



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:02 PM UTC

PDB ID : 1FX0 / pdb_00001fx0
Title : Crystal structure of the chloroplast F1-ATPase from spinach
Authors : Groth, G.; Pohl, E.
Deposited on : 2000-09-25
Resolution : 3.20 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

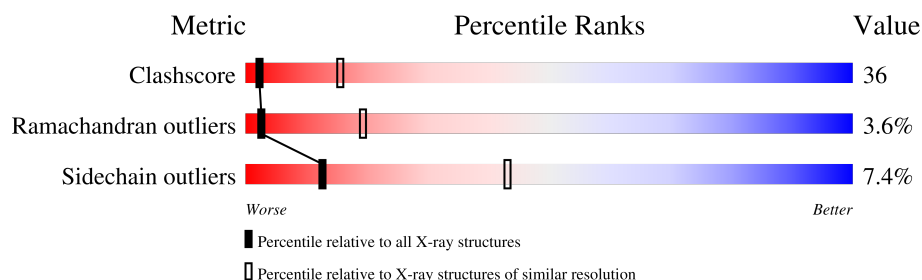
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	507	 41% 46% 7% • 6%
2	B	498	 39% 47% 8% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7187 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 ATP SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	133	0	0
			3647	2296	628	710	13			

- Molecule 2 is a protein called ATP SYNTHASE BETA CHAIN.

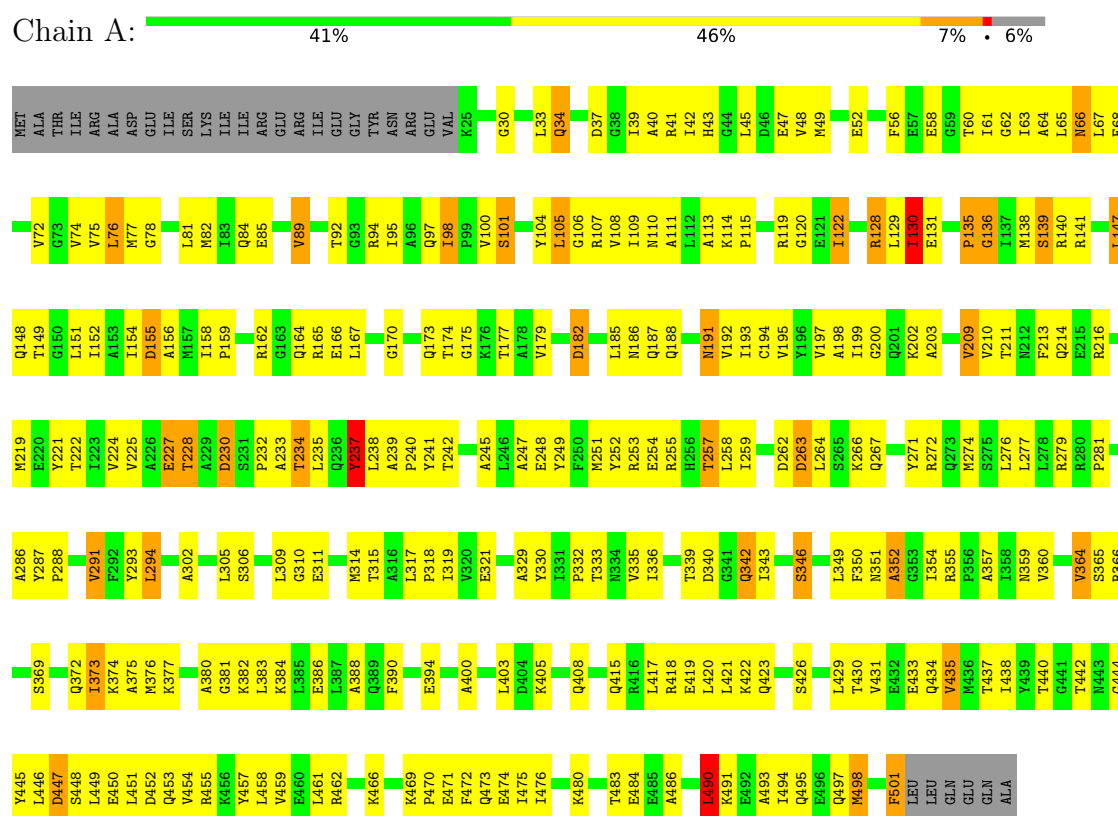
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	467	Total	C	N	O	S	89	0	0
			3540	2234	612	680	14			

3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: ATP SYNTHASE ALPHA CHAIN



• Molecule 2: ATP SYNTHASE BETA CHAIN



R429	F430	L431	F436	F436	V437	A438	F439	V440	L451	T454	L466	L469	E471	Q472	A473	V477	L480	A483	T484	LYS	A485	ALA	MET	ASN	LEU	GLU	MET	GLU	SER	LYS	LEU	LYS	LYS	A357	Y362	P363	A364	V365	D366	F367	L368	D369	S370	T371	M374	L375	Q376	P377	R378	I379	V380	E383	E386	I387	A388	Q389	R390	V391	K392	E393	T394	L395	Q396	R397	Y398	K399	E400	L401	Q402	D403	I404	L408	G409	L410	L413	E416	D417	R418	L419	R423	A424	R425	R426	I427	E428
V202	G203	E204	R206	T206	R207	E208	G209	L212	E215	M216	V221	I222	N223	E224	I227	K231	V232	A233	L234	V235	Y236	G237	Q238	M239	N240	E241	P242	P243	G244	A245	R246	M247	R248	V249	G250	L251	T252	T255	M256	A257	E258	Y259	F260	N264	E265	Q266	D267	V268	L269	L270	F271																																		
A274	I275	F276	R277	F278		A281	G282	V285	S286	A287	L288	L289	G290	R291	M292		A295	V296	G297	Y298	Q299	P300	L301	L302	E305	M306	G307	S308	L309	Q310	E311	R312	I313	T314	T322	S323	I324	Q325	A326	V327	Y328	D336	P337	T342	F343	L346	T350	V351	L352	S353	L356																																		

4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	147.70 Å 147.70 Å 385.05 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.319 , 0.350	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7187	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/3695	0.98	12/5002 (0.2%)
2	B	0.39	0/3598	1.08	25/4883 (0.5%)
All	All	0.38	0/7293	1.03	37/9885 (0.4%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	312	ARG	N-CA-C	-12.25	98.85	114.04
2	B	50	LYS	N-CA-C	9.89	125.50	113.23
2	B	53	ASP	N-CA-C	9.45	123.83	110.50
1	A	264	LEU	N-CA-C	-9.44	101.52	113.23
2	B	227	ILE	N-CA-C	-9.14	102.29	112.80
2	B	165	GLY	N-CA-C	-8.37	104.33	115.21
2	B	247	MET	N-CA-C	-8.32	103.12	113.28
1	A	498	MET	N-CA-C	-8.24	102.49	112.54
1	A	294	LEU	N-CA-C	-8.16	102.92	113.12
1	A	490	LEU	N-CA-C	-7.76	104.33	113.88
2	B	396	GLN	N-CA-C	-7.53	103.70	113.12
2	B	189	ILE	N-CA-C	7.46	118.38	112.12
2	B	106	THR	N-CA-C	-7.35	106.24	114.62
2	B	224	GLU	N-CA-C	-6.94	103.77	111.82
2	B	236	TYR	N-CA-C	6.84	119.67	108.52
1	A	237	TYR	N-CA-C	-6.80	102.37	111.96
1	A	213	PHE	N-CA-C	-6.39	105.61	113.41
1	A	130	ILE	N-CA-C	-6.00	104.66	110.42
2	B	275	ILE	N-CA-C	-5.97	106.92	112.83
2	B	430	PHE	N-CA-C	-5.96	105.97	113.18
2	B	484	THR	N-CA-C	-5.93	96.26	108.53
2	B	357	ALA	N-CA-C	-5.79	106.35	113.41
2	B	418	ARG	N-CA-C	-5.68	106.20	113.01
2	B	113	VAL	N-CA-C	-5.67	104.62	112.50
1	A	281	PRO	N-CA-C	5.51	117.42	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	ALA	N-CA-C	-5.50	107.12	113.88
2	B	323	SER	N-CA-C	5.42	117.07	108.67
2	B	437	VAL	N-CA-C	-5.27	107.63	111.90
2	B	250	GLY	N-CA-C	-5.21	106.10	112.77
2	B	314	THR	N-CA-C	5.19	116.18	108.60
2	B	204	GLU	N-CA-C	5.18	116.17	108.86
2	B	75	ARG	N-CA-C	-5.14	102.58	110.14
1	A	47	GLU	N-CA-C	5.12	118.79	112.54
1	A	346	SER	N-CA-C	5.09	117.70	109.40
2	B	52	ARG	N-CA-C	5.07	121.59	110.80
1	A	501	PHE	N-CA-C	5.06	125.16	111.00
2	B	252	THR	N-CA-C	-5.01	105.48	112.45

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	3647	0	3715	272	0
2	B	3540	0	3589	258	0
All	All	7187	0	7304	507	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 36.

All (507) 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:202:LYS:HZ3	2:B:167:LYS:HD3	1.04	1.13
1:A:210:VAL:HG13	1:A:219:MET:HE1	1.31	1.11
2:B:19:ASN:HB3	2:B:39:LYS:HD3	1.39	0.98
1:A:202:LYS:NZ	2:B:167:LYS:HZ3	1.67	0.93
2:B:244:GLY:HA2	2:B:247:MET:HE2	1.51	0.92
1:A:373:ILE:HG22	1:A:374:LYS:H	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LYS:NZ	2:B:167:LYS:HD3	1.83	0.90
1:A:237:TYR:OH	1:A:274:MET:HB2	1.73	0.89
2:B:185:LEU:HD13	2:B:324:ILE:HG21	1.55	0.88
1:A:202:LYS:HZ3	2:B:167:LYS:CD	1.86	0.87
1:A:151:LEU:HA	1:A:423:GLN:HE22	1.37	0.87
1:A:39:ILE:HD11	1:A:277:LEU:HB3	1.58	0.86
1:A:352:ALA:HA	2:B:393:GLU:HG2	1.58	0.86
1:A:263:ASP:H	1:A:319:ILE:HB	1.41	0.85
1:A:457:TYR:HA	1:A:501:PHE:CZ	2.12	0.84
2:B:85:LEU:HD22	2:B:89:MET:HE1	1.58	0.83
2:B:152:GLY:H	2:B:157:ASN:HD21	1.26	0.83
1:A:158:ILE:HG21	1:A:343:ILE:HG12	1.62	0.82
1:A:336:ILE:HG23	1:A:342:GLN:HE22	1.46	0.81
1:A:437:THR:HG21	1:A:462:ARG:HH21	1.43	0.81
1:A:174:THR:HA	1:A:350:PHE:CZ	2.16	0.80
1:A:364:VAL:HG12	1:A:365:SER:H	1.44	0.80
1:A:495:GLN:HA	1:A:498:MET:HE2	1.64	0.79
1:A:237:TYR:CE2	1:A:271:TYR:HA	2.17	0.79
2:B:399:LYS:HA	2:B:402:GLN:HE21	1.48	0.79
1:A:42:ILE:HG21	1:A:45:LEU:HD12	1.65	0.78
2:B:101:PRO:HB2	2:B:126:THR:HG21	1.66	0.78
2:B:246:ARG:HH12	2:B:281:ALA:HB2	1.49	0.78
2:B:238:GLN:HE21	2:B:238:GLN:HA	1.48	0.77
1:A:152:ILE:H	1:A:423:GLN:NE2	1.83	0.77
2:B:36:PRO:HD2	2:B:39:LYS:HB2	1.65	0.76
1:A:351:ASN:HA	2:B:389:GLN:HE21	1.49	0.76
1:A:182:ASP:HA	1:A:185:LEU:HD12	1.68	0.76
2:B:251:LEU:HD21	2:B:309:LEU:HD22	1.66	0.76
1:A:202:LYS:HZ1	2:B:167:LYS:HZ3	1.33	0.76
1:A:440:THR:HG22	1:A:446:LEU:HG	1.67	0.75
1:A:195:VAL:HB	1:A:259:ILE:HG13	1.69	0.75
1:A:210:VAL:HG13	1:A:219:MET:CE	2.13	0.75
1:A:122:ILE:HD13	1:A:122:ILE:H	1.52	0.74
1:A:346:SER:HB3	1:A:359:ASN:HD21	1.53	0.74
1:A:135:PRO:HB2	1:A:140:ARG:HE	1.51	0.74
1:A:39:ILE:CD1	1:A:277:LEU:HB3	2.17	0.74
2:B:110:ILE:HB	2:B:119:ASP:HB3	1.71	0.73
2:B:35:PHE:HB3	2:B:36:PRO:HD2	1.69	0.73
2:B:171:PHE:HZ	2:B:342:THR:HB	1.53	0.72
2:B:435:PHE:HB2	2:B:438:ALA:HB3	1.71	0.71
2:B:243:PRO:HA	2:B:246:ARG:NH2	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:THR:HA	1:A:350:PHE:HZ	1.52	0.71
2:B:86:THR:H	2:B:89:MET:HE2	1.54	0.71
2:B:310:GLN:HE22	2:B:325:GLN:HE22	1.38	0.70
2:B:216:MET:HE1	2:B:232:VAL:HG21	1.73	0.70
1:A:262:ASP:HA	1:A:319:ILE:HD12	1.71	0.70
2:B:275:ILE:O	2:B:278:PHE:HB3	1.92	0.69
1:A:174:THR:HG23	1:A:350:PHE:CZ	2.26	0.69
2:B:132:ILE:HA	2:B:255:THR:OG1	1.93	0.69
2:B:121:LEU:O	2:B:122:ARG:HB2	1.92	0.68
2:B:394:THR:HG22	2:B:424:ALA:HB2	1.75	0.68
2:B:306:MET:HE1	2:B:342:THR:OG1	1.94	0.68
1:A:39:ILE:HD11	1:A:277:LEU:HD13	1.75	0.68
1:A:37:ASP:CG	2:B:291:ARG:HE	2.01	0.68
2:B:425:ARG:HD3	2:B:471:GLU:OE2	1.94	0.68
2:B:43:ILE:HG22	2:B:44:TYR:CD1	2.28	0.68
1:A:78:GLY:HA2	1:A:232:PRO:HG3	1.75	0.67
1:A:461:LEU:HD22	1:A:497:GLN:HB3	1.76	0.67
1:A:167:LEU:H	1:A:339:THR:HG21	1.60	0.67
2:B:247:MET:SD	2:B:282:GLY:HA2	2.34	0.67
1:A:100:VAL:HA	1:A:104:TYR:HE1	1.58	0.67
2:B:302:LEU:O	2:B:302:LEU:HD23	1.94	0.67
1:A:109:ILE:HG12	1:A:113:ALA:HA	1.76	0.67
1:A:166:GLU:O	1:A:317:LEU:HA	1.93	0.67
1:A:75:VAL:HG11	1:A:274:MET:SD	2.35	0.66
1:A:369:SER:HB2	1:A:377:LYS:HE2	1.78	0.66
2:B:246:ARG:NH1	2:B:281:ALA:HB2	2.10	0.65
2:B:343:PHE:HA	2:B:346:LEU:HD12	1.79	0.65
2:B:203:GLY:O	2:B:277:ARG:HG3	1.97	0.65
1:A:174:THR:HG23	1:A:350:PHE:HZ	1.60	0.65
2:B:197:SER:OG	2:B:269:LEU:HB2	1.97	0.65
1:A:40:ALA:HB2	1:A:76:LEU:HD21	1.80	0.64
2:B:429:ARG:HE	2:B:472:GLN:HE22	1.45	0.64
2:B:423:ARG:O	2:B:427:ILE:HG13	1.97	0.64
1:A:445:TYR:HB3	1:A:498:MET:SD	2.37	0.64
2:B:155:VAL:HG22	2:B:431:LEU:HD22	1.77	0.64
1:A:336:ILE:HG23	1:A:342:GLN:NE2	2.12	0.64
1:A:349:LEU:O	1:A:354:ILE:HB	1.98	0.64
2:B:103:GLY:HA2	2:B:259:TYR:CE2	2.32	0.64
1:A:422:LYS:NZ	1:A:455:ARG:HH21	1.96	0.63
1:A:376:MET:SD	1:A:435:VAL:HG22	2.38	0.63
1:A:187:GLN:HE22	1:A:258:LEU:HD23	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LYS:HZ3	2:B:167:LYS:HZ3	1.45	0.63
1:A:167:LEU:HD22	1:A:335:VAL:HG12	1.80	0.63
1:A:249:TYR:O	1:A:253:ARG:HG3	1.98	0.63
2:B:243:PRO:O	2:B:247:MET:HG3	1.99	0.63
1:A:135:PRO:HB2	1:A:140:ARG:NE	2.13	0.62
2:B:151:THR:HG22	2:B:189:ILE:HD11	1.80	0.62
2:B:48:ILE:HG13	2:B:62:THR:HG23	1.80	0.62
2:B:134:ARG:H	2:B:312:ARG:NH1	1.96	0.62
2:B:310:GLN:HE21	2:B:313:ILE:HD12	1.63	0.62
2:B:158:LEU:HD22	2:B:454:THR:HG22	1.81	0.62
2:B:299:GLN:H	2:B:299:GLN:NE2	1.98	0.62
1:A:437:THR:HG21	1:A:462:ARG:NH2	2.15	0.62
2:B:41:PRO:HB2	2:B:65:VAL:HG21	1.81	0.62
1:A:446:LEU:HA	1:A:449:LEU:HD12	1.82	0.61
2:B:285:VAL:O	2:B:289:LEU:HG	2.00	0.61
1:A:258:LEU:C	1:A:259:ILE:HD12	2.25	0.61
1:A:449:LEU:HD13	1:A:457:TYR:CE2	2.35	0.61
2:B:391:VAL:HG13	2:B:427:ILE:HG21	1.81	0.61
1:A:373:ILE:HG22	1:A:374:LYS:N	2.13	0.61
1:A:457:TYR:HA	1:A:501:PHE:CE2	2.36	0.61
2:B:41:PRO:HG2	2:B:74:VAL:HG11	1.81	0.61
2:B:101:PRO:HA	2:B:129:THR:HA	1.81	0.61
2:B:246:ARG:HB2	2:B:246:ARG:CZ	2.31	0.61
2:B:271:PHE:HE1	2:B:324:ILE:HD12	1.66	0.61
1:A:130:ILE:HG21	1:A:238:LEU:HD22	1.82	0.61
2:B:105:PRO:HG3	2:B:126:THR:HA	1.81	0.60
1:A:450:GLU:HB2	1:A:453:GLN:OE1	2.01	0.60
1:A:354:ILE:HG22	1:A:357:ALA:HA	1.82	0.60
1:A:58:GLU:CD	1:A:82:MET:HB3	2.26	0.60
2:B:389:GLN:O	2:B:393:GLU:HG3	2.02	0.60
1:A:216:ARG:NH2	1:A:426:SER:HB2	2.17	0.59
1:A:340:ASP:HA	1:A:366:ARG:HD2	1.85	0.59
2:B:124:VAL:HG12	2:B:126:THR:HG23	1.83	0.59
2:B:274:ASN:H	2:B:326:ALA:HB3	1.67	0.59
1:A:156:ALA:O	1:A:380:ALA:HB1	2.03	0.59
1:A:187:GLN:OE1	1:A:192:VAL:HB	2.03	0.59
1:A:430:THR:HB	1:A:433:GLU:HG3	1.84	0.59
2:B:179:THR:O	2:B:183:MET:HG2	2.02	0.59
2:B:183:MET:SD	2:B:212:LEU:HD13	2.42	0.59
1:A:98:ILE:HD13	1:A:130:ILE:HG13	1.83	0.59
2:B:183:MET:HE1	2:B:212:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:VAL:HG12	2:B:197:SER:N	2.17	0.59
2:B:203:GLY:HA3	2:B:277:ARG:HB3	1.84	0.59
2:B:240:ASN:HD22	2:B:241:GLU:H	1.51	0.59
2:B:105:PRO:HG2	2:B:126:THR:HG22	1.84	0.58
2:B:19:ASN:O	2:B:92:ILE:HA	2.02	0.58
2:B:113:VAL:HG22	2:B:249:VAL:HG12	1.84	0.58
2:B:237:GLY:HA3	2:B:249:VAL:HG11	1.85	0.58
2:B:148:ILE:HA	2:B:374:MET:HE1	1.86	0.58
2:B:246:ARG:NH1	2:B:246:ARG:HB2	2.18	0.58
2:B:146:LEU:HD13	2:B:163:ARG:NH2	2.18	0.58
1:A:257:THR:HB	1:A:314:MET:HG3	1.84	0.58
2:B:204:GLU:O	2:B:239:MET:HG3	2.03	0.58
1:A:461:LEU:CD2	1:A:497:GLN:HB3	2.33	0.57
2:B:179:THR:O	2:B:182:ILE:HG22	2.03	0.57
1:A:34:GLN:HG3	1:A:41:ARG:HB2	1.86	0.57
1:A:440:THR:HG23	1:A:494:ILE:HG21	1.85	0.57
2:B:104:GLY:N	2:B:105:PRO:HD2	2.19	0.57
2:B:162:TYR:CZ	2:B:168:ILE:HG21	2.39	0.57
2:B:395:LEU:HD21	2:B:428:GLU:HG2	1.85	0.57
2:B:299:GLN:HE21	2:B:299:GLN:N	2.01	0.57
2:B:310:GLN:HE22	2:B:325:GLN:NE2	2.02	0.57
1:A:100:VAL:HA	1:A:104:TYR:CE1	2.40	0.57
1:A:433:GLU:OE2	1:A:466:LYS:HE2	2.05	0.57
1:A:293:TYR:CD1	1:A:293:TYR:N	2.72	0.57
2:B:30:VAL:HG23	2:B:288:LEU:HD13	1.87	0.57
2:B:131:PRO:HD2	2:B:134:ARG:HH21	1.70	0.57
2:B:201:GLY:O	2:B:249:VAL:HG21	2.05	0.57
2:B:466:LEU:HB3	2:B:469:LEU:HD12	1.86	0.57
2:B:222:ILE:HG22	2:B:223:ASN:H	1.69	0.56
1:A:434:GLN:O	1:A:438:ILE:HG12	2.05	0.56
1:A:152:ILE:H	1:A:423:GLN:HE22	1.53	0.56
2:B:419:LEU:O	2:B:423:ARG:HG3	2.05	0.56
1:A:166:GLU:HB3	1:A:317:LEU:HD23	1.87	0.56
1:A:233:ALA:C	1:A:237:TYR:HE1	2.13	0.56
2:B:122:ARG:HB3	2:B:123:PRO:HD2	1.86	0.56
2:B:171:PHE:CZ	2:B:342:THR:HB	2.39	0.56
2:B:199:PHE:HB3	2:B:234:LEU:HD23	1.87	0.56
1:A:216:ARG:NH1	1:A:426:SER:HB2	2.21	0.56
1:A:258:LEU:HD12	1:A:315:THR:O	2.05	0.56
1:A:259:ILE:HD13	1:A:314:MET:CG	2.36	0.56
2:B:310:GLN:HA	2:B:313:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:PHE:O	1:A:476:ILE:HG12	2.06	0.56
2:B:102:VAL:HG12	2:B:256:MET:HG3	1.88	0.55
2:B:276:PHE:CD2	2:B:328:TYR:HB3	2.41	0.55
2:B:207:ARG:HB3	2:B:207:ARG:NH1	2.21	0.55
1:A:259:ILE:HD12	1:A:259:ILE:N	2.22	0.55
1:A:45:LEU:HB3	1:A:48:VAL:HG13	1.88	0.55
1:A:216:ARG:HH22	1:A:426:SER:HB2	1.71	0.55
2:B:113:VAL:HG13	2:B:249:VAL:HG12	1.89	0.55
1:A:287:TYR:HB3	1:A:291:VAL:HG21	1.89	0.54
1:A:187:GLN:HE22	1:A:258:LEU:CD2	2.21	0.54
1:A:247:ALA:HB1	1:A:259:ILE:HD11	1.88	0.54
1:A:276:LEU:HA	2:B:292:MET:CE	2.38	0.54
2:B:163:ARG:HE	2:B:374:MET:HB2	1.72	0.54
2:B:238:GLN:O	2:B:246:ARG:HD3	2.07	0.54
1:A:227:GLU:OE1	1:A:239:ALA:HB2	2.07	0.54
2:B:240:ASN:HD22	2:B:240:ASN:N	2.03	0.54
1:A:61:ILE:HG22	1:A:77:MET:SD	2.46	0.54
1:A:141:ARG:HG3	1:A:306:SER:HB3	1.88	0.54
2:B:163:ARG:HH21	2:B:374:MET:HG3	1.72	0.54
2:B:425:ARG:HH12	2:B:429:ARG:HH22	1.54	0.54
2:B:184:GLU:HG3	2:B:188:ASN:OD1	2.08	0.54
1:A:237:TYR:HE2	1:A:271:TYR:HA	1.68	0.54
1:A:405:LYS:HA	1:A:408:GLN:HB2	1.89	0.54
1:A:451:LEU:C	1:A:453:GLN:H	2.15	0.54
1:A:194:CYS:SG	1:A:258:LEU:HB3	2.48	0.54
1:A:233:ALA:O	1:A:237:TYR:CE1	2.61	0.54
1:A:259:ILE:HD13	1:A:314:MET:HG3	1.90	0.54
2:B:61:VAL:HG21	2:B:85:LEU:HD21	1.91	0.54
2:B:353:SER:HB3	2:B:356:LEU:HB2	1.89	0.54
1:A:346:SER:OG	1:A:349:LEU:HB2	2.08	0.53
1:A:30:GLY:O	1:A:89:VAL:HG23	2.08	0.53
1:A:110:ASN:HB2	1:A:114:LYS:O	2.08	0.53
1:A:431:VAL:O	1:A:435:VAL:HG23	2.08	0.53
1:A:420:LEU:HD22	1:A:458:LEU:HD11	1.89	0.53
2:B:376:GLN:O	2:B:380:VAL:HG22	2.08	0.53
1:A:302:ALA:HA	1:A:314:MET:HE2	1.90	0.53
1:A:429:LEU:HD11	1:A:462:ARG:CZ	2.39	0.53
2:B:68:LEU:HD23	2:B:74:VAL:HG12	1.91	0.53
1:A:162:ARG:HA	1:A:315:THR:OG1	2.08	0.53
1:A:422:LYS:HZ3	1:A:455:ARG:HH21	1.57	0.53
1:A:437:THR:HG23	1:A:458:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:LEU:HD21	2:B:196:VAL:HG13	1.91	0.52
2:B:147:SER:O	2:B:374:MET:HE1	2.09	0.52
1:A:167:LEU:N	1:A:339:THR:HG21	2.22	0.52
1:A:339:THR:HG22	1:A:340:ASP:N	2.24	0.52
2:B:43:ILE:HG22	2:B:44:TYR:HD1	1.71	0.52
2:B:222:ILE:HG22	2:B:223:ASN:N	2.24	0.52
2:B:121:LEU:O	2:B:122:ARG:CB	2.57	0.52
1:A:200:GLY:HA3	1:A:266:LYS:HD3	1.91	0.52
1:A:234:THR:O	1:A:234:THR:HG22	2.10	0.52
2:B:260:PHE:HB2	2:B:268:VAL:HG21	1.92	0.52
1:A:210:VAL:O	1:A:214:GLN:HG3	2.10	0.52
2:B:149:PHE:HB3	2:B:162:TYR:HB2	1.91	0.52
1:A:37:ASP:O	1:A:39:ILE:HD12	2.10	0.52
1:A:494:ILE:O	1:A:498:MET:HG3	2.10	0.52
2:B:466:LEU:HD13	2:B:480:ILE:HD11	1.91	0.52
1:A:39:ILE:HD12	1:A:39:ILE:N	2.25	0.52
1:A:199:ILE:N	1:A:199:ILE:HD12	2.24	0.52
1:A:419:GLU:OE2	1:A:451:LEU:HB3	2.10	0.52
1:A:138:MET:C	1:A:140:ARG:H	2.17	0.52
1:A:197:VAL:HA	1:A:225:VAL:O	2.10	0.51
1:A:241:TYR:HE1	1:A:267:GLN:HE22	1.58	0.51
1:A:239:ALA:HB3	1:A:240:PRO:CD	2.40	0.51
2:B:163:ARG:HE	2:B:374:MET:CB	2.23	0.51
2:B:429:ARG:HD2	2:B:471:GLU:HB3	1.91	0.51
1:A:42:ILE:HG13	1:A:89:VAL:HG21	1.93	0.51
1:A:417:LEU:O	1:A:421:LEU:HG	2.10	0.51
2:B:278:PHE:CZ	2:B:309:LEU:HD12	2.45	0.51
1:A:219:MET:O	1:A:219:MET:HG2	2.11	0.51
1:A:276:LEU:HD23	2:B:292:MET:HE3	1.91	0.51
2:B:473:ALA:O	2:B:477:VAL:HG11	2.10	0.51
2:B:33:VAL:HG13	2:B:91:VAL:HG21	1.93	0.51
2:B:69:LEU:CD1	2:B:75:ARG:HH21	2.24	0.51
2:B:118:VAL:HG12	2:B:118:VAL:O	2.10	0.51
1:A:188:GLN:HB2	1:A:191:ASN:HD22	1.75	0.51
1:A:95:ILE:HG12	1:A:95:ILE:O	2.10	0.51
1:A:100:VAL:O	1:A:101:SER:HB3	2.11	0.51
1:A:225:VAL:HG11	1:A:242:THR:HB	1.93	0.51
2:B:35:PHE:HB3	2:B:36:PRO:CD	2.40	0.51
2:B:195:GLY:O	2:B:231:LYS:HE2	2.11	0.51
2:B:299:GLN:H	2:B:299:GLN:HE21	1.57	0.51
1:A:166:GLU:O	1:A:318:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:TYR:HA	2:B:363:PRO:C	2.36	0.51
1:A:199:ILE:HG12	1:A:240:PRO:HD3	1.94	0.50
2:B:260:PHE:HD1	2:B:264:ASN:ND2	2.08	0.50
1:A:139:SER:HB2	1:A:309:LEU:HD11	1.93	0.50
2:B:275:ILE:HG22	2:B:327:VAL:HG22	1.93	0.50
2:B:286:SER:HA	2:B:291:ARG:NH1	2.26	0.50
1:A:279:ARG:HA	2:B:292:MET:HE2	1.92	0.50
1:A:471:GLU:O	1:A:475:ILE:HG12	2.11	0.50
1:A:216:ARG:CZ	1:A:426:SER:HB2	2.41	0.50
2:B:271:PHE:CE1	2:B:324:ILE:HD12	2.45	0.50
1:A:165:ARG:O	1:A:339:THR:HG23	2.11	0.50
1:A:400:ALA:HB1	1:A:403:LEU:HG	1.94	0.50
2:B:186:ILE:O	2:B:191:LYS:HG3	2.12	0.50
1:A:198:ALA:HA	1:A:262:ASP:HB2	1.94	0.50
1:A:233:ALA:O	1:A:235:LEU:N	2.44	0.50
2:B:207:ARG:C	2:B:209:GLY:H	2.20	0.50
2:B:387:ILE:HA	2:B:390:ARG:HD2	1.94	0.50
2:B:386:GLU:O	2:B:390:ARG:HG3	2.11	0.49
1:A:455:ARG:O	1:A:459:VAL:HG23	2.12	0.49
1:A:486:ALA:O	1:A:490:LEU:HB2	2.12	0.49
2:B:100:VAL:HG11	2:B:252:THR:HG23	1.93	0.49
1:A:216:ARG:HH12	1:A:426:SER:HB2	1.76	0.49
1:A:381:GLY:HA2	1:A:384:LYS:HD2	1.93	0.49
1:A:431:VAL:O	1:A:434:GLN:HB2	2.12	0.49
2:B:106:THR:HB	2:B:256:MET:HE3	1.93	0.49
1:A:173:GLN:HG3	2:B:371:THR:OG1	2.12	0.49
2:B:104:GLY:N	2:B:105:PRO:CD	2.76	0.49
2:B:106:THR:HA	2:B:111:PHE:HZ	1.78	0.49
2:B:301:THR:O	2:B:305:GLU:HG3	2.12	0.49
2:B:50:LYS:HG2	2:B:59:MET:HE1	1.94	0.49
2:B:251:LEU:CG	2:B:309:LEU:HD13	2.43	0.49
1:A:37:ASP:C	1:A:39:ILE:HD12	2.37	0.49
1:A:491:LYS:O	1:A:495:GLN:HB2	2.12	0.49
1:A:420:LEU:CD2	1:A:458:LEU:HD11	2.43	0.48
2:B:398:TYR:O	2:B:402:GLN:HG3	2.13	0.48
1:A:233:ALA:C	1:A:235:LEU:H	2.21	0.48
1:A:350:PHE:HB3	1:A:355:ARG:CZ	2.44	0.48
2:B:260:PHE:HD1	2:B:264:ASN:HD22	1.61	0.48
1:A:122:ILE:HD13	1:A:122:ILE:N	2.23	0.48
2:B:50:LYS:HG2	2:B:59:MET:CE	2.43	0.48
2:B:216:MET:SD	2:B:221:VAL:HG21	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:LEU:HD12	1:A:417:LEU:HD13	1.96	0.48
1:A:380:ALA:O	1:A:384:LYS:HG3	2.14	0.48
2:B:98:LEU:HD21	2:B:114:LEU:HD22	1.94	0.48
1:A:49:MET:HG3	1:A:52:GLU:OE1	2.13	0.48
2:B:397:ARG:O	2:B:401:LEU:HG	2.14	0.48
1:A:230:ASP:OD1	2:B:311:GLU:HG3	2.13	0.48
1:A:158:ILE:HD11	1:A:360:VAL:HG13	1.96	0.48
2:B:425:ARG:HH12	2:B:429:ARG:NH2	2.12	0.48
1:A:65:LEU:HD12	1:A:75:VAL:HG21	1.95	0.48
1:A:128:ARG:HH12	1:A:252:TYR:HE1	1.61	0.48
1:A:234:THR:HA	1:A:237:TYR:CE1	2.49	0.48
1:A:350:PHE:HB3	1:A:355:ARG:NH2	2.28	0.48
2:B:52:ARG:HG2	2:B:53:ASP:N	2.27	0.48
1:A:45:LEU:HB3	1:A:48:VAL:CG1	2.44	0.47
1:A:148:GLN:HE21	1:A:431:VAL:CG2	2.27	0.47
1:A:185:LEU:C	1:A:187:GLN:H	2.22	0.47
1:A:382:LYS:O	1:A:386:GLU:HG3	2.14	0.47
2:B:189:ILE:O	2:B:193:HIS:HB2	2.15	0.47
1:A:115:PRO:HD3	1:A:122:ILE:HD12	1.95	0.47
1:A:151:LEU:CA	1:A:423:GLN:HE22	2.20	0.47
1:A:159:PRO:HB3	1:A:372:GLN:HE21	1.79	0.47
1:A:383:LEU:CD1	1:A:417:LEU:HD13	2.43	0.47
2:B:251:LEU:HG	2:B:309:LEU:HD13	1.96	0.47
2:B:255:THR:HA	2:B:258:GLU:HG2	1.96	0.47
2:B:390:ARG:HA	2:B:393:GLU:OE1	2.13	0.47
2:B:96:ALA:HB1	2:B:97:PRO:HD2	1.96	0.47
2:B:182:ILE:O	2:B:186:ILE:HG13	2.13	0.47
2:B:302:LEU:HD23	2:B:302:LEU:C	2.38	0.47
2:B:240:ASN:N	2:B:240:ASN:ND2	2.58	0.47
2:B:327:VAL:HG21	2:B:342:THR:HG21	1.97	0.47
1:A:104:TYR:O	1:A:105:LEU:C	2.57	0.47
1:A:107:ARG:CZ	1:A:119:ARG:HB2	2.44	0.47
1:A:174:THR:HG22	1:A:174:THR:O	2.14	0.47
2:B:25:GLN:HB2	2:B:32:ASN:HB2	1.96	0.47
2:B:102:VAL:HG11	2:B:255:THR:HG22	1.96	0.47
2:B:138:ALA:HB3	2:B:141:GLN:HG3	1.95	0.47
2:B:148:ILE:HA	2:B:374:MET:CE	2.45	0.47
2:B:298:TYR:CD2	2:B:337:PRO:HB2	2.49	0.47
2:B:378:ARG:O	2:B:379:ILE:HD13	2.15	0.47
2:B:383:GLU:O	2:B:387:ILE:HD12	2.14	0.47
1:A:63:ILE:O	1:A:74:VAL:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:471:GLU:C	2:B:473:ALA:H	2.21	0.47
2:B:53:ASP:OD1	2:B:58:PRO:HG3	2.15	0.47
2:B:105:PRO:CG	2:B:126:THR:HA	2.45	0.47
2:B:238:GLN:HE21	2:B:238:GLN:CA	2.17	0.47
2:B:240:ASN:HD22	2:B:241:GLU:N	2.12	0.47
2:B:248:ARG:HG2	2:B:248:ARG:HH11	1.80	0.47
2:B:43:ILE:O	2:B:44:TYR:HB2	2.13	0.46
1:A:271:TYR:CE2	1:A:294:LEU:HD21	2.50	0.46
1:A:369:SER:O	1:A:372:GLN:HG3	2.15	0.46
2:B:99:SER:HB2	2:B:129:THR:HB	1.97	0.46
2:B:388:ALA:O	2:B:392:LYS:HG3	2.15	0.46
2:B:42:ASN:HB2	2:B:45:ASN:OD1	2.15	0.46
2:B:270:LEU:HD23	2:B:313:ILE:HG23	1.98	0.46
1:A:106:GLY:HA2	1:A:219:MET:HG2	1.97	0.46
2:B:103:GLY:C	2:B:105:PRO:HD2	2.40	0.46
1:A:390:PHE:O	1:A:394:GLU:HG3	2.15	0.46
1:A:469:LYS:HB3	1:A:472:PHE:CD1	2.51	0.46
2:B:23:ILE:HD12	2:B:31:LEU:HD13	1.97	0.46
2:B:278:PHE:HE2	2:B:306:MET:HA	1.81	0.46
1:A:84:GLN:OE1	2:B:40:MET:HE3	2.15	0.46
1:A:152:ILE:HG23	1:A:438:ILE:HD11	1.96	0.46
1:A:237:TYR:CZ	1:A:274:MET:HB2	2.49	0.46
1:A:263:ASP:HA	1:A:319:ILE:O	2.16	0.46
1:A:66:ASN:HD22	1:A:68:GLU:CD	2.22	0.46
1:A:233:ALA:O	1:A:237:TYR:CD1	2.69	0.46
1:A:386:GLU:OE2	1:A:442:THR:HG23	2.16	0.46
2:B:68:LEU:O	2:B:70:GLY:N	2.49	0.46
1:A:108:VAL:HA	1:A:224:VAL:HB	1.97	0.46
2:B:169:GLY:HA3	2:B:346:LEU:HD13	1.98	0.46
2:B:336:ASP:OD2	2:B:337:PRO:HD2	2.16	0.46
2:B:477:VAL:HG21	2:B:483:ALA:HB2	1.99	0.46
2:B:85:LEU:CD2	2:B:89:MET:HE1	2.38	0.45
2:B:167:LYS:HZ1	2:B:310:GLN:CD	2.24	0.45
1:A:115:PRO:HG3	1:A:120:GLY:O	2.17	0.45
2:B:429:ARG:HE	2:B:472:GLN:NE2	2.13	0.45
1:A:139:SER:HB2	1:A:309:LEU:CD1	2.46	0.45
1:A:210:VAL:HG22	1:A:224:VAL:HG21	1.99	0.45
2:B:82:THR:HB	2:B:85:LEU:HD12	1.98	0.45
1:A:444:GLY:HA2	1:A:447:ASP:CG	2.42	0.45
2:B:107:LEU:HD21	2:B:196:VAL:CG1	2.47	0.45
2:B:176:VAL:HG23	2:B:352:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:GLY:HA3	2:B:277:ARG:CB	2.46	0.45
1:A:105:LEU:HD22	1:A:221:TYR:HA	1.98	0.45
2:B:248:ARG:HG2	2:B:248:ARG:NH1	2.31	0.45
2:B:298:TYR:HB3	2:B:302:LEU:HD12	1.98	0.45
1:A:67:LEU:HD23	1:A:72:VAL:HG13	1.99	0.45
1:A:152:ILE:HG22	1:A:421:LEU:HD23	1.99	0.45
1:A:310:GLY:O	1:A:311:GLU:HB2	2.17	0.45
1:A:466:LYS:HA	1:A:473:GLN:OE1	2.17	0.45
2:B:149:PHE:HB2	2:B:162:TYR:O	2.17	0.45
1:A:209:VAL:HG12	1:A:210:VAL:N	2.30	0.45
2:B:298:TYR:HE2	2:B:336:ASP:OD2	2.00	0.45
2:B:19:ASN:O	2:B:92:ILE:HG13	2.17	0.45
1:A:139:SER:O	1:A:305:LEU:HA	2.17	0.44
1:A:154:ILE:HD12	1:A:154:ILE:N	2.32	0.44
1:A:237:TYR:O	1:A:240:PRO:HD2	2.17	0.44
1:A:470:PRO:O	1:A:474:GLU:HG3	2.17	0.44
2:B:199:PHE:HB3	2:B:234:LEU:CD2	2.47	0.44
1:A:152:ILE:CG2	1:A:438:ILE:HD11	2.48	0.44
1:A:351:ASN:HB3	2:B:392:LYS:HB2	1.99	0.44
2:B:106:THR:HA	2:B:111:PHE:CZ	2.53	0.44
2:B:86:THR:HG22	2:B:87:ARG:N	2.31	0.44
1:A:39:ILE:HD11	1:A:277:LEU:CB	2.36	0.44
2:B:438:ALA:C	2:B:440:VAL:H	2.25	0.44
1:A:203:ALA:HB1	2:B:142:LEU:HD11	2.00	0.44
1:A:248:GLU:HG2	1:A:251:MET:CE	2.48	0.44
1:A:254:GLU:HG2	1:A:310:GLY:HA3	1.99	0.44
2:B:204:GLU:O	2:B:238:GLN:NE2	2.51	0.43
1:A:122:ILE:HG12	1:A:122:ILE:O	2.18	0.43
1:A:235:LEU:C	1:A:237:TYR:H	2.26	0.43
2:B:170:LEU:HD11	2:B:324:ILE:HG22	2.00	0.43
1:A:202:LYS:HZ3	2:B:167:LYS:NZ	2.13	0.43
1:A:451:LEU:O	1:A:453:GLN:N	2.49	0.43
1:A:130:ILE:HG23	1:A:241:TYR:HB3	2.00	0.43
1:A:483:THR:HG22	1:A:484:GLU:N	2.33	0.43
2:B:33:VAL:O	2:B:73:ARG:HG3	2.18	0.43
2:B:20:LEU:HA	2:B:91:VAL:O	2.18	0.43
2:B:187:ASN:C	2:B:187:ASN:HD22	2.25	0.43
2:B:202:VAL:HG22	2:B:249:VAL:HG23	2.00	0.43
2:B:243:PRO:C	2:B:245:ALA:H	2.26	0.43
1:A:63:ILE:HG22	1:A:64:ALA:N	2.33	0.43
1:A:109:ILE:HD11	1:A:113:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLY:O	1:A:179:VAL:HG23	2.18	0.43
2:B:207:ARG:C	2:B:209:GLY:N	2.75	0.43
1:A:97:GLN:HG2	1:A:129:LEU:HD23	1.99	0.43
1:A:111:ALA:HB2	1:A:227:GLU:CD	2.44	0.43
1:A:245:ALA:O	1:A:248:GLU:N	2.52	0.43
2:B:103:GLY:HA2	2:B:259:TYR:CD2	2.54	0.43
1:A:33:LEU:HD11	1:A:43:HIS:HB2	2.01	0.43
2:B:245:ALA:O	2:B:249:VAL:HG13	2.19	0.43
1:A:107:ARG:NH2	1:A:115:PRO:HB3	2.35	0.42
1:A:154:ILE:C	1:A:156:ALA:H	2.27	0.42
1:A:230:ASP:OD1	2:B:311:GLU:HB2	2.19	0.42
2:B:268:VAL:HG12	2:B:269:LEU:N	2.34	0.42
2:B:429:ARG:HH11	2:B:429:ARG:HG3	1.84	0.42
1:A:98:ILE:O	1:A:98:ILE:HG22	2.20	0.42
1:A:100:VAL:HG21	1:A:249:TYR:HB2	2.01	0.42
1:A:457:TYR:HA	1:A:501:PHE:HZ	1.75	0.42
2:B:167:LYS:NZ	2:B:310:GLN:CD	2.77	0.42
2:B:209:GLY:HA2	2:B:236:TYR:OH	2.19	0.42
2:B:264:ASN:HB2	2:B:266:GLN:HG3	2.00	0.42
2:B:396:GLN:O	2:B:400:GLU:HG3	2.19	0.42
1:A:305:LEU:HD22	1:A:309:LEU:CD1	2.50	0.42
2:B:25:GLN:CB	2:B:32:ASN:HD22	2.33	0.42
2:B:260:PHE:HA	2:B:264:ASN:HD22	1.84	0.42
1:A:56:PHE:HD2	1:A:60:THR:HB	1.84	0.42
1:A:61:ILE:HG22	1:A:62:GLY:N	2.35	0.42
1:A:158:ILE:O	1:A:158:ILE:HG22	2.19	0.42
1:A:272:ARG:HD2	1:A:286:ALA:HB3	2.01	0.42
2:B:308:SER:C	2:B:309:LEU:HD23	2.44	0.42
2:B:68:LEU:CD2	2:B:74:VAL:HG12	2.49	0.42
1:A:415:GLN:HA	1:A:418:ARG:HD2	2.01	0.42
2:B:164:ARG:C	2:B:166:GLY:H	2.28	0.42
2:B:172:GLY:HA3	2:B:176:VAL:HG21	2.01	0.42
2:B:185:LEU:HD13	2:B:324:ILE:CG2	2.39	0.42
2:B:404:ILE:HG23	2:B:408:LEU:HD12	2.01	0.42
1:A:109:ILE:CG2	1:A:225:VAL:HG22	2.50	0.42
1:A:493:ALA:HB1	1:A:497:GLN:NE2	2.35	0.42
2:B:33:VAL:HG12	2:B:34:ALA:N	2.35	0.42
1:A:329:ALA:O	1:A:332:PRO:HD2	2.20	0.41
2:B:29:PRO:HG3	2:B:243:PRO:HG3	2.02	0.41
2:B:69:LEU:HD13	2:B:75:ARG:HH21	1.85	0.41
2:B:269:LEU:HD22	2:B:322:THR:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:ALA:O	2:B:337:PRO:HG2	2.20	0.41
2:B:410:LEU:O	2:B:413:LEU:HB2	2.20	0.41
1:A:164:GLN:O	1:A:315:THR:HG23	2.20	0.41
1:A:440:THR:HG23	1:A:494:ILE:CG2	2.50	0.41
2:B:196:VAL:CG1	2:B:197:SER:N	2.82	0.41
1:A:230:ASP:CG	2:B:308:SER:HA	2.45	0.41
2:B:64:GLU:CD	2:B:248:ARG:HE	2.28	0.41
2:B:196:VAL:HG23	2:B:266:GLN:OE1	2.20	0.41
1:A:109:ILE:CG1	1:A:113:ALA:HA	2.47	0.41
1:A:135:PRO:CB	1:A:140:ARG:HE	2.26	0.41
2:B:26:ILE:HG23	2:B:31:LEU:CD2	2.50	0.41
2:B:350:THR:HA	2:B:370:SER:OG	2.20	0.41
1:A:170:GLY:O	1:A:321:GLU:HA	2.21	0.41
1:A:81:LEU:HA	2:B:43:ILE:HB	2.03	0.41
1:A:305:LEU:HD22	1:A:309:LEU:HD12	2.03	0.41
1:A:381:GLY:O	1:A:384:LYS:HB2	2.21	0.41
1:A:415:GLN:O	1:A:419:GLU:HG3	2.20	0.41
1:A:193:ILE:HD11	1:A:255:ARG:HH11	1.86	0.41
1:A:329:ALA:C	1:A:332:PRO:HD2	2.46	0.41
1:A:440:THR:O	1:A:445:TYR:HB2	2.21	0.41
2:B:24:ALA:HB3	2:B:32:ASN:O	2.21	0.41
2:B:109:ARG:NE	2:B:119:ASP:OD2	2.52	0.41
2:B:251:LEU:HD21	2:B:309:LEU:HD13	2.03	0.41
2:B:310:GLN:HE21	2:B:313:ILE:CD1	2.32	0.41
1:A:271:TYR:CD2	1:A:294:LEU:HD11	2.55	0.41
1:A:419:GLU:HA	1:A:422:LYS:CD	2.51	0.41
2:B:186:ILE:HA	2:B:190:ALA:HB3	2.02	0.41
2:B:435:PHE:HB2	2:B:438:ALA:CB	2.47	0.41
1:A:45:LEU:O	1:A:48:VAL:HG22	2.20	0.40
1:A:37:ASP:O	1:A:277:LEU:HD13	2.22	0.40
1:A:39:ILE:HD11	1:A:277:LEU:CD1	2.47	0.40
1:A:209:VAL:C	1:A:211:THR:N	2.78	0.40
1:A:247:ALA:CB	1:A:259:ILE:HD11	2.50	0.40
1:A:276:LEU:HA	2:B:292:MET:HE2	2.03	0.40
1:A:430:THR:HG22	1:A:431:VAL:N	2.36	0.40
2:B:160:ALA:HB2	2:B:370:SER:O	2.21	0.40
2:B:298:TYR:HE2	2:B:337:PRO:HD2	1.85	0.40
1:A:136:GLY:O	1:A:140:ARG:HG3	2.21	0.40
1:A:194:CYS:O	1:A:222:THR:HA	2.21	0.40
2:B:163:ARG:HH21	2:B:374:MET:HA	1.87	0.40
1:A:61:ILE:N	1:A:61:ILE:HD12	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:THR:C	1:A:94:ARG:H	2.28	0.40
1:A:104:TYR:O	1:A:106:GLY:N	2.54	0.40
1:A:147:LEU:HG	1:A:162:ARG:HG2	2.03	0.40
1:A:109:ILE:HG21	1:A:225:VAL:HG22	2.04	0.40
1:A:149:THR:H	1:A:155:ASP:CG	2.28	0.40
1:A:228:THR:HG22	2:B:311:GLU:OE2	2.22	0.40
1:A:339:THR:CG2	1:A:340:ASP:N	2.84	0.40
1:A:375:ALA:HB2	1:A:480:LYS:O	2.21	0.40
2:B:366:ASP:OD1	2:B:368:LEU:HB2	2.22	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	475/507 (94%)	372 (78%)	86 (18%)	17 (4%)	2	19
2	B	465/498 (93%)	380 (82%)	68 (15%)	17 (4%)	2	18
All	All	940/1005 (94%)	752 (80%)	154 (16%)	34 (4%)	2	19

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	234	THR
1	A	447	ASP
1	A	85	GLU
1	A	186	ASN
1	A	448	SER
1	A	454	VAL
2	B	54	THR
2	B	69	LEU

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Mol	Chain	Res	Type
2	B	154	LYS
2	B	286	SER
1	A	139	SER
1	A	288	PRO
1	A	452	ASP
2	B	297	GLY
2	B	310	GLN
2	B	472	GLN
1	A	101	SER
1	A	136	GLY
1	A	155	ASP
1	A	263	ASP
1	A	352	ALA
2	B	52	ARG
2	B	55	ALA
2	B	364	ALA
2	B	451	LEU
1	A	330	TYR
2	B	274	ASN
2	B	122	ARG
2	B	156	VAL
1	A	373	ILE
2	B	58	PRO
2	B	175	GLY
2	B	161	PRO

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	388/414 (94%)	362 (93%)	26 (7%)	15	47
2	B	381/410 (93%)	350 (92%)	31 (8%)	11	39
All	All	769/824 (93%)	712 (93%)	57 (7%)	13	43

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	66	ASN
1	A	76	LEU
1	A	89	VAL
1	A	98	ILE
1	A	122	ILE
1	A	128	ARG
1	A	130	ILE
1	A	131	GLU
1	A	135	PRO
1	A	147	LEU
1	A	177	THR
1	A	182	ASP
1	A	191	ASN
1	A	209	VAL
1	A	227	GLU
1	A	228	THR
1	A	230	ASP
1	A	237	TYR
1	A	257	THR
1	A	291	VAL
1	A	333	THR
1	A	342	GLN
1	A	364	VAL
1	A	435	VAL
1	A	490	LEU
2	B	48	ILE
2	B	57	GLN
2	B	59	MET
2	B	71	ASN
2	B	94	THR
2	B	98	LEU
2	B	113	VAL
2	B	129	THR
2	B	140	THR
2	B	149	PHE
2	B	167	LYS
2	B	184	GLU
2	B	197	SER
2	B	206	THR
2	B	215	GLU
2	B	238	GLN
2	B	240	ASN

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Mol	Chain	Res	Type
2	B	268	VAL
2	B	274	ASN
2	B	288	LEU
2	B	299	GLN
2	B	306	MET
2	B	309	LEU
2	B	322	THR
2	B	325	GLN
2	B	342	THR
2	B	352	LEU
2	B	374	MET
2	B	395	LEU
2	B	416	GLU
2	B	417	ASP

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	43	HIS
1	A	70	ASN
1	A	187	GLN
1	A	208	GLN
1	A	267	GLN
1	A	273	GLN
1	A	295	HIS
1	A	415	GLN
1	A	423	GLN
1	A	425	GLN
1	A	434	GLN
1	A	443	ASN
2	B	19	ASN
2	B	57	GLN
2	B	66	GLN
2	B	187	ASN
2	B	238	GLN
2	B	240	ASN
2	B	264	ASN
2	B	299	GLN
2	B	310	GLN
2	B	325	GLN
2	B	389	GLN
2	B	396	GLN

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Mol	Chain	Res	Type
2	B	402	GLN
2	B	472	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.