



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:41 PM UTC

PDB ID : 1GQQ / pdb_00001gqq
Title : MURC - Crystal structure of the apo-enzyme from Haemophilus influenzae
Authors : Skarzynski, T.; Cleasby, A.; Domenici, E.; Gevi, M.; Shaw, J.
Deposited on : 2001-12-03
Resolution : 3.10 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

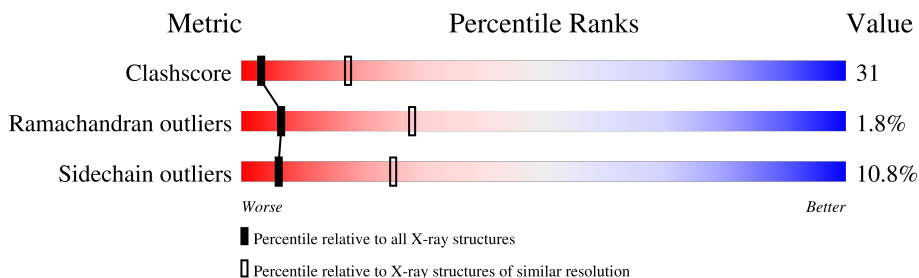
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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	475	
1	B	475	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6578 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 UDP-N-ACETYLMURAMATE-L-ALANINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3292	2081	573	623	15			
1	B	427	Total	C	N	O	S	0	0	0
			3286	2078	572	621	15			



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.51Å 99.48Å 180.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 3.10	Depositor
% Data completeness (in resolution range)	100.0 (19.88-3.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.239 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6578	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	1.74	53/3346 (1.6%)	1.77	70/4525 (1.5%)
1	B	1.34	27/3341 (0.8%)	1.50	39/4519 (0.9%)
All	All	1.55	80/6687 (1.2%)	1.64	109/9044 (1.2%)

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	ILE	CA-CB	-13.82	1.36	1.53
1	A	357	ILE	CA-CB	-11.23	1.41	1.54
1	A	400	MET	SD-CE	-10.57	1.53	1.79
1	A	473	TRP	C-O	-10.35	1.11	1.24
1	B	411	ILE	CA-CB	-8.54	1.44	1.54
1	A	371	MET	SD-CE	-8.10	1.59	1.79
1	A	472	SER	CA-C	-8.07	1.42	1.52
1	B	209	MET	SD-CE	7.67	1.98	1.79
1	B	403	VAL	CA-CB	-7.50	1.47	1.54
1	A	370	VAL	CA-CB	-7.48	1.45	1.54
1	A	329	GLN	C-O	-7.46	1.14	1.24
1	A	403	VAL	CA-CB	-7.36	1.47	1.54
1	B	389	VAL	CA-CB	-7.33	1.45	1.54
1	B	308	ILE	CA-CB	-7.32	1.44	1.54
1	A	471	GLU	C-O	-7.13	1.15	1.24
1	B	454	ILE	CA-CB	-6.71	1.46	1.54
1	A	430	ASP	CB-CG	6.61	1.68	1.52
1	A	45	ILE	C-O	-6.38	1.17	1.24
1	A	110	MET	CA-C	-6.33	1.44	1.52
1	A	456	ALA	CA-CB	-6.32	1.45	1.53
1	A	470	ALA	CA-CB	-6.32	1.43	1.53
1	A	460	GLY	C-O	-6.23	1.15	1.23
1	B	31	MET	SD-CE	-6.19	1.64	1.79
1	A	273	VAL	CA-C	-6.11	1.45	1.52
1	A	107	ARG	NE-CZ	6.10	1.39	1.33
1	B	115	MET	SD-CE	-6.10	1.64	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	ASP	C-O	-6.06	1.21	1.23
1	B	316	ALA	CA-CB	-6.02	1.44	1.53
1	A	35	ALA	CA-CB	-6.00	1.44	1.53
1	A	135	MET	SD-CE	-5.97	1.64	1.79
1	B	194	MET	SD-CE	-5.95	1.64	1.79
1	B	412	VAL	CA-CB	-5.95	1.48	1.54
1	A	348	HIS	CA-CB	-5.93	1.45	1.53
1	B	122	ALA	CA-CB	-5.80	1.44	1.53
1	A	470	ALA	C-O	-5.75	1.17	1.24
1	A	26	ILE	CA-CB	-5.72	1.48	1.54
1	A	400	MET	CG-SD	-5.69	1.66	1.80
1	A	64	ALA	CA-C	-5.67	1.45	1.53
1	B	345	ASP	CA-C	5.64	1.59	1.52
1	A	132	THR	CA-CB	-5.61	1.44	1.53
1	B	259	ILE	CA-CB	5.60	1.60	1.54
1	A	367	LYS	CE-NZ	5.58	1.66	1.49
1	B	246	VAL	CA-CB	-5.57	1.47	1.54
1	A	429	VAL	CA-CB	-5.51	1.47	1.54
1	A	344	ASP	CB-CG	-5.50	1.38	1.52
1	A	301	ALA	CA-C	-5.49	1.46	1.52
1	A	356	THR	CA-CB	-5.49	1.44	1.53
1	A	78	ALA	CA-CB	-5.47	1.44	1.53
1	A	405	ALA	CA-CB	-5.45	1.44	1.53
1	B	410	PRO	CA-C	5.44	1.59	1.52
1	A	288	PRO	CA-C	-5.42	1.47	1.52
1	A	302	VAL	CA-CB	-5.41	1.48	1.54
1	A	460	GLY	CA-C	-5.37	1.44	1.51
1	A	459	ALA	CA-CB	-5.37	1.41	1.53
1	B	149	PHE	CA-C	-5.37	1.46	1.52
1	B	121	ILE	CA-CB	-5.35	1.47	1.53
1	A	466	SER	C-O	-5.31	1.17	1.24
1	A	356	THR	N-CA	-5.31	1.39	1.46
1	B	328	ASP	CA-C	-5.26	1.46	1.52
1	A	467	ARG	NE-CZ	5.25	1.38	1.33
1	B	429	VAL	CA-CB	-5.25	1.50	1.55
1	A	445	ASP	CA-C	-5.23	1.45	1.52
1	A	236	MET	SD-CE	-5.22	1.66	1.79
1	B	323	ALA	CA-CB	-5.21	1.45	1.53
1	A	360	ALA	CA-C	-5.21	1.46	1.52
1	A	187	MET	SD-CE	5.20	1.92	1.79
1	B	414	ALA	CA-CB	-5.18	1.45	1.53
1	A	447	ILE	CA-CB	-5.13	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	349	HIS	CA-C	-5.13	1.46	1.52
1	A	326	ARG	C-O	-5.12	1.17	1.24
1	A	283	VAL	CA-CB	-5.10	1.47	1.54
1	B	171	ILE	CA-C	-5.09	1.46	1.52
1	A	37	ILE	CA-CB	-5.09	1.47	1.54
1	A	174	ALA	CA-CB	-5.09	1.46	1.53
1	B	135	MET	SD-CE	-5.05	1.67	1.79
1	A	409	ALA	CA-CB	-5.04	1.44	1.53
1	B	192	THR	CA-CB	-5.03	1.45	1.53
1	B	417	LYS	CD-CE	5.03	1.67	1.52
1	A	34	ILE	CA-C	-5.02	1.46	1.52
1	A	457	GLN	C-O	5.00	1.30	1.24

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	SER	N-CA-C	-11.65	98.38	112.59
1	B	252	SER	N-CA-C	9.39	123.39	109.59
1	A	336	PRO	CA-C-N	-8.67	109.08	122.60
1	A	336	PRO	C-N-CA	-8.67	109.08	122.60
1	B	349	HIS	N-CA-C	-8.08	100.84	110.13
1	A	359	ALA	N-CA-C	-7.98	102.66	111.36
1	A	352	GLU	N-CA-C	-7.92	102.59	111.14
1	A	381	THR	N-CA-C	-7.63	102.61	112.23
1	A	455	LEU	CA-C-N	-7.38	112.61	122.42
1	A	455	LEU	C-N-CA	-7.38	112.61	122.42
1	A	56	THR	CA-C-N	-7.18	109.40	120.31
1	A	56	THR	C-N-CA	-7.18	109.40	120.31
1	A	242	VAL	N-CA-C	7.11	117.21	110.53
1	B	283	VAL	N-CA-C	7.04	118.02	108.17
1	B	45	ILE	N-CA-C	6.99	119.13	108.71
1	B	266	GLY	N-CA-C	-6.92	99.14	112.02
1	A	428	LYS	N-CA-C	-6.87	102.90	112.45
1	B	370	VAL	CB-CA-C	-6.80	100.69	110.83
1	B	190	VAL	CB-CA-C	-6.75	101.11	111.31
1	A	301	ALA	N-CA-C	-6.75	103.53	111.03
1	A	433	LEU	CA-C-N	-6.72	114.80	122.93
1	A	433	LEU	C-N-CA	-6.72	114.80	122.93
1	B	398	LEU	CA-C-N	-6.64	114.95	123.19
1	B	398	LEU	C-N-CA	-6.64	114.95	123.19
1	A	251	PHE	N-CA-C	-6.64	105.00	113.23
1	A	298	ALA	N-CA-C	-6.64	103.97	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	PRO	CB-CA-C	-6.59	102.31	110.95
1	B	29	ALA	N-CA-C	-6.47	99.98	110.20
1	A	331	GLY	CA-C-O	-6.40	114.67	122.15
1	A	191	VAL	CB-CA-C	-6.26	103.28	110.73
1	A	364	TRP	CA-C-N	-6.24	116.09	123.08
1	A	364	TRP	C-N-CA	-6.24	116.09	123.08
1	A	389	VAL	CB-CA-C	-6.23	103.91	111.88
1	A	29	ALA	N-CA-C	-6.19	102.36	110.53
1	A	370	VAL	CB-CA-C	-6.18	101.93	110.96
1	A	375	PRO	CA-C-O	-6.18	114.30	121.34
1	B	41	GLU	N-CA-C	-6.11	104.68	111.71
1	B	298	ALA	N-CA-C	-6.10	104.70	111.71
1	A	271	TYR	N-CA-C	6.07	117.37	108.14
1	A	283	VAL	N-CA-C	6.02	118.02	108.87
1	A	254	GLN	N-CA-C	6.00	120.30	112.92
1	A	246	VAL	N-CA-C	5.95	116.44	107.75
1	A	34	ILE	N-CA-C	-5.95	104.71	110.72
1	A	293	ALA	N-CA-C	-5.95	104.70	111.07
1	B	398	LEU	N-CA-C	5.92	118.06	108.34
1	B	331	GLY	N-CA-C	5.91	120.44	112.17
1	A	214	VAL	N-CA-C	-5.91	104.59	110.62
1	A	474	LYS	CD-CE-NZ	-5.91	93.00	111.90
1	B	417	LYS	N-CA-C	-5.90	104.97	111.82
1	A	453	LEU	CB-CA-C	-5.90	100.13	109.80
1	B	382	ARG	NE-CZ-NH1	-5.89	115.61	121.50
1	A	134	ALA	N-CA-C	-5.88	104.79	111.14
1	B	406	ALA	CA-C-N	-5.86	116.47	123.44
1	B	406	ALA	C-N-CA	-5.86	116.47	123.44
1	B	405	ALA	N-CA-C	5.84	118.42	111.71
1	A	439	GLN	N-CA-C	5.82	120.11	112.89
1	A	85	SER	N-CA-C	-5.80	106.16	113.18
1	B	457	GLN	N-CA-C	5.78	117.83	108.41
1	B	415	ASP	CA-C-N	-5.75	111.53	121.66
1	B	415	ASP	C-N-CA	-5.75	111.53	121.66
1	A	252	SER	N-CA-C	5.67	118.24	110.24
1	A	68	ILE	CA-CB-CG1	-5.66	100.78	110.40
1	A	465	ILE	CB-CA-C	-5.63	104.45	112.22
1	B	372	ILE	N-CA-C	-5.62	99.54	107.75
1	A	372	ILE	CB-CA-C	-5.62	103.69	110.99
1	B	224	GLY	CA-C-O	-5.61	116.10	122.33
1	A	420	CYS	N-CA-C	-5.60	105.26	111.36
1	A	468	GLY	N-CA-C	-5.59	105.47	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	GLU	N-CA-C	-5.55	105.12	113.89
1	A	245	GLN	CA-C-N	-5.54	115.73	123.10
1	A	245	GLN	C-N-CA	-5.54	115.73	123.10
1	A	434	VAL	N-CA-C	5.48	114.26	106.53
1	A	81	VAL	N-CA-C	-5.48	100.17	108.17
1	B	468	GLY	N-CA-C	-5.43	105.81	112.77
1	B	122	ALA	CA-C-N	-5.42	116.08	123.12
1	B	122	ALA	C-N-CA	-5.42	116.08	123.12
1	B	102	ILE	CA-C-O	5.41	122.70	119.19
1	A	44	GLN	CA-C-N	-5.37	115.65	123.06
1	A	44	GLN	C-N-CA	-5.37	115.65	123.06
1	A	138	MET	N-CA-C	-5.36	104.84	111.33
1	A	303	ALA	N-CA-C	5.35	116.80	111.07
1	A	428	LYS	CA-C-N	-5.34	115.52	122.94
1	A	428	LYS	C-N-CA	-5.34	115.52	122.94
1	B	124	ALA	N-CA-C	5.31	117.48	109.41
1	A	52	ASP	CB-CA-C	-5.28	102.33	110.78
1	A	375	PRO	CB-CA-C	-5.28	104.65	111.46
1	A	417	LYS	N-CA-C	-5.27	105.54	111.28
1	A	340	VAL	CA-C-O	-5.26	115.71	121.28
1	A	406	ALA	CA-C-N	-5.24	111.14	121.41
1	A	406	ALA	C-N-CA	-5.24	111.14	121.41
1	A	457	GLN	N-CA-C	5.23	117.49	109.07
1	A	398	LEU	CA-C-N	-5.22	116.71	123.19
1	A	398	LEU	C-N-CA	-5.22	116.71	123.19
1	B	62	ALA	N-CA-C	-5.22	106.92	113.28
1	B	238	LEU	N-CA-C	-5.21	107.09	113.50
1	B	283	VAL	CB-CA-C	-5.21	103.07	110.83
1	B	88	LYS	N-CA-C	5.20	117.31	109.41
1	B	355	VAL	N-CA-C	-5.18	105.44	110.42
1	A	79	SER	N-CA-C	-5.17	107.53	113.88
1	B	232	ASP	CA-C-N	5.16	124.33	118.97
1	B	232	ASP	C-N-CA	5.16	124.33	118.97
1	A	73	GLU	N-CA-C	-5.16	106.83	113.02
1	A	28	GLY	N-CA-C	-5.07	105.59	112.14
1	B	432	ILE	CA-C-N	-5.06	115.73	122.72
1	B	432	ILE	C-N-CA	-5.06	115.73	122.72
1	A	106	GLN	N-CA-C	5.06	117.38	110.55
1	B	422	SER	N-CA-C	-5.05	105.66	111.07
1	A	104	VAL	CB-CA-C	-5.02	104.28	111.31
1	A	386	ASP	N-CA-C	-5.01	105.26	111.33

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	3292	0	3295	180	0
1	B	3286	0	3288	230	0
All	All	6578	0	6583	404	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 31.

All (404) 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:A:105:ILE:HD11	1:A:110:MET:HG2	1.23	1.16
1:A:417:LYS:HD3	1:A:417:LYS:N	1.66	1.08
1:B:39:LEU:HD13	1:B:45:ILE:HG12	1.42	1.02
1:B:287:VAL:HG12	1:B:288:PRO:HD2	1.39	0.99
1:B:80:VAL:HG21	1:B:105:ILE:HD12	1.44	0.98
1:A:105:ILE:HD11	1:A:110:MET:CG	1.97	0.95
1:B:275:CYS:SG	1:B:281:ILE:HD12	2.08	0.94
1:B:287:VAL:CG1	1:B:288:PRO:HD2	1.97	0.93
1:A:105:ILE:CD1	1:A:110:MET:HG2	1.98	0.93
1:B:368:ARG:NH2	1:B:452:ASP:OD2	2.00	0.92
1:A:417:LYS:HD3	1:A:417:LYS:H	1.31	0.91
1:A:194:MET:HE3	1:A:235:LEU:CD2	2.02	0.90
1:B:108:ALA:O	1:B:109:GLN:C	2.16	0.89
1:A:436:ASP:OD1	1:A:438:SER:OG	1.91	0.89
1:B:265:THR:HB	1:B:270:HIS:CE1	2.07	0.88
1:B:181:PHE:CD2	1:B:181:PHE:N	2.41	0.87
1:B:255:ALA:HB3	1:B:258:ARG:HB2	1.55	0.86
1:B:135:MET:SD	1:B:296:ALA:HA	2.15	0.86
1:B:340:VAL:HG12	1:B:452:ASP:HB2	1.55	0.86
1:A:334:ILE:HG12	1:A:339:LYS:HG3	1.57	0.85
1:B:249:TYR:CZ	1:B:298:ALA:HB2	2.10	0.85
1:A:113:GLU:OE2	1:B:221:PRO:HA	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:MET:HE3	1:A:235:LEU:HD23	1.59	0.84
1:B:19:GLN:HG3	1:B:44:GLN:HG3	1.58	0.83
1:A:317:LEU:N	1:A:317:LEU:HD23	1.91	0.82
1:A:275:CYS:HB3	1:A:276:PRO:CD	2.10	0.82
1:A:124:ALA:O	1:A:191:VAL:HA	1.81	0.81
1:B:71:ALA:O	1:B:73:GLU:N	2.14	0.80
1:B:108:ALA:O	1:B:111:LEU:N	2.14	0.80
1:B:230:ALA:HA	1:B:236:MET:SD	2.22	0.80
1:B:306:GLU:O	1:B:306:GLU:HG3	1.81	0.80
1:B:268:GLN:HE21	1:B:286:ASN:HA	1.46	0.80
1:B:252:SER:O	1:B:254:GLN:N	2.15	0.80
1:A:436:ASP:CG	1:A:438:SER:HG	1.89	0.80
1:A:111:LEU:HD12	1:A:111:LEU:O	1.83	0.78
1:B:287:VAL:HG12	1:B:288:PRO:CD	2.14	0.78
1:B:181:PHE:N	1:B:181:PHE:HD2	1.79	0.77
1:B:116:ARG:HG2	1:B:117:PHE:N	2.00	0.77
1:A:402:ASP:OD1	1:A:417:LYS:NZ	2.18	0.76
1:A:275:CYS:SG	1:A:281:ILE:HD11	2.26	0.75
1:B:26:ILE:HG21	1:B:66:ILE:HD12	1.67	0.75
1:B:233:PRO:O	1:B:237:GLU:HB2	1.87	0.74
1:A:275:CYS:HB3	1:A:276:PRO:HD2	1.68	0.74
1:B:243:GLY:C	1:B:244:ARG:HG2	2.14	0.73
1:A:176:GLU:HG2	1:A:213:TYR:OH	1.87	0.73
1:B:230:ALA:HB2	1:B:248:THR:HB	1.70	0.73
1:A:376:HIS:O	1:A:377:ARG:HB2	1.87	0.72
1:A:460:GLY:H	1:A:462:VAL:HG12	1.54	0.72
1:B:184:LEU:O	1:B:186:PRO:HD3	1.88	0.72
1:A:377:ARG:HG2	1:A:377:ARG:HH11	1.53	0.72
1:B:285:LEU:HD12	1:B:286:ASN:N	2.05	0.71
1:B:461:SER:O	1:B:465:ILE:HD12	1.91	0.71
1:B:267:PHE:CE1	1:B:363:GLY:HA3	2.26	0.71
1:A:88:LYS:O	1:A:90:ASP:N	2.22	0.71
1:A:304:LYS:NZ	1:A:310:ASN:OD1	2.22	0.71
1:B:281:ILE:HG23	1:B:314:LEU:HD11	1.74	0.70
1:B:75:ILE:HG23	1:B:75:ILE:O	1.90	0.70
1:B:341:ARG:HD2	1:B:364:TRP:CH2	2.27	0.70
1:B:72:GLU:HB3	1:B:96:THR:HG21	1.72	0.70
1:B:275:CYS:SG	1:B:281:ILE:CD1	2.79	0.69
1:B:218:HIS:O	1:B:220:LEU:N	2.25	0.69
1:A:370:VAL:O	1:A:454:ILE:HA	1.93	0.68
1:B:80:VAL:CG2	1:B:105:ILE:HD12	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ARG:HB2	1:B:185:GLN:OE1	1.93	0.68
1:B:287:VAL:CG1	1:B:288:PRO:CD	2.70	0.68
1:A:275:CYS:SG	1:A:281:ILE:CD1	2.82	0.68
1:A:230:ALA:HB2	1:A:248:THR:HB	1.76	0.68
1:A:417:LYS:HD2	1:A:433:LEU:HD21	1.74	0.67
1:A:243:GLY:O	1:A:244:ARG:HD3	1.94	0.67
1:B:33:GLY:O	1:B:37:ILE:HG13	1.94	0.67
1:A:176:GLU:CD	1:A:176:GLU:H	2.04	0.66
1:A:375:PRO:HB2	1:A:403:VAL:HG22	1.77	0.66
1:A:391:VAL:CG1	1:A:392:LEU:N	2.58	0.66
1:B:285:LEU:HD12	1:B:286:ASN:H	1.61	0.66
1:B:364:TRP:CD1	1:B:367:LYS:HB2	2.30	0.66
1:B:140:TYR:HB3	1:B:147:PRO:HG3	1.77	0.66
1:B:449:GLN:O	1:B:450:ASP:C	2.37	0.66
1:B:308:ILE:HG22	1:B:309:ALA:N	2.11	0.65
1:B:209:MET:O	1:B:212:THR:N	2.28	0.65
1:B:21:ILE:HD13	1:B:38:LEU:HD13	1.78	0.65
1:B:109:GLN:OE1	1:B:183:HIS:NE2	2.30	0.65
1:A:405:ALA:O	1:A:406:ALA:HB3	1.96	0.64
1:B:67:TYR:HB3	1:B:74:HIS:CE1	2.32	0.64
1:B:67:TYR:CD2	1:B:74:HIS:HB3	2.33	0.64
1:B:207:GLU:OE1	1:B:210:LYS:HD3	1.96	0.64
1:A:71:ALA:HB3	1:A:74:HIS:CE1	2.34	0.63
1:A:417:LYS:N	1:A:417:LYS:CD	2.52	0.63
1:A:247:ILE:HG13	1:A:305:GLU:OE1	1.98	0.62
1:B:262:TYR:C	1:B:262:TYR:CD2	2.77	0.62
1:B:20:GLN:HB3	1:B:78:ALA:HA	1.80	0.62
1:A:232:ASP:OD2	1:A:234:VAL:HB	2.01	0.61
1:A:391:VAL:HG13	1:A:392:LEU:N	2.13	0.61
1:A:385:PHE:O	1:A:386:ASP:C	2.43	0.61
1:B:126:THR:OG1	1:B:194:MET:HA	1.99	0.61
1:B:27:GLY:HA3	1:B:49:ASP:OD2	2.01	0.60
1:A:239:VAL:HB	1:A:240:PRO:HD3	1.83	0.60
1:B:56:THR:HB	1:B:66:ILE:HG21	1.82	0.60
1:B:135:MET:SD	1:B:296:ALA:CA	2.88	0.60
1:B:265:THR:HB	1:B:270:HIS:HE1	1.64	0.60
1:A:417:LYS:O	1:A:421:ARG:HG3	2.01	0.60
1:B:247:ILE:HD12	1:B:257:TYR:HE1	1.67	0.60
1:B:357:ILE:O	1:B:358:LYS:C	2.41	0.60
1:B:415:ASP:OD1	1:B:415:ASP:C	2.44	0.59
1:A:244:ARG:HH22	1:B:109:GLN:NE2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLY:O	1:B:129:LYS:NZ	2.32	0.59
1:A:167:SER:OG	1:A:168:ARG:N	2.32	0.59
1:A:400:MET:O	1:A:433:LEU:HD12	2.02	0.59
1:A:312:ALA:O	1:A:313:ILE:C	2.43	0.59
1:A:417:LYS:HD2	1:A:433:LEU:CD2	2.31	0.59
1:A:243:GLY:C	1:B:103:PRO:HB3	2.28	0.58
1:A:335:ARG:HB3	1:A:336:PRO:HD2	1.85	0.58
1:A:335:ARG:HD3	1:A:473:TRP:CD2	2.38	0.58
1:B:281:ILE:CG2	1:B:314:LEU:HD21	2.33	0.58
1:A:185:GLN:HB3	1:B:116:ARG:HH22	1.69	0.58
1:B:19:GLN:N	1:B:79:SER:HG	2.00	0.58
1:B:121:ILE:HD12	1:B:171:ILE:HD13	1.85	0.58
1:A:34:ILE:HD11	1:A:111:LEU:HB2	1.85	0.58
1:B:105:ILE:HG21	1:B:110:MET:HG2	1.86	0.58
1:B:385:PHE:O	1:B:389:VAL:HG23	2.03	0.58
1:A:113:GLU:OE2	1:B:221:PRO:CA	2.51	0.58
1:A:258:ARG:O	1:A:273:VAL:HA	2.04	0.57
1:A:39:LEU:CD1	1:A:45:ILE:HB	2.34	0.57
1:A:229:CYS:O	1:A:236:MET:HE3	2.03	0.57
1:B:265:THR:CB	1:B:270:HIS:CE1	2.83	0.57
1:A:460:GLY:N	1:A:462:VAL:HG12	2.19	0.57
1:B:75:ILE:HD11	1:B:97:SER:OG	2.05	0.57
1:B:108:ALA:O	1:B:110:MET:N	2.38	0.56
1:B:243:GLY:O	1:B:244:ARG:HG2	2.04	0.56
1:A:115:MET:HE3	1:A:184:LEU:HD22	1.87	0.56
1:B:119:HIS:O	1:B:119:HIS:ND1	2.38	0.56
1:B:146:ASP:N	1:B:147:PRO:HD3	2.20	0.56
1:B:434:VAL:HG12	1:B:434:VAL:O	2.03	0.56
1:A:26:ILE:HG21	1:A:66:ILE:HD13	1.86	0.56
1:A:332:GLU:HG2	1:A:341:ARG:HG3	1.86	0.56
1:A:434:VAL:HG12	1:A:434:VAL:O	2.05	0.56
1:B:242:VAL:HG12	1:B:244:ARG:N	2.20	0.56
1:A:18:VAL:HG21	1:B:222:PHE:HE1	1.71	0.56
1:B:39:LEU:HD13	1:B:45:ILE:CG1	2.27	0.55
1:A:176:GLU:CG	1:A:213:TYR:OH	2.54	0.55
1:B:83:VAL:HG12	1:B:84:SER:O	2.06	0.55
1:A:288:PRO:O	1:A:292:ASN:ND2	2.40	0.55
1:B:218:HIS:C	1:B:220:LEU:N	2.64	0.55
1:A:84:SER:OG	1:A:85:SER:N	2.40	0.55
1:B:71:ALA:C	1:B:73:GLU:H	2.15	0.54
1:B:275:CYS:HG	1:B:281:ILE:HD12	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:VAL:HA	1:A:105:ILE:O	2.08	0.54
1:B:105:ILE:HG22	1:B:106:GLN:O	2.07	0.54
1:B:184:LEU:C	1:B:186:PRO:HD3	2.32	0.54
1:B:249:TYR:CE1	1:B:298:ALA:HB2	2.42	0.54
1:B:126:THR:HG21	1:B:195:GLU:O	2.07	0.54
1:A:349:HIS:O	1:A:350:PRO:C	2.51	0.54
1:A:243:GLY:C	1:A:244:ARG:HG2	2.32	0.54
1:A:142:GLN:C	1:A:144:LYS:H	2.15	0.53
1:B:19:GLN:NE2	1:B:44:GLN:OE1	2.40	0.53
1:B:20:GLN:NE2	1:B:77:GLY:O	2.40	0.53
1:B:341:ARG:HH11	1:B:364:TRP:HH2	1.54	0.53
1:A:429:VAL:HG22	1:A:430:ASP:N	2.24	0.53
1:B:83:VAL:HG13	1:B:87:ILE:HG13	1.90	0.53
1:B:335:ARG:HB3	1:B:336:PRO:HD2	1.90	0.53
1:A:127:HIS:O	1:A:193:ASN:ND2	2.39	0.53
1:B:72:GLU:HB3	1:B:96:THR:CG2	2.38	0.53
1:A:300:LEU:C	1:A:300:LEU:HD23	2.33	0.53
1:B:25:GLY:N	1:B:48:SER:O	2.42	0.52
1:B:228:MET:HE2	1:B:235:LEU:HD22	1.91	0.52
1:B:308:ILE:CG2	1:B:309:ALA:N	2.72	0.52
1:A:429:VAL:O	1:A:431:PRO:HD3	2.10	0.52
1:A:350:PRO:HD3	1:A:388:PHE:CZ	2.45	0.52
1:A:360:ALA:O	1:A:361:ARG:C	2.49	0.52
1:A:106:GLN:O	1:A:107:ARG:C	2.49	0.52
1:B:218:HIS:C	1:B:220:LEU:H	2.17	0.52
1:A:71:ALA:HB3	1:A:74:HIS:NE2	2.25	0.52
1:A:100:LYS:O	1:A:101:ARG:CB	2.58	0.52
1:A:49:ASP:O	1:A:68:ILE:HA	2.10	0.52
1:A:22:HIS:HA	1:A:46:SER:O	2.11	0.51
1:B:190:VAL:HG12	1:B:191:VAL:N	2.24	0.51
1:A:303:ALA:O	1:A:304:LYS:C	2.52	0.51
1:A:41:GLU:OE1	1:A:118:ARG:NH2	2.43	0.51
1:B:235:LEU:C	1:B:237:GLU:H	2.18	0.51
1:A:96:THR:HG22	1:A:100:LYS:HD2	1.93	0.51
1:A:148:THR:HB	1:A:170:LEU:HD12	1.91	0.51
1:B:287:VAL:HG21	1:B:320:PHE:HD2	1.75	0.51
1:B:67:TYR:CG	1:B:74:HIS:CG	2.99	0.51
1:A:88:LYS:C	1:A:90:ASP:H	2.19	0.51
1:A:304:LYS:HD3	1:A:313:ILE:HD12	1.93	0.51
1:B:108:ALA:HA	1:B:111:LEU:HB3	1.93	0.51
1:B:140:TYR:CB	1:B:147:PRO:HG3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:VAL:HG13	1:B:288:PRO:HD2	1.87	0.51
1:B:264:GLN:NE2	1:B:267:PHE:HD1	2.08	0.50
1:B:340:VAL:CG1	1:B:452:ASP:HB2	2.34	0.50
1:A:340:VAL:HG11	1:A:448:ILE:HD13	1.94	0.50
1:B:20:GLN:NE2	1:B:77:GLY:C	2.69	0.50
1:B:109:GLN:HG3	1:B:183:HIS:CD2	2.46	0.50
1:B:346:TYR:O	1:B:347:GLY:C	2.55	0.50
1:B:355:VAL:CG2	1:B:356:THR:N	2.75	0.50
1:B:355:VAL:O	1:B:356:THR:C	2.53	0.50
1:A:233:PRO:O	1:A:234:VAL:C	2.53	0.50
1:B:67:TYR:CD1	1:B:74:HIS:CD2	3.00	0.50
1:B:248:THR:N	1:B:256:ASP:OD1	2.38	0.50
1:A:37:ILE:HG21	1:A:114:ILE:HD13	1.94	0.49
1:A:31:MET:O	1:A:32:SER:C	2.49	0.49
1:A:111:LEU:HD12	1:A:111:LEU:C	2.36	0.49
1:A:377:ARG:HH11	1:A:377:ARG:CG	2.19	0.49
1:B:242:VAL:HG12	1:B:244:ARG:H	1.77	0.49
1:B:34:ILE:HD11	1:B:111:LEU:HB2	1.93	0.49
1:B:94:LEU:O	1:B:94:LEU:HD12	2.12	0.49
1:B:209:MET:O	1:B:210:LYS:C	2.54	0.49
1:A:52:ASP:HA	1:A:56:THR:OG1	2.13	0.49
1:A:262:TYR:HA	1:A:271:TYR:HB3	1.94	0.49
1:B:270:HIS:ND1	1:B:270:HIS:N	2.60	0.49
1:A:440:LEU:O	1:A:441:GLY:C	2.52	0.49
1:B:57:GLN:O	1:B:61:GLN:HG3	2.12	0.49
1:A:22:HIS:CE1	1:A:47:GLY:HA2	2.48	0.49
1:A:137:SER:O	1:A:138:MET:C	2.55	0.49
1:A:190:VAL:HG22	1:A:227:VAL:HB	1.95	0.49
1:B:287:VAL:HG21	1:B:320:PHE:CD2	2.47	0.49
1:B:72:GLU:CB	1:B:96:THR:HG21	2.43	0.49
1:B:243:GLY:O	1:B:244:ARG:NH1	2.28	0.48
1:A:280:ARG:C	1:A:281:ILE:HG13	2.37	0.48
1:B:26:ILE:HG21	1:B:66:ILE:CD1	2.40	0.48
1:B:207:GLU:OE1	1:B:207:GLU:HA	2.12	0.48
1:B:338:GLY:CA	1:B:450:ASP:HA	2.43	0.48
1:A:112:ALA:HB2	1:A:183:HIS:HB3	1.95	0.48
1:B:109:GLN:OE1	1:B:183:HIS:CD2	2.66	0.48
1:B:114:ILE:HG22	1:B:115:MET:N	2.28	0.48
1:B:258:ARG:HD3	1:B:260:GLU:OE2	2.14	0.48
1:B:306:GLU:O	1:B:306:GLU:CG	2.58	0.48
1:A:140:TYR:N	1:A:140:TYR:CD1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:MET:HE3	1:A:235:LEU:HD21	1.90	0.48
1:A:364:TRP:CD1	1:A:367:LYS:HD2	2.49	0.48
1:A:184:LEU:C	1:A:186:PRO:HD3	2.39	0.48
1:B:277:ASN:C	1:B:279:GLU:H	2.20	0.48
1:B:21:ILE:HB	1:B:45:ILE:HD12	1.96	0.48
1:B:244:ARG:O	1:B:246:VAL:HG23	2.13	0.47
1:B:206:PHE:O	1:B:207:GLU:C	2.57	0.47
1:B:252:SER:O	1:B:253:GLU:C	2.57	0.47
1:A:58:ARG:O	1:A:59:LEU:C	2.54	0.47
1:A:335:ARG:HD3	1:A:473:TRP:CE2	2.49	0.47
1:B:249:TYR:CE2	1:B:298:ALA:HB2	2.50	0.47
1:B:235:LEU:C	1:B:237:GLU:N	2.70	0.47
1:B:244:ARG:O	1:B:245:GLN:C	2.57	0.47
1:A:115:MET:O	1:A:118:ARG:N	2.40	0.47
1:A:334:ILE:HG12	1:A:339:LYS:CG	2.38	0.47
1:B:421:ARG:O	1:B:422:SER:C	2.58	0.47
1:A:309:ALA:O	1:A:310:ASN:C	2.56	0.47
1:B:134:ALA:O	1:B:135:MET:C	2.56	0.46
1:B:346:TYR:CE1	1:B:348:HIS:HE1	2.34	0.46
1:A:39:LEU:HD13	1:A:45:ILE:HB	1.97	0.46
1:A:142:GLN:C	1:A:144:LYS:N	2.72	0.46
1:B:20:GLN:HB3	1:B:77:GLY:O	2.15	0.46
1:B:243:GLY:O	1:B:244:ARG:HD3	2.16	0.46
1:B:274:ILE:HG22	1:B:274:ILE:O	2.15	0.46
1:B:284:LEU:O	1:B:318:ALA:HA	2.15	0.46
1:B:304:LYS:HD2	1:B:304:LYS:HA	1.76	0.46
1:A:67:TYR:C	1:A:68:ILE:HG13	2.40	0.46
1:A:119:HIS:HD2	1:A:187:MET:HB2	1.80	0.46
1:A:214:VAL:O	1:A:215:LYS:C	2.53	0.46
1:A:378:TYR:O	1:A:379:SER:C	2.58	0.46
1:B:277:ASN:C	1:B:279:GLU:N	2.73	0.46
1:A:317:LEU:O	1:A:318:ALA:C	2.57	0.46
1:A:23:PHE:HB2	1:A:26:ILE:HD12	1.98	0.46
1:B:228:MET:CE	1:B:235:LEU:HD22	2.45	0.46
1:A:100:LYS:O	1:A:101:ARG:HB2	2.15	0.46
1:B:294:LEU:HA	1:B:294:LEU:HD23	1.66	0.46
1:B:83:VAL:HG13	1:B:87:ILE:CG1	2.45	0.46
1:B:341:ARG:HD2	1:B:364:TRP:HH2	1.78	0.45
1:A:20:GLN:HE22	1:A:77:GLY:HA3	1.81	0.45
1:A:296:ALA:HB1	1:A:317:LEU:HD13	1.98	0.45
1:B:239:VAL:HB	1:B:240:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASP:OD1	1:A:57:GLN:NE2	2.40	0.45
1:A:322:GLY:O	1:A:323:ALA:HB3	2.16	0.45
1:A:346:TYR:CZ	1:A:459:ALA:HB1	2.51	0.45
1:B:432:ILE:HD13	1:B:432:ILE:HG21	1.74	0.45
1:B:436:ASP:OD1	1:B:436:ASP:C	2.59	0.45
1:A:449:GLN:O	1:A:450:ASP:C	2.57	0.45
1:B:129:LYS:O	1:B:130:THR:C	2.57	0.45
1:B:38:LEU:HA	1:B:38:LEU:HD23	1.69	0.45
1:A:249:TYR:HB2	1:A:297:THR:HG22	1.98	0.45
1:B:96:THR:O	1:B:97:SER:C	2.60	0.45
1:B:403:VAL:CG1	1:B:404:TYR:N	2.74	0.45
1:B:133:THR:O	1:B:134:ALA:C	2.59	0.45
1:A:277:ASN:O	1:A:278:ASN:HB2	2.16	0.45
1:A:285:LEU:HD12	1:A:285:LEU:HA	1.58	0.45
1:B:252:SER:O	1:B:255:ALA:N	2.45	0.45
1:A:23:PHE:O	1:A:47:GLY:CA	2.65	0.44
1:A:53:GLY:O	1:A:54:VAL:C	2.60	0.44
1:B:218:HIS:O	1:B:219:ASN:C	2.57	0.44
1:B:274:ILE:N	1:B:274:ILE:HD12	2.31	0.44
1:A:436:ASP:CG	1:A:438:SER:OG	2.51	0.44
1:B:110:MET:SD	1:B:110:MET:O	2.75	0.44
1:B:59:LEU:O	1:B:60:ALA:C	2.61	0.44
1:B:108:ALA:C	1:B:110:MET:N	2.72	0.44
1:A:25:GLY:N	1:A:48:SER:O	2.44	0.44
1:A:44:GLN:O	1:A:45:ILE:HD13	2.17	0.44
1:A:108:ALA:O	1:A:109:GLN:C	2.56	0.44
1:A:283:VAL:HG12	1:A:284:LEU:N	2.31	0.44
1:B:464:LYS:O	1:B:467:ARG:HG2	2.18	0.44
1:B:60:ALA:HA	1:B:64:ALA:O	2.17	0.44
1:A:38:LEU:HG	1:A:114:ILE:HD11	1.99	0.44
1:B:102:ILE:HA	1:B:103:PRO:HD3	1.88	0.44
1:B:447:ILE:HG21	1:B:447:ILE:HD13	1.69	0.44
1:B:94:LEU:HD12	1:B:94:LEU:C	2.43	0.44
1:A:61:GLN:HA	1:A:61:GLN:NE2	2.32	0.44
1:A:304:LYS:O	1:A:307:GLY:N	2.32	0.44
1:A:442:ASP:O	1:A:443:VAL:C	2.57	0.44
1:A:88:LYS:C	1:A:90:ASP:N	2.75	0.44
1:B:21:ILE:HB	1:B:45:ILE:CD1	2.48	0.44
1:B:283:VAL:HG12	1:B:284:LEU:N	2.33	0.44
1:A:90:ASP:OD1	1:A:90:ASP:O	2.36	0.43
1:A:420:CYS:SG	1:A:431:PRO:HB2	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ARG:HH21	1:B:452:ASP:CG	2.11	0.43
1:A:352:GLU:O	1:A:353:VAL:C	2.62	0.43
1:B:116:ARG:HD3	1:B:117:PHE:CE1	2.53	0.43
1:B:244:ARG:HG2	1:B:244:ARG:HH11	1.83	0.43
1:B:429:VAL:O	1:B:429:VAL:HG13	2.18	0.43
1:B:285:LEU:HD12	1:B:285:LEU:HA	1.35	0.43
1:B:375:PRO:HB2	1:B:403:VAL:HG22	2.00	0.43
1:A:428:LYS:HB3	1:A:428:LYS:HE2	1.69	0.43
1:B:243:GLY:O	1:B:244:ARG:CG	2.66	0.43
1:A:56:THR:O	1:A:57:GLN:C	2.59	0.43
1:A:123:VAL:HG12	1:A:129:LYS:HA	1.99	0.43
1:A:140:TYR:N	1:A:140:TYR:HD1	2.17	0.43
1:A:377:ARG:CG	1:A:377:ARG:NH1	2.79	0.43
1:A:380:ARG:HH11	1:A:380:ARG:HD3	1.54	0.43
1:B:55:VAL:HB	1:B:56:THR:H	1.65	0.43
1:B:470:ALA:O	1:B:471:GLU:C	2.62	0.43
1:B:168:ARG:O	1:B:168:ARG:CG	2.67	0.43
1:A:335:ARG:HB3	1:A:336:PRO:CD	2.49	0.43
1:B:187:MET:HE3	1:B:187:MET:HB3	1.89	0.43
1:B:319:ASP:O	1:B:319:ASP:CG	2.61	0.43
1:A:102:ILE:HA	1:A:103:PRO:HD2	1.87	0.43
1:A:455:LEU:HA	1:A:455:LEU:HD23	1.68	0.43
1:B:270:HIS:O	1:B:271:TYR:HB3	2.19	0.43
1:B:147:PRO:HB3	1:B:169:TYR:HB2	2.01	0.43
1:A:145:LEU:O	1:A:146:ASP:C	2.61	0.42
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.77	0.42
1:A:470:ALA:O	1:A:471:GLU:C	2.60	0.42
1:A:252:SER:O	1:A:253:GLU:C	2.61	0.42
1:B:115:MET:O	1:B:116:ARG:C	2.62	0.42
1:B:119:HIS:HA	1:B:187:MET:HG3	2.00	0.42
1:B:426:LEU:HD23	1:B:426:LEU:HA	1.67	0.42
1:B:19:GLN:HG3	1:B:44:GLN:CG	2.40	0.42
1:B:255:ALA:HB3	1:B:258:ARG:CB	2.39	0.42
1:A:228:MET:O	1:A:248:THR:HA	2.19	0.42
1:B:217:LEU:HD23	1:B:217:LEU:HA	1.49	0.42
1:A:113:GLU:O	1:A:114:ILE:C	2.61	0.42
1:A:125:GLY:O	1:A:129:LYS:NZ	2.41	0.42
1:A:458:GLY:C	1:A:462:VAL:HG11	2.44	0.42
1:B:55:VAL:O	1:B:58:ARG:N	2.53	0.42
1:A:129:LYS:HB2	1:A:129:LYS:HE2	1.77	0.42
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LEU:O	1:B:239:VAL:C	2.62	0.42
1:B:338:GLY:HA3	1:B:450:ASP:HA	2.02	0.42
1:A:19:GLN:O	1:A:44:GLN:HB2	2.20	0.42
1:B:232:ASP:HA	1:B:233:PRO:HD3	1.88	0.42
1:B:398:LEU:HA	1:B:398:LEU:HD12	1.77	0.42
1:B:411:ILE:O	1:B:412:VAL:C	2.58	0.42
1:A:304:LYS:O	1:A:306:GLU:N	2.52	0.42
1:B:45:ILE:HG22	1:B:46:SER:N	2.34	0.42
1:A:52:ASP:CG	1:A:57:GLN:HE21	2.25	0.42
1:A:301:ALA:O	1:A:302:VAL:C	2.59	0.42
1:A:364:TRP:CG	1:A:367:LYS:HD2	2.55	0.41
1:B:291:HIS:CG	1:B:292:ASN:N	2.88	0.41
1:B:315:GLU:O	1:B:319:ASP:HB3	2.20	0.41
1:A:34:ILE:HG21	1:A:34:ILE:HD13	1.65	0.41
1:B:94:LEU:O	1:B:98:LYS:HG3	2.20	0.41
1:B:190:VAL:HA	1:B:227:VAL:O	2.20	0.41
1:B:235:LEU:HD23	1:B:235:LEU:HA	1.75	0.41
1:B:424:ARG:O	1:B:427:GLY:N	2.53	0.41
1:B:455:LEU:HA	1:B:455:LEU:HD23	1.88	0.41
1:B:114:ILE:CG2	1:B:115:MET:N	2.81	0.41
1:A:367:LYS:HG3	1:A:451:GLY:O	2.20	0.41
1:A:399:ILE:HG21	1:A:399:ILE:HD13	1.83	0.41
1:B:243:GLY:C	1:B:244:ARG:HH11	2.21	0.41
1:A:127:HIS:HB2	1:A:193:ASN:HD21	1.84	0.41
1:A:188:VAL:HG12	1:A:189:SER:N	2.36	0.41
1:B:182:LEU:O	1:B:219:ASN:ND2	2.52	0.41
1:B:376:HIS:O	1:B:377:ARG:HB2	2.19	0.41
1:B:252:SER:C	1:B:254:GLN:N	2.79	0.41
1:B:323:ALA:O	1:B:324:GLY:C	2.61	0.41
1:A:91:ASN:OD1	1:A:93:GLU:N	2.47	0.41
1:A:248:THR:O	1:A:256:ASP:HB2	2.20	0.41
1:A:384:LEU:O	1:A:385:PHE:C	2.63	0.41
1:B:39:LEU:HD12	1:B:39:LEU:HA	1.74	0.41
1:B:91:ASN:O	1:B:95:VAL:HG12	2.21	0.41
1:B:96:THR:O	1:B:100:LYS:N	2.53	0.41
1:B:335:ARG:HH11	1:B:335:ARG:HD2	1.72	0.41
1:A:262:TYR:HA	1:A:270:HIS:O	2.21	0.41
1:B:267:PHE:CE1	1:B:363:GLY:CA	3.00	0.41
1:B:270:HIS:N	1:B:270:HIS:HD1	2.19	0.41
1:A:65:LYS:HE2	1:A:67:TYR:OH	2.20	0.40
1:A:391:VAL:O	1:A:394:GLN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:GLN:NE2	1:B:267:PHE:CD1	2.89	0.40
1:A:75:ILE:CG2	1:A:102:ILE:HD12	2.52	0.40
1:A:388:PHE:O	1:A:389:VAL:C	2.63	0.40
1:B:228:MET:HE2	1:B:228:MET:HB3	1.95	0.40
1:B:436:ASP:O	1:B:437:THR:C	2.63	0.40
1:B:238:LEU:C	1:B:240:PRO:HD2	2.47	0.40
1:A:134:ALA:O	1:A:135:MET:C	2.61	0.40
1:A:232:ASP:O	1:A:236:MET:HG2	2.22	0.40
1:B:429:VAL:HG22	1:B:430:ASP:N	2.36	0.40
1:A:290:LYS:O	1:A:293:ALA:N	2.55	0.40
1:B:55:VAL:O	1:B:56:THR:C	2.64	0.40
1:B:313:ILE:O	1:B:316:ALA:HB3	2.22	0.40
1:B:353:VAL:O	1:B:356:THR:HB	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	420/475 (88%)	384 (91%)	30 (7%)	6 (1%)	9	34
1	B	419/475 (88%)	376 (90%)	34 (8%)	9 (2%)	5	25
All	All	839/950 (88%)	760 (91%)	64 (8%)	15 (2%)	6	28

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	B	55	VAL
1	B	72	GLU
1	B	253	GLU
1	B	219	ASN

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Mol	Chain	Res	Type
1	A	116	ARG
1	A	305	GLU
1	B	89	ASP
1	B	278	ASN
1	B	365	GLY
1	A	54	VAL
1	A	377	ARG
1	B	347	GLY
1	A	55	VAL
1	B	54	VAL

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	349/387 (90%)	313 (90%)	36 (10%)	7	27
1	B	348/387 (90%)	309 (89%)	39 (11%)	6	24
All	All	697/774 (90%)	622 (89%)	75 (11%)	6	25

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	44	GLN
1	A	57	GLN
1	A	66	ILE
1	A	81	VAL
1	A	101	ARG
1	A	105	ILE
1	A	110	MET
1	A	114	ILE
1	A	116	ARG
1	A	138	MET
1	A	168	ARG
1	A	195	GLU

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Mol	Chain	Res	Type
1	A	252	SER
1	A	261	ASP
1	A	263	GLU
1	A	274	ILE
1	A	279	GLU
1	A	306	GLU
1	A	313	ILE
1	A	321	GLN
1	A	329	GLN
1	A	339	LYS
1	A	341	ARG
1	A	350	PRO
1	A	367	LYS
1	A	379	SER
1	A	380	ARG
1	A	391	VAL
1	A	417	LYS
1	A	426	LEU
1	A	448	ILE
1	A	461	SER
1	A	462	VAL
1	A	463	SER
1	A	467	ARG
1	B	32	SER
1	B	34	ILE
1	B	44	GLN
1	B	50	ILE
1	B	54	VAL
1	B	72	GLU
1	B	75	ILE
1	B	95	VAL
1	B	101	ARG
1	B	110	MET
1	B	111	LEU
1	B	114	ILE
1	B	118	ARG
1	B	131	THR
1	B	171	ILE
1	B	181	PHE
1	B	182	LEU
1	B	207	GLU
1	B	225	LEU

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Mol	Chain	Res	Type
1	B	228	MET
1	B	247	ILE
1	B	270	HIS
1	B	279	GLU
1	B	280	ARG
1	B	285	LEU
1	B	297	THR
1	B	311	GLU
1	B	326	ARG
1	B	329	GLN
1	B	348	HIS
1	B	355	VAL
1	B	358	LYS
1	B	368	ARG
1	B	426	LEU
1	B	448	ILE
1	B	453	LEU
1	B	465	ILE
1	B	469	LEU
1	B	475	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	20	GLN
1	A	44	GLN
1	A	61	GLN
1	A	99	GLN
1	A	106	GLN
1	A	219	ASN
1	A	254	GLN
1	A	268	GLN
1	A	278	ASN
1	A	291	HIS
1	A	439	GLN
1	A	446	GLN
1	A	449	GLN
1	B	19	GLN
1	B	20	GLN
1	B	61	GLN
1	B	74	HIS

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Mol	Chain	Res	Type
1	B	99	GLN
1	B	264	GLN
1	B	268	GLN
1	B	282	ASN
1	B	292	ASN
1	B	295	ASN
1	B	337	ASN
1	B	449	GLN

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

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.