



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:30 PM GMT

PDB ID : 1FX0
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

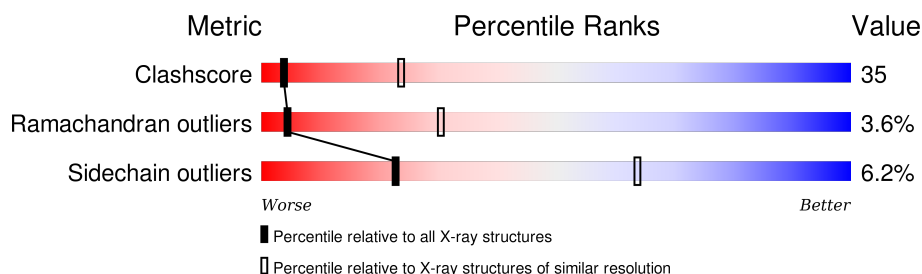
1 Overall quality at a glance

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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	507	
2	B	498	

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.

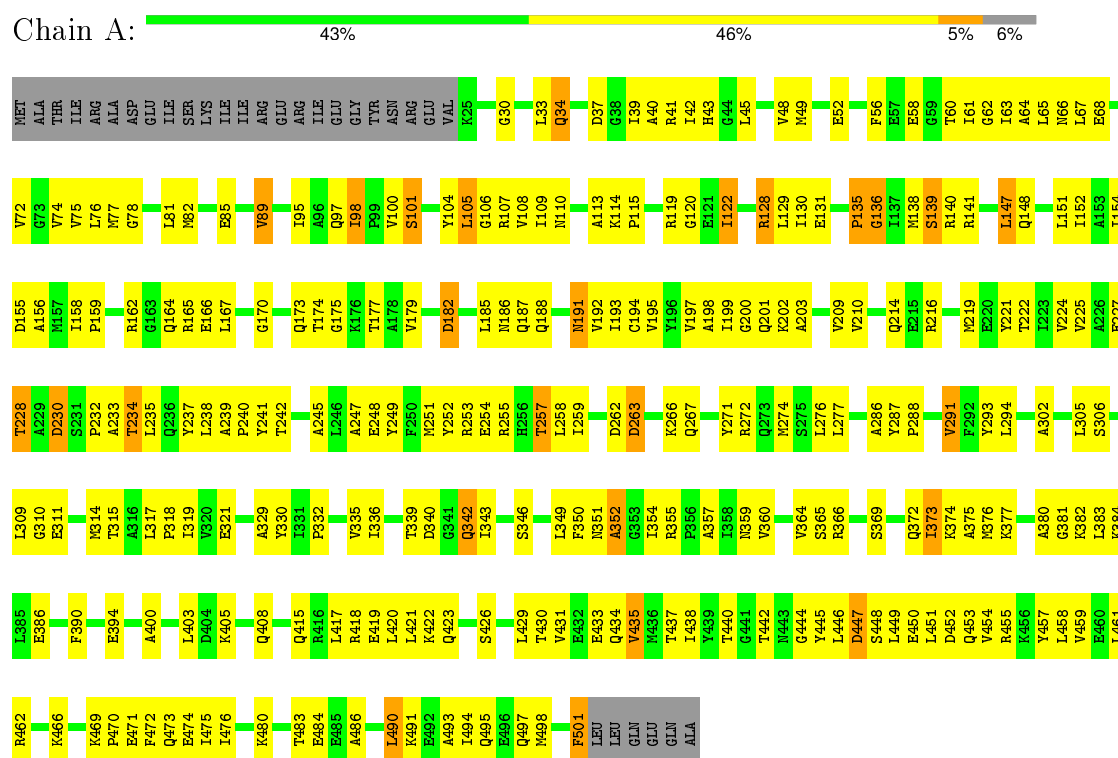
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	467	Total	C	N	O	S	89	0	0
			3540	2234	612	680	14			

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: ATP SYNTHASE ALPHA CHAIN



• Molecule 2: ATP SYNTHASE BETA CHAIN



V440	L368	G282	R207
L451	D369	G285	E208
T454	S370	S286	G209
L466	T371	A287	L212
L469	K374	L288	L215
P470	L375	L289	E216
E471	Q376	G290	R231
Q472	P377	R291	M232
A473	R378	M292	V221
V477	V380	A295	I222
I480	E383	V296	I223
D481	E386	G297	G231
P482	I387	Y298	V232
A483	A388	Q299	A233
A485	Q389	P300	L234
I484	R390	T301	V235
LYS	V391	L302	V236
ALA	R392	E305	G237
MET	E393	M306	Q238
ASN	T394	L309	M239
LEU	L395	Q310	N240
GLU	Q396	E311	E241
MET	R397	R312	P242
SER	Y398	I313	P243
LYS	R399	T322	G244
LEU	L401	R246	A245
LYS	Q402	S323	M247
LYS	P403	I324	R248
LYS	L404	Q325	V249
	L408	A326	G250
	G409	V327	L251
	L410	Y328	T252
	L413	D332	T255
	E416	D336	M256
	D417	P337	A257
	R418	T342	E258
	L419	F343	Y259
	R423	L346	F260
	A424		N264
	R425	Q266	E265
	V426	T267	Q266
	I427	V351	D267
	E428	L352	V268
	R429	S353	L269
	L431	L356	L270
	F435	Y362	F271
	A438	P363	N274
	E439	F276	I275
		A364	P277
		V365	R277
		D366	F278
		P367	A281

4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	147.70Å 147.70Å 385.05Å 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	0.32	1/3695 (0.0%)	0.63	1/5002 (0.0%)
2	B	0.31	0/3598	0.67	2/4883 (0.0%)
All	All	0.31	1/7293 (0.0%)	0.65	3/9885 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	501	PHE	CD2-CE2	-6.27	1.26	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	484	THR	N-CA-C	-5.46	96.26	111.00
2	B	50	LYS	N-CA-C	5.37	125.50	111.00
1	A	501	PHE	N-CA-C	5.24	125.16	111.00

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	262	0
2	B	3540	0	3589	247	0
All	All	7187	0	7304	490	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (490) 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	1.02	1.10
2:B:19:ASN:HB3	2:B:39:LYS:HD3	1.39	0.98
1:A:202:LYS:NZ	2:B:167:LYS:HZ2	1.67	0.93
1:A:202:LYS:HZ1	2:B:167:LYS:HZ2	0.95	0.93
1:A:373:ILE:HG22	1:A:374:LYS:H	1.35	0.91
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:210:VAL:HG13	1:A:219:MET:HE1	1.54	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: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: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
2:B:101:PRO:HB2	2:B:126:THR:HG21	1.66	0.78
1:A:42:ILE:HG21	1:A:45:LEU:HD12	1.65	0.78
1:A:210:VAL:HG13	1:A:219:MET:CE	2.13	0.78
2:B:246:ARG:HH12	2:B:281:ALA:HB2	1.49	0.78
2:B:238:GLN:HA	2:B:238:GLN:HE21	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: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:122:ILE:H	1:A:122:ILE:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:174:THR:HA	1:A:350:PHE:HZ	1.52	0.71
2:B:310:GLN:HE22	2:B:325:GLN:HE22	1.38	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
1:A:39:ILE:HD11	1:A:277:LEU:HD13	1.75	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
2:B:247:MET:SD	2:B:282:GLY:HA2	2.34	0.67
1:A:167:LEU:H	1:A:339:THR:HG21	1.60	0.67
1:A:100:VAL:HA	1:A:104:TYR:HE1	1.58	0.67
2:B:302:LEU:HD23	2:B:302:LEU:O	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
2:B:429:ARG:HE	2:B:472:GLN:HE22	1.45	0.64
1:A:40:ALA:HB2	1:A:76:LEU:HD21	1.80	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
2:B:103:GLY:HA2	2:B:259:TYR:CE2	2.32	0.64
1:A:349:LEU:O	1:A:354:ILE:HB	1.98	0.64
1:A:37:ASP:CG	2:B:291:ARG:HE	2.01	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:310:GLN:HE21	2:B:313:ILE:HD12	1.63	0.62
2:B:134:ARG:H	2:B:312:ARG:NH1	1.96	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: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:101:PRO:HA	2:B:129:THR:HA	1.81	0.61
2:B:41:PRO:HG2	2:B:74:VAL:HG11	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
2:B:389:GLN:O	2:B:393:GLU:HG3	2.02	0.60
2:B:124:VAL:HG12	2:B:126:THR:HG23	1.83	0.59
1:A:340:ASP:HA	1:A:366:ARG:HD2	1.85	0.59
2:B:274:ASN:H	2:B:326:ALA:HB3	1.67	0.59
1:A:216:ARG:NH2	1:A:426:SER:HB2	2.17	0.59
1:A:430:THR:HB	1:A:433:GLU:HG3	1.84	0.59
1:A:187:GLN:OE1	1:A:192:VAL:HB	2.03	0.59
1:A:156:ALA:O	1:A:380:ALA:HB1	2.03	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:196:VAL:HG12	2:B:197:SER:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:246:ARG:HB2	2:B:246:ARG:NH1	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: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
1:A:34:GLN:HG3	1:A:41:ARG:HB2	1.86	0.57
2:B:299:GLN:N	2:B:299:GLN:HE21	2.01	0.57
2:B:310:GLN:HE22	2:B:325:GLN:NE2	2.02	0.57
1:A:202:LYS:HZ3	2:B:167:LYS:CD	1.95	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
2:B:30:VAL:HG23	2:B:288:LEU:HD13	1.87	0.57
1:A:293:TYR:N	1:A:293:TYR:CD1	2.72	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
1:A:258:LEU:C	1:A:259:ILE:HD12	2.25	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:302:ALA:HA	1:A:314:MET:HE2	1.87	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
2:B:171:PHE:CZ	2:B:342:THR:HB	2.39	0.56
2:B:122:ARG:HB3	2:B:123:PRO:HD2	1.86	0.56
1:A:166:GLU:HB3	1:A:317:LEU:HD23	1.87	0.56
2:B:199:PHE:HB3	2:B:234:LEU:HD23	1.87	0.56
1:A:276:LEU:HA	2:B:292:MET:HE2	1.88	0.56
1:A:258:LEU:HD12	1:A:315:THR:O	2.05	0.56
1:A:216:ARG:NH1	1:A:426:SER:HB2	2.21	0.56
1:A:259:ILE:HD13	1:A:314:MET:CG	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:GLN:HA	2:B:313:ILE:HD12	1.87	0.56
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
1:A:58:GLU:CD	1:A:82:MET:HB3	2.26	0.55
2:B:207:ARG:HB3	2:B:207:ARG:NH1	2.21	0.55
1:A:259:ILE:N	1:A:259:ILE:HD12	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
2:B:238:GLN:O	2:B:246:ARG:HD3	2.07	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
2:B:163:ARG:HE	2:B:374:MET:HB2	1.72	0.54
1:A:276:LEU:HA	2:B:292:MET:CE	2.38	0.54
1:A:227:GLU:OE1	1:A:239:ALA:HB2	2.07	0.54
2:B:240:ASN:N	2:B:240:ASN:HD22	2.03	0.54
1:A:61:ILE:HG22	1:A:77:MET:SD	2.46	0.54
2:B:425:ARG:HH12	2:B:429:ARG:HH22	1.54	0.54
2:B:163:ARG:HH21	2:B:374:MET:HG3	1.72	0.54
1:A:141:ARG:HG3	1:A:306:SER:HB3	1.88	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:233:ALA:O	1:A:237:TYR:CE1	2.61	0.54
1:A:194:CYS:SG	1:A:258:LEU:HB3	2.48	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:431:VAL:O	1:A:435:VAL:HG23	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: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:429:LEU:HD11	1:A:462:ARG:CZ	2.39	0.53
2:B:247:MET:HE2	2:B:285:VAL:HG11	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:THR:HG23	1:A:458:LEU:HD22	1.91	0.52
2:B:107:LEU:HD21	2:B:196:VAL:HG13	1.91	0.52
2:B:43:ILE:HG22	2:B:44:TYR:HD1	1.71	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: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:234:THR:HG22	1:A:234:THR:O	2.10	0.52
2:B:260:PHE:HB2	2:B:268:VAL:HG21	1.92	0.52
1:A:200:GLY:HA3	1:A:266:LYS:HD3	1.91	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:199:ILE:N	1:A:199:ILE:HD12	2.24	0.52
1:A:39:ILE:HD12	1:A:39:ILE:N	2.25	0.52
1:A:419:GLU:OE2	1:A:451:LEU:HB3	2.10	0.52
2:B:240:ASN:N	2:B:240:ASN:ND2	2.58	0.52
1:A:233:ALA:C	1:A:237:TYR:HE1	2.13	0.51
1:A:197:VAL:HA	1:A:225:VAL:O	2.10	0.51
2:B:148:ILE:HA	2:B:374:MET:HE1	1.93	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:429:ARG:HD2	2:B:471:GLU:HB3	1.91	0.51
2:B:163:ARG:HE	2:B:374:MET:CB	2.23	0.51
1:A:417:LEU:O	1:A:421:LEU:HG	2.10	0.51
1:A:42:ILE:HG13	1:A:89:VAL:HG21	1.93	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
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:118:VAL:O	2:B:118:VAL:HG12	2.10	0.51
2:B:69:LEU:CD1	2:B:75:ARG:HH21	2.24	0.51
1:A:188:GLN:HB2	1:A:191:ASN:HD22	1.75	0.51
2:B:35:PHE:HB3	2:B:36:PRO:CD	2.40	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:299:GLN:H	2:B:299:GLN:HE21	1.57	0.51
2:B:195:GLY:O	2:B:231:LYS:HE2	2.11	0.51
1:A:95:ILE:O	1:A:95:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:O	1:A:318:PRO:HD2	2.11	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
2:B:286:SER:HA	2:B:291:ARG:NH1	2.26	0.50
2:B:275:ILE:HG22	2:B:327:VAL:HG22	1.93	0.50
2:B:50:LYS:HG2	2:B:59:MET:HE1	1.93	0.50
1:A:139:SER:HB2	1:A:309:LEU:HD11	1.93	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
2:B:186:ILE:O	2:B:191:LYS:HG3	2.12	0.50
1:A:400:ALA:HB1	1:A:403:LEU:HG	1.94	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: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:431:VAL:O	1:A:434:GLN:HB2	2.12	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
2:B:104:GLY:N	2:B:105:PRO:CD	2.76	0.49
1:A:173:GLN:HG3	2:B:371:THR:OG1	2.12	0.49
2:B:106:THR:HA	2:B:111:PHE:HZ	1.78	0.49
1:A:451:LEU:C	1:A:453:GLN:H	2.15	0.49
2:B:301:THR:O	2:B:305:GLU:HG3	2.12	0.49
2:B:251:LEU:CG	2:B:309:LEU:HD13	2.43	0.49
1:A:491:LYS:O	1:A:495:GLN:HB2	2.12	0.49
1:A:276:LEU:HD23	2:B:292:MET:HE3	1.95	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: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:N	1:A:122:ILE:HD13	2.23	0.48
2:B:147:SER:O	2:B:374:MET:HE1	2.13	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:LEU:HD21	2:B:114:LEU:HD22	1.94	0.48
2:B:244:GLY:HA2	2:B:247:MET:CE	2.44	0.48
2:B:397:ARG:O	2:B:401:LEU:HG	2.14	0.48
1:A:49:MET:HG3	1:A:52:GLU:OE1	2.13	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:234:THR:HA	1:A:237:TYR:CE1	2.49	0.48
1:A:65:LEU:HD12	1:A:75:VAL:HG21	1.95	0.48
2:B:216:MET:HE1	2:B:232:VAL:HG21	1.95	0.48
1:A:128:ARG:HH12	1:A:252:TYR:HE1	1.61	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:148:GLN:HE21	1:A:431:VAL:CG2	2.27	0.47
1:A:45:LEU:HB3	1:A:48:VAL:CG1	2.44	0.47
2:B:189:ILE:O	2:B:193:HIS:HB2	2.15	0.47
1:A:382:LYS:O	1:A:386:GLU:HG3	2.14	0.47
1:A:383:LEU:CD1	1:A:417:LEU:HD13	2.43	0.47
1:A:151:LEU:CA	1:A:423:GLN:HE22	2.20	0.47
2:B:251:LEU:HG	2:B:309:LEU:HD13	1.96	0.47
1:A:115:PRO:HD3	1:A:122:ILE:HD12	1.95	0.47
1:A:159:PRO:HB3	1:A:372:GLN:HE21	1.79	0.47
2:B:390:ARG:HA	2:B:393:GLU:OE1	2.13	0.47
2:B:255:THR:HA	2:B:258:GLU:HG2	1.96	0.47
2:B:182:ILE:O	2:B:186:ILE:HG13	2.13	0.47
2:B:96:ALA:HB1	2:B:97:PRO:HD2	1.96	0.47
2:B:327:VAL:HG21	2:B:342:THR:HG21	1.97	0.47
1:A:138:MET:C	1:A:140:ARG:H	2.17	0.47
2:B:383:GLU:O	2:B:387:ILE:HD12	2.14	0.47
1:A:174:THR:HG22	1:A:174:THR:O	2.14	0.47
1:A:107:ARG:CZ	1:A:119:ARG:HB2	2.44	0.47
2:B:102:VAL:HG11	2:B:255:THR:HG22	1.96	0.47
2:B:298:TYR:CD2	2:B:337:PRO:HB2	2.49	0.47
2:B:148:ILE:HA	2:B:374:MET:CE	2.45	0.47
2:B:378:ARG:O	2:B:379:ILE:HD13	2.15	0.47
2:B:138:ALA:HB3	2:B:141:GLN:HG3	1.95	0.47
2:B:25:GLN:HB2	2:B:32:ASN:HB2	1.96	0.47
1:A:63:ILE:O	1:A:74:VAL:HG13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:ASP:OD1	2:B:58:PRO:HG3	2.15	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
2:B:388:ALA:O	2:B:392:LYS:HG3	2.15	0.46
2:B:99:SER:HB2	2:B:129:THR:HB	1.97	0.46
1:A:369:SER:O	1:A:372:GLN:HG3	2.15	0.46
2:B:270:LEU:HD23	2:B:313:ILE:HG23	1.98	0.46
2:B:42:ASN:HB2	2:B:45:ASN:OD1	2.15	0.46
1:A:106:GLY:HA2	1:A:219:MET:HG2	1.97	0.46
2:B:278:PHE:HE2	2:B:306:MET:HA	1.81	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
1:A:390:PHE:O	1:A:394:GLU:HG3	2.15	0.46
1:A:237:TYR:CZ	1:A:274:MET:HB2	2.49	0.46
1:A:152:ILE:HG23	1:A:438:ILE:HD11	1.96	0.46
1:A:263:ASP:HA	1:A:319:ILE:O	2.16	0.46
1:A:233:ALA:O	1:A:237:TYR:CD1	2.69	0.46
2:B:68:LEU:O	2:B:70:GLY:N	2.49	0.46
1:A:386:GLU:OE2	1:A:442:THR:HG23	2.16	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
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
2:B:86:THR:HG22	2:B:87:ARG:N	2.31	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:139:SER:HB2	1:A:309:LEU:CD1	2.46	0.45
2:B:203:GLY:HA3	2:B:277:ARG:CB	2.46	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
1:A:105:LEU:HD22	1:A:221:TYR:HA	1.98	0.45
2:B:298:TYR:HB3	2:B:302:LEU:HD12	1.98	0.45
2:B:248:ARG:NH1	2:B:248:ARG:HG2	2.31	0.45
1:A:495:GLN:HA	1:A:498:MET:CE	2.46	0.45
2:B:86:THR:H	2:B:89:MET:CE	2.29	0.45
1:A:152:ILE:HG22	1:A:421:LEU:HD23	1.99	0.45
2:B:207:ARG:C	2:B:209:GLY:H	2.20	0.45
1:A:67:LEU:HD23	1:A:72:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:237:TYR:O	1:A:240:PRO:HD2	2.17	0.44
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
2:B:362:TYR:HA	2:B:363:PRO:C	2.36	0.44
2:B:199:PHE:HB3	2:B:234:LEU:CD2	2.47	0.44
1:A:470:PRO:O	1:A:474:GLU:HG3	2.17	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
1:A:39:ILE:HD11	1:A:277:LEU:CB	2.36	0.44
1:A:37:ASP:C	1:A:39:ILE:HD12	2.37	0.44
1:A:233:ALA:C	1:A:235:LEU:H	2.21	0.44
2:B:85:LEU:HD22	2:B:89:MET:HE1	2.00	0.44
1:A:254:GLU:HG2	1:A:310:GLY:HA3	1.99	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
2:B:204:GLU:O	2:B:238:GLN:NE2	2.51	0.43
2:B:170:LEU:HD11	2:B:324:ILE:HG22	2.00	0.43
1:A:122:ILE:O	1:A:122:ILE:HG12	2.18	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
2:B:33:VAL:O	2:B:73:ARG:HG3	2.18	0.43
1:A:483:THR:HG22	1:A:484:GLU:N	2.33	0.43
2:B:202:VAL:HG22	2:B:249:VAL:HG23	2.00	0.43
2:B:20:LEU:HA	2:B:91:VAL:O	2.18	0.43
1:A:109:ILE:HD11	1:A:113:ALA:HB1	2.00	0.43
1:A:63:ILE:HG22	1:A:64:ALA:N	2.33	0.43
1:A:175:GLY:O	1:A:179:VAL:HG23	2.18	0.43
1:A:97:GLN:HG2	1:A:129:LEU:HD23	1.99	0.43
1:A:202:LYS:NZ	2:B:167:LYS:NZ	2.52	0.43
2:B:103:GLY:HA2	2:B:259:TYR:CD2	2.54	0.43
1:A:185:LEU:C	1:A:187:GLN:H	2.22	0.43
1:A:245:ALA:O	1:A:248:GLU:N	2.52	0.43
2:B:245:ALA:O	2:B:249:VAL:HG13	2.19	0.43
1:A:33:LEU:HD11	1:A:43:HIS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:NH2	1:A:115:PRO:HB3	2.35	0.42
2:B:429:ARG:HG3	2:B:429:ARG:HH11	1.84	0.42
2:B:471:GLU:C	2:B:473:ALA:H	2.21	0.42
2:B:268:VAL:HG12	2:B:269:LEU:N	2.34	0.42
1:A:230:ASP:OD1	2:B:311:GLU:HB2	2.19	0.42
2:B:302:LEU:C	2:B:302:LEU:HD23	2.38	0.42
1:A:495:GLN:HA	1:A:498:MET:HE3	2.01	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:104:TYR:O	1:A:105:LEU:C	2.57	0.42
1:A:457:TYR:HA	1:A:501:PHE:HZ	1.75	0.42
2:B:264:ASN:HB2	2:B:266:GLN:HG3	2.00	0.42
2:B:209:GLY:HA2	2:B:236:TYR:OH	2.19	0.42
2:B:396:GLN:O	2:B:400:GLU:HG3	2.19	0.42
2:B:260:PHE:HA	2:B:264:ASN:HD22	1.84	0.42
2:B:85:LEU:HB3	2:B:89:MET:HE1	2.01	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
1:A:158:ILE:HG22	1:A:158:ILE:O	2.19	0.42
1:A:61:ILE:HG22	1:A:62:GLY:N	2.35	0.42
1:A:56:PHE:HD2	1:A:60:THR:HB	1.84	0.42
1:A:272:ARG:HD2	1:A:286:ALA:HB3	2.01	0.42
2:B:68:LEU:CD2	2:B:74:VAL:HG12	2.49	0.42
2:B:185:LEU:HD13	2:B:324:ILE:CG2	2.39	0.42
1:A:415:GLN:HA	1:A:418:ARG:HD2	2.01	0.42
2:B:172:GLY:HA3	2:B:176:VAL:HG21	2.01	0.42
2:B:404:ILE:HG23	2:B:408:LEU:HD12	2.01	0.42
1:A:493:ALA:HB1	1:A:497:GLN:NE2	2.35	0.42
1:A:109:ILE:CG2	1:A:225:VAL:HG22	2.50	0.42
2:B:33:VAL:HG12	2:B:34:ALA:N	2.35	0.42
2:B:29:PRO:HG3	2:B:243:PRO:HG3	2.02	0.41
2:B:269:LEU:HD22	2:B:322:THR:HB	2.01	0.41
2:B:69:LEU:HD13	2:B:75:ARG:HH21	1.85	0.41
1:A:329:ALA:O	1:A:332:PRO:HD2	2.20	0.41
2:B:103:GLY:C	2:B:105:PRO:HD2	2.40	0.41
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:440:THR:HG23	1:A:494:ILE:CG2	2.50	0.41
1:A:164:GLN:O	1:A:315:THR:HG23	2.20	0.41
2:B:196:VAL:CG1	2:B:197:SER:N	2.82	0.41
2:B:196:VAL:HG23	2:B:266:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PRO:CB	1:A:140:ARG:HE	2.26	0.41
1:A:109:ILE:CG1	1:A:113:ALA:HA	2.47	0.41
2:B:26:ILE:HG23	2:B:31:LEU:CD2	2.50	0.41
1:A:66:ASN:HD22	1:A:68:GLU:CD	2.22	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:381:GLY:O	1:A:384:LYS:HB2	2.21	0.41
1:A:305:LEU:HD22	1:A:309:LEU:HD12	2.03	0.41
1:A:415:GLN:O	1:A:419:GLU:HG3	2.20	0.41
1:A:440:THR:O	1:A:445:TYR:HB2	2.21	0.41
2:B:251:LEU:HD21	2:B:309:LEU:HD13	2.03	0.41
2:B:109:ARG:NE	2:B:119:ASP:OD2	2.52	0.41
2:B:310:GLN:HE21	2:B:313:ILE:CD1	2.32	0.41
2:B:163:ARG:HA	2:B:374:MET:HE1	2.02	0.41
2:B:24:ALA:HB3	2:B:32:ASN:O	2.21	0.41
1:A:193:ILE:HD11	1:A:255:ARG:HH11	1.86	0.41
1:A:271:TYR:CD2	1:A:294:LEU:HD11	2.55	0.41
2:B:435:PHE:HB2	2:B:438:ALA:CB	2.47	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
1:A:45:LEU:O	1:A:48:VAL:HG22	2.20	0.40
2:B:438:ALA:C	2:B:440:VAL:H	2.25	0.40
1:A:444:GLY:HA2	1:A:447:ASP:CG	2.42	0.40
1:A:430:THR:HG22	1:A:431:VAL:N	2.36	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:247:ALA:CB	1:A:259:ILE:HD11	2.50	0.40
2:B:298:TYR:HE2	2:B:337:PRO:HD2	1.85	0.40
2:B:160:ALA:HB2	2:B:370:SER:O	2.21	0.40
1:A:194:CYS:O	1:A:222:THR:HA	2.21	0.40
1:A:136:GLY:O	1:A:140:ARG:HG3	2.21	0.40
2:B:163:ARG:HH21	2:B:374:MET:HA	1.87	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:61:ILE:HD12	1:A:61:ILE:N	2.37	0.40
2:B:85:LEU:HD22	2:B:89:MET:CE	2.52	0.40
2:B:244:GLY:HA2	2:B:247:MET:HE2	2.04	0.40
1:A:339:THR:CG2	1:A:340:ASP:N	2.84	0.40
1:A:109:ILE:HG21	1:A:225:VAL:HG22	2.04	0.40
1:A:228:THR:HG22	2:B:311:GLU:OE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	4	30
2	B	465/498 (93%)	380 (82%)	68 (15%)	17 (4%)	4	29
All	All	940/1005 (94%)	752 (80%)	154 (16%)	34 (4%)	4	30

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
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

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Mol	Chain	Res	Type
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%)	369 (95%)	19 (5%)	31	72
2	B	381/410 (93%)	352 (92%)	29 (8%)	16	55
All	All	769/824 (93%)	721 (94%)	48 (6%)	23	64

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	89	VAL
1	A	98	ILE
1	A	122	ILE
1	A	128	ARG

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Mol	Chain	Res	Type
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	201	GLN
1	A	228	THR
1	A	230	ASP
1	A	257	THR
1	A	291	VAL
1	A	342	GLN
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	129	THR
2	B	140	THR
2	B	149	PHE
2	B	167	LYS
2	B	184	GLU
2	B	187	ASN
2	B	197	SER
2	B	215	GLU
2	B	238	GLN
2	B	240	ASN
2	B	274	ASN
2	B	288	LEU
2	B	299	GLN
2	B	322	THR
2	B	325	GLN
2	B	332	ASP
2	B	342	THR
2	B	352	LEU
2	B	374	MET
2	B	395	LEU
2	B	416	GLU
2	B	417	ASP

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Mol	Chain	Res	Type
2	B	481	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	267	GLN
1	A	273	GLN
1	A	295	HIS
1	A	359	ASN
1	A	423	GLN
1	A	443	ASN
1	A	473	GLN
2	B	19	ASN
2	B	67	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	345	HIS
2	B	389	GLN
2	B	396	GLN
2	B	402	GLN
2	B	472	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.