ILE:HG22	1:A:297:LEU:CD1	2.49	0.42
1:A:36:VAL:O	1:A:64:THR:HA	2.19	0.42
1:A:78:LEU:HG	1:A:83:ILE:HG12	2.00	0.42
1:A:152:ILE:O	1:A:181:SER:N	2.52	0.42
1:A:165:MET:CA	1:A:170:THR:HB	2.47	0.42
1:A:290:PRO:HB3	1:A:318:LEU:HD12	2.01	0.42
1:B:44:THR:OG1	1:B:272:LEU:HD11	2.18	0.42
1:B:56:ILE:HG22	1:B:57:LEU:N	2.34	0.42
1:B:183:GLU:HG2	1:B:187:LEU:HD12	2.01	0.42
1:B:130:LEU:HD12	1:B:199:PRO:HG2	2.01	0.42
1:B:297:LEU:HA	1:B:300:VAL:CG2	2.49	0.42
1:B:301:ALA:HB1	1:B:305:GLY:C	2.44	0.42
1:B:290:PRO:HB3	1:B:318:LEU:HB2	2.02	0.42
1:A:225:VAL:HG12	1:A:226:PHE:CD1	2.54	0.42
1:B:294:GLU:N	1:B:295:PRO:HD2	2.34	0.42
1:A:205:TRP:CD1	2:A:1:ACH:H91	2.55	0.42
1:B:90:TRP:HB2	1:B:94:MET:CE	2.38	0.42
1:A:119:TYR:HD1	1:A:205:TRP:HB3	1.84	0.42
1:B:87:LEU:HB2	3:B:332:HOH:O	2.19	0.42
1:B:189:GLN:O	1:B:192:ARG:N	2.53	0.41
1:A:208:HIS:HB3	1:A:210:MET:HG2	2.02	0.41
1:B:182:SER:HB2	1:B:184:GLN:NE2	2.35	0.41
1:A:156:ASN:HD21	2:A:1:ACH:C5	2.34	0.41
1:A:195:LYS:HE3	1:A:195:LYS:HB2	1.91	0.41
1:B:141:HIS:HB3	1:B:144:GLU:OE1	2.19	0.41
1:B:192:ARG:HH11	1:B:192:ARG:HD3	1.52	0.41
1:A:239:VAL:HG13	1:A:243:TYR:HB3	2.03	0.41
1:B:120:THR:HG22	1:B:218:TYR:HD2	1.86	0.41
1:A:162:ILE:HD11	1:A:203:LEU:HD21	2.02	0.41
1:A:208:HIS:HA	1:A:268:MET:CE	2.51	0.41
1:B:70:SER:OG	1:B:72:PRO:HD2	2.21	0.41
1:B:285:TRP:CE3	1:B:286:LEU:HD23	2.56	0.41
1:A:263:MET:HG3	1:A:285:TRP:CZ2	2.56	0.41
1:B:157:ASP:OD1	1:B:157:ASP:N	2.50	0.41
1:A:187:LEU:HD23	1:A:190:VAL:HG21	2.03	0.41
1:B:87:LEU:HD23	1:B:237:THR:OG1	2.21	0.41
1:A:46:ILE:HG23	1:A:47:THR:N	2.36	0.40
1:A:247:CYS:HB3	1:A:250:VAL:HG23	2.02	0.40
1:B:152:ILE:CG2	1:B:183:GLU:HA	2.51	0.40
1:A:93:THR:O	1:A:160:ARG:NH2	2.51	0.40
1:A:142:LYS:O	1:A:145:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:HG	1:B:83:ILE:CD1	2.51	0.40
1:A:84:ASP:HA	1:A:240:ARG:CG	2.51	0.40
1:A:87:LEU:HD23	1:A:87:LEU:HA	1.80	0.40
1:A:99:ALA:HA	1:A:102:ARG:HD3	2.03	0.40
1:B:40:ASP:OD2	1:B:47:THR:HA	2.22	0.40
1:B:51:ALA:HA	1:B:54:THR:OG1	2.21	0.40
1:B:99:ALA:O	1:B:102:ARG:HG3	2.22	0.40
1:B:156:ASN:ND2	2:B:1:ACH:O7	2.50	0.40
1:B:162:ILE:HD11	1:B:203:LEU:HG	2.03	0.40
1:B:256:ASN:HB2	1:B:296:TRP:O	2.22	0.40
1:A:223:ASP:HA	1:A:227:GLY:O	2.21	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	286/298 (96%)	251 (88%)	30 (10%)	5 (2%)	7	2
1	B	286/298 (96%)	263 (92%)	21 (7%)	2 (1%)	18	8
All	All	572/596 (96%)	514 (90%)	51 (9%)	7 (1%)	10	3

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	B	257	LEU
1	B	152	ILE
1	A	139	ALA
1	A	298	SER
1	A	152	ILE
1	A	197	GLY

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	231/240 (96%)	195 (84%)	36 (16%)	2	0
1	B	231/240 (96%)	188 (81%)	43 (19%)	1	0
All	All	462/480 (96%)	383 (83%)	79 (17%)	2	0

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	36	VAL
1	A	37	ARG
1	A	47	THR
1	A	55	THR
1	A	56	ILE
1	A	66	VAL
1	A	67	LYS
1	A	74	THR
1	A	77	SER
1	A	78	LEU
1	A	83	ILE
1	A	98	ILE
1	A	105	LYS
1	A	111	ARG
1	A	130	LEU
1	A	142	LYS
1	A	144	GLU
1	A	174	LYS
1	A	195	LYS
1	A	209	PRO
1	A	215	LYS
1	A	216	LEU
1	A	230	TYR
1	A	239	VAL
1	A	240	ARG
1	A	245	THR

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Mol	Chain	Res	Type
1	A	250	VAL
1	A	254	LEU
1	A	255	GLN
1	A	261	LEU
1	A	270	LYS
1	A	280	LYS
1	A	303	LYS
1	A	316	LEU
1	A	318	LEU
1	B	38	PHE
1	B	39	SER
1	B	46	ILE
1	B	56	ILE
1	B	57	LEU
1	B	63	GLU
1	B	95	GLU
1	B	102	ARG
1	B	105	LYS
1	B	111	ARG
1	B	118	LYS
1	B	126	LYS
1	B	133	LYS
1	B	134	ASP
1	B	142	LYS
1	B	143	ASP
1	B	148	LYS
1	B	149	ILE
1	B	152	ILE
1	B	157	ASP
1	B	162	ILE
1	B	164	ASP
1	B	168	LYS
1	B	177	GLU
1	B	179	VAL
1	B	184	GLN
1	B	192	ARG
1	B	195	LYS
1	B	196	SER
1	B	200	ILE
1	B	214	PHE
1	B	215	LYS
1	B	216	LEU

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Mol	Chain	Res	Type
1	B	217	THR
1	B	223	ASP
1	B	225	VAL
1	B	257	LEU
1	B	262	GLN
1	B	271	ILE
1	B	276	GLU
1	B	293	ILE
1	B	309	LEU
1	B	318	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	141	HIS
1	A	211	ASN
1	A	213	ASN
1	A	236	HIS
1	A	238	ASN
1	A	255	GLN
1	A	273	ASN
1	A	289	ASN
1	B	80	ASN
1	B	184	GLN
1	B	213	ASN
1	B	262	GLN
1	B	291	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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACH	A	1	-	9,9,9	0.79	0	12,12,12	1.18	2 (16%)
2	ACH	B	1	-	9,9,9	0.91	0	12,12,12	1.14	1 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACH	A	1	-	-	6/7/7/7	-
2	ACH	B	1	-	-	4/7/7/7	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	ACH	C3-O4-C5	-2.97	103.89	117.14
2	A	1	ACH	C3-O4-C5	-2.64	105.37	117.14
2	A	1	ACH	C3-C2-N1	-2.00	109.40	115.82

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	ACH	N1-C2-C3-O4
2	B	1	ACH	N1-C2-C3-O4
2	A	1	ACH	C6-C5-O4-C3
2	A	1	ACH	O7-C5-O4-C3
2	B	1	ACH	O7-C5-O4-C3

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Mol	Chain	Res	Type	Atoms
2	B	1	ACH	C6-C5-O4-C3
2	B	1	ACH	C2-C3-O4-C5
2	A	1	ACH	C3-C2-N1-C10
2	A	1	ACH	C3-C2-N1-C9
2	A	1	ACH	C3-C2-N1-C8

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	ACH	13	0
2	B	1	ACH	9	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	288/298 (96%)	-0.27	4 (1%) 73 73	0, 7, 18, 38	0
1	B	288/298 (96%)	-0.29	1 (0%) 90 90	0, 7, 18, 40	0
All	All	576/596 (96%)	-0.28	5 (0%) 81 81	0, 7, 18, 40	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	GLY	3.2
1	A	299	GLY	3.0
1	A	283	ALA	2.9
1	A	308	GLY	2.4
1	B	292	SER	2.3

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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACH	A	1	10/10	0.95	0.06	0,0,13,14	0
2	ACH	B	1	10/10	0.96	0.10	0,19,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.