



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:56 AM GMT

PDB ID : 1FPM
Title : MONOVALENT CATION BINDING SITES IN N10-FORMYLTETRAHYDROFOLATESYNTHEASE FROM MOORELLA THERMOACETICA
Authors : Radfar, R.; Leapheart, A.; Brewer, J.M.; Minor, W.; Odom, J.D.
Deposited on : 2000-08-31
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

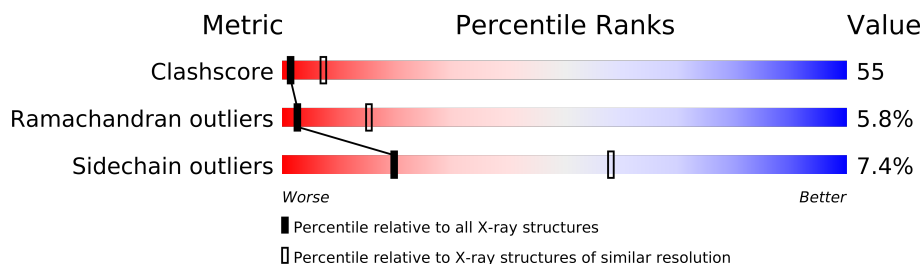
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	557	
1	B	557	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8585 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

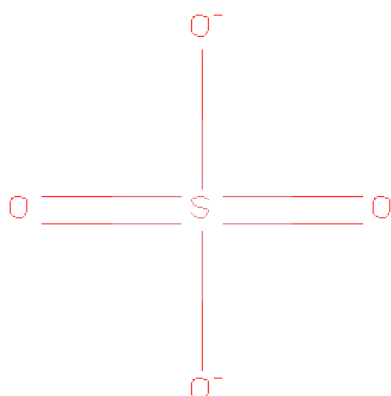
- Molecule 1 is a protein called FORMATE--TETRAHYDROFOLATELIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4133	2617	715	780	21			
1	B	548	Total	C	N	O	S	0	0	0
			4125	2613	714	777	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	DELETION	UNP P21164
A	?	-	VAL	DELETION	UNP P21164
B	?	-	GLU	DELETION	UNP P21164
B	?	-	VAL	DELETION	UNP P21164

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cs 1 1	0	0
3	A	1	Total Cs 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	200	Total O 200 200	0	0
4	B	70	Total O 70 70	0	0

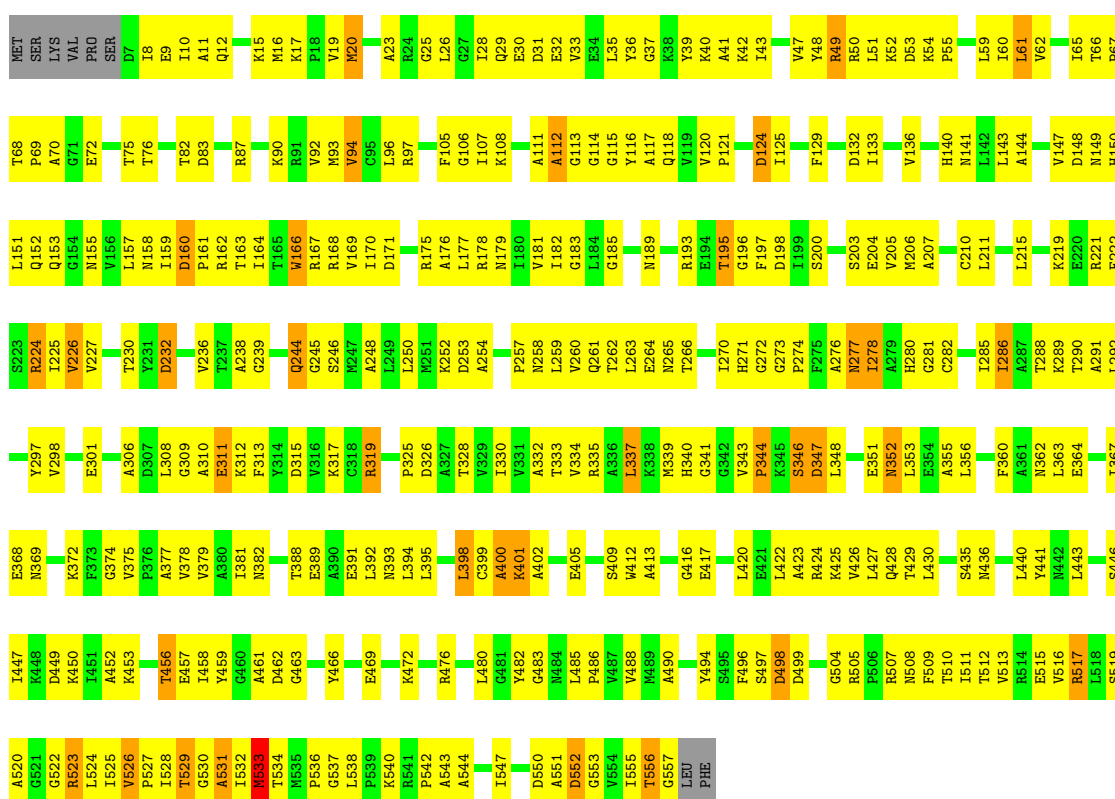
3 Residue-property plots

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.

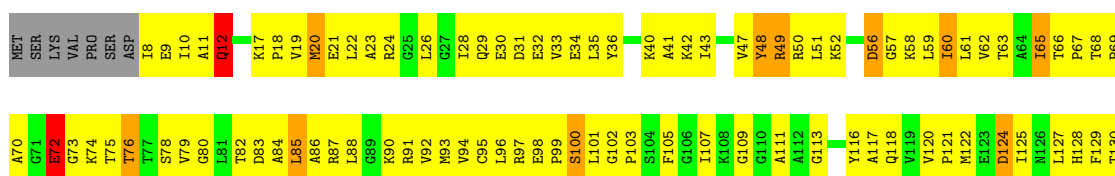
• Molecule 1: FORMATE--TETRAHYDROFOLATELIGASE

Chain A:



• Molecule 1: FORMATE--TETRAHYDROFOLATELIGASE

Chain B:



A520	I454	D387	P325	K265	F197	G131
G521	A455	T388	D326	T266	D198	D132
G522	T456	E389	A327	P267	I199	I133
R523	E457	T328	T328	A268	S200	H134
I524	I458	L392	I329	F269	V201	A135
I525	Y459	N393	I330	L270	A202	V136
V526	G460	L394	V331	H271	S203	
P527	A461	L395	A332	G272	E204	H140
I528	D462	L396	T333	G273	V205	N141
T529	G463	E397	V334	P274	M206	L142
		L398	R335	F275	A207	L143
	Y466	C399	A336	A276	C208	A144
I532		A400	L337	N277	L209	A145
M535	A470	K401	K338	I278	C210	H146
	D471	A402	M339	A279	L211	V147
L538	K472	G403	H340	H280	A212	D148
P539	A473	A404	G341	G281	N149	N149
K540	I474	E405	G342	C282	H150	H150
R541	G475		V343	N283	L151	L151
P542	R476	L408	P344	S284	Q152	Q152
A543	Y477	S409		I285	Q153	Q153
	E478	V412	D347	L286	G154	G154
I547	S479	A413	L348	A287	F221	F221
D548	L480	K414	A349	T288	S223	S223
I549	G481	G415	T350	K289	R224	L157
D550	Y482	G416	E351	T290	I225	N158
A551	G483	E417	N352	A291	I159	I159
D552	N484	G418	L353	L292	D160	D160
G553	G485	G419	E354	K293	T230	P161
V554	P486	L420	A355	L294	Y231	R162
I555	V487	E421	L356	A295	D232	T163
T556	V488	L422	R357	D296	V236	I164
G557	M489	A423	E358	I297	G239	T165
LEU	K490	R424	G359	V298	D240	W166
PHE	K491	K425	F360	V299	R167	R167
	T492	V426	A361	T300	R168	R168
	Q493		N362	E301	V169	V169
	Y494	T429	L363	A302		
	S495	L430	E364	G303	L172	L172
	S497		K365	F304	N173	N173
	D498	R433	H366	G305	D174	D174
		S435	I367	A306	G245	G245
	G503	V436	E368	D307	S246	R175
	R504	F437	N369	L308	M247	A176
	R505	L440	I370	G309	A248	L177
	P506	Y441	F373	A310	L249	R178
	N507	N442	G374	E311	L250	
	F509	L443	V375	K312	M251	I182
T510	T510	D444	P376	V314	D253	G185
T511	L445		A377	D315	A254	G186
T512	S446	L446	V378	V316	I255	K187
V513	I447	T447	V379	K317	K256	A188
R514	K448	D449	A380	C318	P257	N189
E515	E515	D449	I381	N382	N258	G190
V516	V516	K450	N382	A321	L259	V191
R517	R517	I451	A383	F322	Q261	P192
L518	L518	A452	P384	F323	T262	R193
S519	S519	K453	T386	K324	L263	E194
					T195	T195
					E264	G196

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	160.88Å 160.88Å 256.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00	Depositor
% Data completeness (in resolution range)	84.0 (40.00-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.266 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8585	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CS, SO4

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	0.52	0/4201	0.72	0/5690
1	B	0.43	0/4193	0.67	0/5679
All	All	0.48	0/8394	0.70	0/11369

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4133	0	4219	382	0
1	B	4125	0	4215	545	1
2	A	35	0	0	10	0
2	B	20	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	200	0	0	27	0
4	B	70	0	0	14	1
All	All	8585	0	8434	927	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 55.

All (927) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:166:TRP:CZ3	1:B:225:ILE:HD11	1.30	1.59
1:A:166:TRP:CZ3	1:A:225:ILE:HD11	1.42	1.53
1:B:166:TRP:CH2	1:B:225:ILE:HD11	1.58	1.38
1:B:166:TRP:CH2	1:B:225:ILE:CD1	2.11	1.34
1:B:166:TRP:CZ3	1:B:225:ILE:CD1	2.10	1.33
1:A:166:TRP:CE3	1:A:225:ILE:HD11	1.64	1.31
1:A:166:TRP:CZ3	1:A:225:ILE:CD1	2.20	1.23
1:B:43:ILE:HD11	1:B:259:LEU:HD22	1.29	1.15
1:B:222:PHE:O	1:B:225:ILE:HG22	1.49	1.13
1:B:109:GLY:O	4:B:580:HOH:O	1.65	1.12
1:B:195:THR:HG22	1:B:196:GLY:H	1.02	1.12
1:A:20:MET:HE3	1:A:30:GLU:HG3	1.33	1.09
1:B:376:PRO:HD3	1:B:435:SER:HB3	1.32	1.07
1:B:523:ARG:H	1:B:523:ARG:NE	1.58	1.00
1:B:368:GLU:HG2	1:B:401:LYS:HE2	1.42	0.99
1:A:179:ASN:OD1	4:A:757:HOH:O	1.81	0.98
1:B:166:TRP:CH2	1:B:225:ILE:HD13	1.96	0.98
1:A:25:GLY:O	4:A:677:HOH:O	1.82	0.96
1:B:277:ASN:ND2	1:B:278:ILE:H	1.65	0.95
1:B:166:TRP:HH2	1:B:225:ILE:CD1	1.81	0.93
1:B:195:THR:HG22	1:B:196:GLY:N	1.83	0.92
1:B:93:MET:HG2	1:B:267:PRO:HB2	1.52	0.92
1:B:365:LYS:HE3	1:B:369:ASN:HD21	1.34	0.91
1:B:338:LYS:HG2	1:B:343:VAL:HG21	1.51	0.91
1:A:35:LEU:HD22	1:A:37:GLY:O	1.71	0.91
1:A:140:HIS:HD2	1:A:203:SER:OG	1.53	0.91
1:A:405:GLU:CD	1:A:422:LEU:HA	1.90	0.91
1:A:222:PHE:O	1:A:225:ILE:HG22	1.71	0.90
1:A:169:VAL:HG23	1:A:198:ASP:O	1.70	0.90
1:A:557:GLY:O	4:A:582:HOH:O	1.91	0.88
1:B:21:GLU:HA	1:B:24:ARG:HD2	1.54	0.88
1:A:257:PRO:HD3	1:A:286:ILE:HD11	1.56	0.86
1:B:447:ILE:HD11	1:B:483:GLY:HA2	1.54	0.86
1:B:517:ARG:HH22	1:B:532:ILE:HG13	1.41	0.86
1:B:555:ILE:O	1:B:556:THR:HB	1.74	0.86
1:A:485:LEU:HD13	1:A:523:ARG:HA	1.58	0.85
1:B:195:THR:CG2	1:B:196:GLY:H	1.85	0.85
1:A:9:GLU:HG2	1:A:115:GLY:H	1.42	0.85
1:B:490:ALA:HB2	1:B:525:ILE:HG22	1.59	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:363:LEU:O	1:B:367:ILE:HG12	1.75	0.85
1:B:185:GLY:HA3	1:B:189:ASN:HD22	1.42	0.84
1:B:265:ASN:HD22	1:B:265:ASN:N	1.76	0.83
1:A:47:VAL:HA	1:A:50:ARG:NH1	1.92	0.83
1:B:277:ASN:HD22	1:B:278:ILE:H	1.22	0.83
1:A:136:VAL:HG21	1:A:206:MET:HE2	1.58	0.83
1:A:277:ASN:HD22	1:A:277:ASN:H	1.26	0.83
1:B:48:TYR:HB2	1:B:290:THR:OG1	1.77	0.83
1:B:394:LEU:O	1:B:398:LEU:HD23	1.78	0.83
1:B:26:LEU:HD23	1:B:28:ILE:HD11	1.59	0.83
1:A:401:LYS:HB2	4:A:748:HOH:O	1.78	0.83
1:A:277:ASN:HD22	1:A:278:ILE:H	1.27	0.82
1:A:169:VAL:HG21	1:A:200:SER:HA	1.61	0.82
1:B:498:ASP:HB3	1:B:528:ILE:HG21	1.61	0.82
1:A:42:LYS:HE3	1:A:258:ASN:OD1	1.80	0.82
1:A:326:ASP:HA	1:A:435:SER:OG	1.80	0.81
1:B:357:ARG:O	1:B:360:PHE:HB3	1.81	0.81
1:B:210:CYS:SG	1:B:274:PRO:HD3	2.21	0.80
1:A:82:THR:HG21	1:A:94:VAL:HG22	1.62	0.80
1:B:33:VAL:HG13	1:B:41:ALA:HB1	1.64	0.80
1:B:40:LYS:HB2	1:B:40:LYS:HZ2	1.44	0.80
1:B:337:LEU:HD21	1:B:363:LEU:HB2	1.61	0.80
1:B:166:TRP:HZ3	1:B:225:ILE:HD11	1.00	0.79
1:B:376:PRO:HG3	1:B:433:ARG:HG2	1.64	0.79
1:A:372:LYS:HE2	4:A:728:HOH:O	1.81	0.79
1:A:447:ILE:HD11	1:A:483:GLY:HA2	1.62	0.79
1:B:557:GLY:HA3	4:B:574:HOH:O	1.81	0.79
1:A:17:LYS:H	1:A:261:GLN:NE2	1.81	0.78
1:B:550:ASP:C	1:B:552:ASP:H	1.85	0.78
1:A:66:THR:HB	1:A:340:HIS:NE2	1.99	0.78
1:A:175:ARG:HD3	2:A:563:SO4:O3	1.84	0.78
1:B:335:ARG:NH2	1:B:349:ALA:HA	1.99	0.77
1:B:286:ILE:HA	1:B:289:LYS:HG2	1.66	0.77
1:B:337:LEU:HD23	1:B:360:PHE:HA	1.65	0.77
1:A:417:GLU:HA	1:A:420:LEU:HD23	1.66	0.77
1:B:215:LEU:HD11	1:B:252:LYS:HA	1.67	0.76
1:B:334:VAL:HG13	1:B:356:LEU:HD21	1.66	0.76
1:A:488:VAL:CG2	1:A:523:ARG:HD3	2.15	0.76
1:B:477:TYR:HE2	1:B:516:VAL:HG12	1.51	0.76
1:B:489:MET:CE	1:B:526:VAL:HG11	2.14	0.76
1:A:210:CYS:SG	1:A:274:PRO:HD3	2.26	0.76
1:B:74:LYS:HB2	1:B:74:LYS:NZ	2.00	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:261:GLN:HB2	1:B:265:ASN:HA	1.69	0.75
1:A:105:PHE:HB3	1:A:544:ALA:HB2	1.66	0.75
1:B:488:VAL:CG2	1:B:523:ARG:HD3	2.17	0.75
1:A:92:VAL:HG23	1:A:297:TYR:O	1.86	0.75
1:B:516:VAL:HA	1:B:527:PRO:HD2	1.67	0.75
1:A:66:THR:HB	1:A:340:HIS:HE2	1.51	0.75
1:A:488:VAL:HG21	1:A:523:ARG:HD3	1.68	0.75
1:A:405:GLU:OE1	1:A:425:LYS:HB2	1.87	0.74
1:B:111:ALA:HB2	1:B:122:MET:SD	2.28	0.74
1:B:488:VAL:HG21	1:B:523:ARG:HD3	1.69	0.74
1:B:47:VAL:HG11	1:B:294:LEU:HD11	1.68	0.74
1:B:136:VAL:HG13	1:B:205:VAL:HG12	1.68	0.74
1:A:96:LEU:O	1:A:270:ILE:HA	1.88	0.74
1:A:498:ASP:HB3	1:A:528:ILE:HG21	1.69	0.74
1:A:486:PRO:O	1:A:523:ARG:HB2	1.86	0.74
1:B:43:ILE:CD1	1:B:259:LEU:HD22	2.15	0.74
1:B:98:GLU:HG2	1:B:99:PRO:HD2	1.70	0.74
1:B:451:ILE:HG12	1:B:489:MET:HE1	1.69	0.74
1:B:23:ALA:HA	1:B:28:ILE:HD12	1.69	0.73
1:A:333:THR:HG22	1:A:382:ASN:HB3	1.69	0.73
1:B:12:GLN:NE2	1:B:263:LEU:HD13	2.03	0.73
1:B:417:GLU:HA	1:B:420:LEU:HD23	1.71	0.73
1:B:61:LEU:HD12	1:B:300:THR:O	1.88	0.73
1:A:446:SER:HB3	1:A:449:ASP:HB2	1.71	0.73
1:B:515:GLU:HB3	1:B:527:PRO:HG2	1.69	0.72
1:A:533:MET:HB2	2:A:561:SO4:O2	1.89	0.72
1:A:488:VAL:HG21	1:A:523:ARG:HH11	1.55	0.72
1:A:530:GLY:C	1:A:532:ILE:H	1.92	0.72
1:B:83:ASP:OD2	1:B:262:THR:HG21	1.90	0.72
1:B:174:ASP:OD1	1:B:177:LEU:HG	1.88	0.72
1:B:376:PRO:HD3	1:B:435:SER:CB	2.15	0.72
1:B:405:GLU:OE1	1:B:421:GLU:HG2	1.89	0.72
1:A:169:VAL:CG2	1:A:200:SER:HA	2.20	0.71
1:A:17:LYS:H	1:A:261:GLN:HE21	1.37	0.71
1:B:144:ALA:HB1	1:B:168:ARG:HH21	1.54	0.71
1:B:449:ASP:O	1:B:452:ALA:HB3	1.90	0.71
1:B:277:ASN:ND2	1:B:278:ILE:N	2.36	0.71
1:A:382:ASN:OD1	2:A:565:SO4:O1	2.08	0.71
1:B:292:LEU:HD23	1:B:298:VAL:HG21	1.73	0.71
1:A:160:ASP:OD1	1:A:163:THR:HG23	1.89	0.71
1:B:285:ILE:N	4:B:611:HOH:O	2.22	0.71
1:A:516:VAL:HG22	1:A:526:VAL:HB	1.72	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:169:VAL:HG11	1:B:200:SER:HA	1.72	0.71
1:B:136:VAL:HG13	1:B:205:VAL:CG1	2.20	0.70
1:A:462:ASP:OD2	1:A:508:ASN:HA	1.91	0.70
1:B:169:VAL:CG1	1:B:200:SER:HA	2.21	0.70
1:B:543:ALA:O	1:B:547:ILE:HG13	1.90	0.70
1:A:257:PRO:HD3	1:A:286:ILE:CD1	2.21	0.70
1:B:173:ASN:HB2	1:B:538:LEU:HD23	1.72	0.70
1:B:472:LYS:HD3	1:B:476:ARG:NH2	2.07	0.70
1:B:75:THR:HB	1:B:113:GLY:HA2	1.73	0.70
1:B:286:ILE:HD12	1:B:287:ALA:N	2.07	0.70
1:A:405:GLU:OE1	1:A:422:LEU:HA	1.92	0.70
1:A:82:THR:HG21	1:A:94:VAL:CG2	2.22	0.70
1:A:264:GLU:O	1:A:265:ASN:HB2	1.90	0.70
1:B:210:CYS:HA	1:B:284:SER:HA	1.74	0.69
1:A:412:TRP:CG	2:A:565:SO4:O4	2.45	0.69
1:A:32:GLU:OE2	1:A:50:ARG:NH1	2.25	0.69
1:A:92:VAL:HB	1:A:297:TYR:HB2	1.74	0.69
1:B:265:ASN:H	1:B:265:ASN:HD22	1.40	0.69
1:A:504:GLY:O	4:A:622:HOH:O	2.10	0.69
1:B:334:VAL:HB	1:B:387:ASP:OD1	1.91	0.69
1:B:85:LEU:HD13	1:B:92:VAL:HG11	1.74	0.69
1:B:353:LEU:HD12	1:B:353:LEU:N	2.07	0.69
1:B:242:GLU:HA	1:B:244:GLN:OE1	1.91	0.69
1:A:148:ASP:OD2	1:A:168:ARG:NH2	2.25	0.69
1:B:257:PRO:HA	1:B:271:HIS:ND1	2.08	0.69
1:B:40:LYS:NZ	1:B:130:THR:HG22	2.08	0.69
1:B:517:ARG:HH12	1:B:532:ILE:HD12	1.57	0.69
1:B:148:ASP:OD1	4:B:591:HOH:O	2.11	0.69
1:B:9:GLU:HG3	1:B:118:GLN:HE22	1.57	0.68
1:A:262:THR:HG22	1:A:263:LEU:H	1.57	0.68
1:B:262:THR:HG22	1:B:263:LEU:H	1.58	0.68
1:A:469:GLU:HG3	4:A:700:HOH:O	1.94	0.68
1:B:306:ALA:O	1:B:310:ALA:HB3	1.93	0.68
1:B:219:LYS:O	1:B:222:PHE:HB2	1.92	0.68
1:A:175:ARG:HG2	1:A:178:ARG:NH2	2.09	0.68
1:A:61:LEU:HD13	1:A:313:PHE:CD2	2.29	0.68
1:A:452:ALA:O	1:A:456:THR:HB	1.94	0.68
1:B:167:ARG:HD3	1:B:198:ASP:OD2	1.94	0.68
1:B:271:HIS:ND1	1:B:286:ILE:HD11	2.10	0.67
1:A:159:ILE:O	1:A:161:PRO:HD3	1.93	0.67
1:B:515:GLU:HB3	1:B:527:PRO:CG	2.24	0.67
1:A:363:LEU:O	1:A:367:ILE:HG12	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:83:ASP:O	1:B:87:ARG:HB2	1.92	0.67
1:B:335:ARG:NH2	1:B:386:THR:HG21	2.10	0.67
1:A:286:ILE:HG23	4:A:627:HOH:O	1.94	0.67
1:B:166:TRP:HZ3	1:B:225:ILE:CD1	1.79	0.67
1:A:167:ARG:NH2	1:A:178:ARG:O	2.27	0.67
1:A:244:GLN:H	1:A:244:GLN:NE2	1.93	0.67
1:B:40:LYS:HB2	1:B:40:LYS:NZ	2.10	0.67
1:B:244:GLN:H	1:B:244:GLN:NE2	1.93	0.67
1:B:40:LYS:HZ3	1:B:130:THR:HG22	1.59	0.67
1:A:498:ASP:CB	1:A:528:ILE:HG21	2.25	0.67
1:B:360:PHE:CE2	1:B:364:GLU:HB2	2.30	0.67
1:A:532:ILE:O	1:A:532:ILE:HG12	1.95	0.67
1:A:83:ASP:OD1	1:A:262:THR:HG21	1.95	0.67
1:B:36:TYR:HB2	1:B:40:LYS:HZ2	1.60	0.67
1:B:63:THR:HG22	1:B:329:VAL:O	1.95	0.66
1:B:185:GLY:HA3	1:B:189:ASN:ND2	2.10	0.66
1:B:523:ARG:HH11	1:B:525:ILE:HD11	1.60	0.66
1:A:82:THR:HG22	1:A:266:THR:HG21	1.76	0.66
1:A:262:THR:HG22	1:A:263:LEU:N	2.09	0.66
1:A:125:ILE:HG12	1:A:129:PHE:CE1	2.30	0.66
1:B:43:ILE:HD11	1:B:259:LEU:CD2	2.17	0.66
1:B:277:ASN:HD22	1:B:278:ILE:N	1.93	0.66
1:A:286:ILE:HA	1:A:289:LYS:HG2	1.78	0.66
1:A:182:ILE:CG2	1:A:183:GLY:N	2.58	0.66
1:B:173:ASN:HB2	1:B:538:LEU:CD2	2.25	0.66
1:A:68:THR:HB	1:A:69:PRO:HD2	1.78	0.66
1:A:164:ILE:HG21	1:A:193:ARG:HH22	1.60	0.66
1:B:276:ALA:HA	1:B:281:GLY:HA3	1.77	0.65
1:A:185:GLY:HA3	1:A:189:ASN:HD22	1.61	0.65
1:A:150:HIS:CE1	1:A:157:LEU:H	2.14	0.65
1:B:488:VAL:HG23	1:B:523:ARG:HG2	1.79	0.65
1:B:337:LEU:HD21	1:B:363:LEU:CB	2.27	0.65
1:B:491:LYS:HB3	1:B:528:ILE:CG1	2.27	0.65
1:B:265:ASN:ND2	1:B:265:ASN:N	2.42	0.65
1:B:550:ASP:C	1:B:552:ASP:N	2.50	0.65
1:B:528:ILE:HG22	1:B:529:THR:N	2.12	0.65
1:B:21:GLU:O	1:B:24:ARG:HB2	1.97	0.65
1:B:470:ALA:O	1:B:474:ILE:HG13	1.96	0.65
1:B:159:ILE:HD11	1:B:236:VAL:HG11	1.79	0.65
1:A:177:LEU:HB3	1:A:197:PHE:HB2	1.78	0.64
1:B:120:VAL:HB	1:B:121:PRO:HA	1.77	0.64
1:B:476:ARG:O	1:B:480:LEU:HD22	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:143:LEU:HD23	1:B:166:TRP:CE2	2.32	0.64
1:A:36:TYR:CE1	1:A:42:LYS:HG3	2.32	0.64
1:B:513:VAL:HG21	1:B:526:VAL:HG23	1.79	0.64
1:A:43:ILE:HD12	1:A:43:ILE:N	2.12	0.64
1:B:369:ASN:OD1	1:B:458:ILE:HA	1.98	0.64
1:A:166:TRP:CE3	1:A:225:ILE:CD1	2.61	0.64
1:B:42:LYS:HD2	1:B:256:LYS:HB2	1.79	0.64
1:B:244:GLN:HG2	1:B:245:GLY:H	1.63	0.64
1:A:286:ILE:HD12	1:A:286:ILE:C	2.18	0.64
1:B:215:LEU:HG	1:B:255:ILE:HG21	1.78	0.64
1:A:153:GLN:HA	1:A:153:GLN:OE1	1.98	0.64
1:A:166:TRP:CZ3	1:A:225:ILE:HD12	2.27	0.64
1:B:459:TYR:CZ	1:B:491:LYS:HD3	2.33	0.64
1:B:498:ASP:CB	1:B:528:ILE:HG21	2.28	0.64
1:B:61:LEU:HD22	1:B:313:PHE:CE2	2.33	0.63
1:A:405:GLU:OE1	1:A:425:LYS:HD3	1.96	0.63
1:A:490:ALA:HB3	1:A:527:PRO:HA	1.79	0.63
1:A:277:ASN:ND2	1:A:278:ILE:H	1.96	0.63
1:B:278:ILE:O	1:B:525:ILE:HD12	1.97	0.63
1:A:59:LEU:N	1:A:326:ASP:OD2	2.28	0.63
1:A:175:ARG:O	1:A:178:ARG:HG3	1.98	0.63
1:A:16:MET:HB2	1:A:39:TYR:CE2	2.34	0.63
1:A:166:TRP:CH2	1:A:225:ILE:CD1	2.82	0.63
1:A:488:VAL:HG21	1:A:523:ARG:NH1	2.14	0.63
1:B:334:VAL:HG13	1:B:356:LEU:CD2	2.29	0.63
1:B:374:GLY:O	1:B:435:SER:HB2	1.99	0.62
1:B:331:VAL:HG12	1:B:332:ALA:H	1.63	0.62
1:A:136:VAL:HG21	1:A:206:MET:CE	2.29	0.62
1:A:82:THR:CG2	1:A:94:VAL:HG22	2.28	0.62
1:A:381:ILE:HD12	1:A:395:LEU:HD21	1.81	0.62
1:A:140:HIS:CD2	1:A:203:SER:OG	2.44	0.62
1:A:239:GLY:HA2	1:A:244:GLN:HE22	1.64	0.62
1:B:42:LYS:HZ1	1:B:254:ALA:HA	1.64	0.62
1:B:258:ASN:O	1:B:269:PHE:HD1	1.81	0.62
1:B:489:MET:HE1	1:B:526:VAL:HG11	1.81	0.62
1:B:350:THR:HG22	1:B:351:GLU:N	2.14	0.62
1:A:532:ILE:O	1:A:534:THR:HG23	1.99	0.62
1:B:100:SER:HB2	1:B:201:VAL:HG21	1.82	0.62
1:B:34:GLU:HB3	1:B:42:LYS:HB2	1.82	0.62
1:B:285:ILE:HD13	1:B:321:ALA:HB2	1.82	0.62
1:B:364:GLU:O	1:B:368:GLU:HG3	1.99	0.62
1:B:555:ILE:O	1:B:555:ILE:HG23	2.00	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:261:GLN:HG3	1:A:265:ASN:HA	1.80	0.62
1:B:65:ILE:HG23	1:B:332:ALA:HB2	1.81	0.61
1:A:277:ASN:HD22	1:A:277:ASN:N	1.89	0.61
1:B:206:MET:O	1:B:209:LEU:HB3	2.00	0.61
1:B:59:LEU:HD13	1:B:292:LEU:HD21	1.81	0.61
1:B:116:TYR:HA	1:B:263:LEU:HD12	1.81	0.61
1:B:338:LYS:CG	1:B:343:VAL:HG21	2.27	0.61
1:A:61:LEU:HD13	1:A:313:PHE:CG	2.35	0.61
1:A:394:LEU:HG	1:A:398:LEU:HD23	1.81	0.61
1:A:425:LYS:O	1:A:429:THR:HG23	2.00	0.61
1:B:487:VAL:CG1	1:B:489:MET:HE2	2.30	0.61
1:B:166:TRP:O	4:B:632:HOH:O	2.16	0.61
1:B:161:PRO:O	4:B:605:HOH:O	2.16	0.61
1:A:405:GLU:OE2	1:A:422:LEU:HD12	2.00	0.61
1:A:523:ARG:HH11	1:A:525:ILE:CD1	2.14	0.61
1:B:159:ILE:HG12	1:B:236:VAL:HG21	1.82	0.61
1:B:82:THR:HG22	1:B:266:THR:HG21	1.83	0.61
1:A:168:ARG:O	1:A:197:PHE:HA	1.99	0.61
1:A:532:ILE:O	1:A:534:THR:N	2.34	0.61
1:B:150:HIS:HE1	1:B:156:VAL:N	1.98	0.61
1:A:523:ARG:NH1	1:A:525:ILE:HD11	2.15	0.61
1:B:286:ILE:O	1:B:290:THR:HB	2.00	0.61
1:A:351:GLU:O	1:A:352:ASN:HB2	2.01	0.61
1:A:36:TYR:O	1:A:40:LYS:HB2	2.01	0.60
1:A:257:PRO:CD	1:A:286:ILE:HD11	2.30	0.60
1:B:62:VAL:HG13	1:B:301:GLU:HB3	1.82	0.60
1:A:551:ALA:O	4:A:759:HOH:O	2.17	0.60
1:B:490:ALA:HB3	1:B:527:PRO:HA	1.82	0.60
1:B:523:ARG:H	1:B:523:ARG:CD	2.15	0.60
1:B:353:LEU:H	1:B:353:LEU:HD12	1.66	0.60
1:A:423:ALA:C	1:A:427:LEU:HD12	2.22	0.60
1:A:551:ALA:C	4:A:759:HOH:O	2.38	0.60
1:B:321:ALA:HB1	1:B:323:PHE:CE2	2.37	0.60
1:A:547:ILE:HD13	1:A:556:THR:O	2.02	0.60
1:A:76:THR:HG23	1:A:117:ALA:HB3	1.83	0.60
1:A:210:CYS:O	4:A:620:HOH:O	2.16	0.60
1:B:95:CYS:O	1:B:283:ASN:ND2	2.34	0.60
1:B:292:LEU:HD23	1:B:298:VAL:CG2	2.32	0.59
1:A:450:LYS:NZ	1:A:485:LEU:O	2.35	0.59
1:A:87:ARG:HG3	4:A:718:HOH:O	2.02	0.59
1:A:476:ARG:CD	4:A:610:HOH:O	2.49	0.59
1:B:36:TYR:O	1:B:40:LYS:HE3	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:36:TYR:HB2	1:B:40:LYS:NZ	2.16	0.59
1:B:116:TYR:HB2	1:B:415:GLY:HA2	1.83	0.59
1:A:450:LYS:NZ	1:A:483:GLY:O	2.33	0.59
1:A:150:HIS:HE1	1:A:157:LEU:H	1.49	0.59
1:A:523:ARG:C	1:A:523:ARG:HD2	2.22	0.59
1:B:262:THR:HG22	1:B:263:LEU:N	2.18	0.59
1:B:204:GLU:O	1:B:207:ALA:HB3	2.03	0.59
1:A:230:THR:C	1:A:232:ASP:H	2.07	0.59
1:A:277:ASN:HD22	1:A:278:ILE:N	1.97	0.59
1:A:276:ALA:HB2	1:A:281:GLY:HA3	1.83	0.59
1:B:344:PRO:HD2	1:B:347:ASP:HB2	1.85	0.59
1:B:49:ARG:O	1:B:52:LYS:HB2	2.03	0.58
1:A:476:ARG:HD3	4:A:610:HOH:O	2.01	0.58
1:A:116:TYR:CD1	1:A:413:ALA:O	2.56	0.58
1:B:72:GLU:CD	1:B:73:GLY:H	2.07	0.58
1:B:88:LEU:HD21	1:B:420:LEU:CD1	2.34	0.58
1:A:152:GLN:OE1	1:A:152:GLN:HA	2.04	0.58
1:A:482:TYR:O	1:A:524:LEU:HD11	2.03	0.58
1:A:159:ILE:HD11	1:A:236:VAL:HG11	1.84	0.58
1:A:70:ALA:HB2	1:A:339:MET:SD	2.42	0.58
1:B:320:TYR:OH	1:B:486:PRO:HG2	2.03	0.58
1:A:422:LEU:O	1:A:426:VAL:HG23	2.04	0.58
1:A:19:VAL:HG13	1:A:39:TYR:HA	1.84	0.58
1:B:20:MET:HE3	1:B:30:GLU:HG3	1.86	0.58
1:B:276:ALA:HA	1:B:281:GLY:CA	2.34	0.58
1:A:550:ASP:N	1:A:553:GLY:O	2.36	0.58
1:A:277:ASN:ND2	1:A:277:ASN:N	2.51	0.58
1:B:116:TYR:HA	1:B:263:LEU:CD1	2.34	0.57
1:A:116:TYR:CZ	2:A:566:SO4:O1	2.57	0.57
1:A:486:PRO:HD2	1:A:523:ARG:HB3	1.86	0.57
1:A:544:ALA:HA	1:A:547:ILE:HG13	1.86	0.57
1:B:133:ILE:O	1:B:136:VAL:N	2.37	0.57
1:A:360:PHE:CD2	1:A:398:LEU:HD12	2.39	0.57
1:A:182:ILE:HG23	1:A:183:GLY:H	1.69	0.57
1:A:424:ARG:O	1:A:428:GLN:HB2	2.04	0.57
1:A:540:LYS:O	1:A:542:PRO:HD3	2.03	0.57
1:B:271:HIS:CE1	1:B:286:ILE:HD11	2.39	0.57
1:A:447:ILE:HD13	1:A:524:LEU:HD13	1.86	0.57
1:A:472:LYS:O	1:A:476:ARG:HG3	2.04	0.57
1:B:167:ARG:HA	1:B:195:THR:CG2	2.34	0.57
1:B:167:ARG:NH2	1:B:196:GLY:HA3	2.19	0.57
1:A:498:ASP:OD2	1:A:511:ILE:HA	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:253:ASP:HB2	4:A:753:HOH:O	2.03	0.57
1:B:166:TRP:CZ3	1:B:225:ILE:CG1	2.86	0.57
1:B:523:ARG:N	1:B:523:ARG:NE	2.41	0.57
1:A:277:ASN:ND2	1:A:277:ASN:H	2.00	0.57
1:A:169:VAL:HG22	1:A:170:ILE:N	2.20	0.57
1:B:288:THR:HG23	1:B:298:VAL:HG11	1.86	0.57
1:A:544:ALA:HA	1:A:547:ILE:CG1	2.35	0.57
1:A:347:ASP:N	1:A:347:ASP:OD2	2.36	0.57
1:A:164:ILE:HG21	1:A:193:ARG:NH2	2.18	0.57
1:B:365:LYS:CE	1:B:369:ASN:HD21	2.12	0.57
1:B:408:LEU:HD13	1:B:414:LYS:CE	2.35	0.57
1:A:20:MET:HE1	1:A:30:GLU:HA	1.86	0.57
1:B:353:LEU:HB3	1:B:394:LEU:HD22	1.87	0.57
1:B:405:GLU:HB2	1:B:422:LEU:HD13	1.85	0.57
1:A:83:ASP:CG	1:A:262:THR:HG21	2.25	0.57
1:A:423:ALA:O	1:A:427:LEU:HD12	2.04	0.57
1:A:311:GLU:HG3	1:A:312:LYS:HG3	1.87	0.57
1:B:485:LEU:HD22	1:B:522:GLY:O	2.05	0.56
1:B:548:ASP:O	1:B:555:ILE:HG22	2.04	0.56
1:B:513:VAL:CG2	1:B:526:VAL:HG23	2.34	0.56
1:A:120:VAL:HB	1:A:121:PRO:HA	1.86	0.56
1:A:167:ARG:NH2	1:A:196:GLY:HA3	2.20	0.56
1:B:331:VAL:HG12	1:B:332:ALA:N	2.20	0.56
1:A:523:ARG:NH1	1:A:525:ILE:CD1	2.68	0.56
1:B:74:LYS:HB2	1:B:74:LYS:HZ2	1.69	0.56
1:A:533:MET:HG3	1:A:533:MET:O	2.05	0.56
1:A:466:TYR:CD2	1:A:513:VAL:HG22	2.41	0.56
1:A:306:ALA:O	1:A:310:ALA:HB3	2.05	0.56
1:A:225:ILE:CG2	1:A:238:ALA:CB	2.84	0.56
1:B:132:ASP:OD2	1:B:254:ALA:HA	2.05	0.56
1:B:426:VAL:O	1:B:430:LEU:HB3	2.04	0.56
1:A:141:ASN:HB3	4:A:598:HOH:O	2.06	0.56
1:B:43:ILE:O	1:B:257:PRO:HD2	2.06	0.56
1:B:199:ILE:HG13	1:B:535:MET:HE1	1.85	0.56
1:B:331:VAL:HA	1:B:380:ALA:HB3	1.87	0.56
1:B:517:ARG:HH22	1:B:532:ILE:CG1	2.16	0.56
1:A:9:GLU:CG	1:A:115:GLY:H	2.17	0.56
1:A:225:ILE:CG2	1:A:238:ALA:HB2	2.36	0.55
1:B:331:VAL:O	1:B:332:ALA:HB2	2.05	0.55
1:A:219:LYS:HG3	1:A:248:ALA:HB2	1.89	0.55
1:B:40:LYS:CB	1:B:40:LYS:NZ	2.69	0.55
1:B:91:ARG:HG2	1:B:295:ALA:HA	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:455:ALA:HB1	1:B:461:ALA:HB3	1.89	0.55
1:B:83:ASP:HB3	1:B:264:GLU:OE2	2.07	0.55
1:A:8:ILE:CG1	1:A:11:ALA:HB2	2.36	0.55
1:A:167:ARG:HH21	1:A:196:GLY:HA3	1.72	0.55
1:A:195:THR:HG21	4:A:596:HOH:O	2.06	0.55
1:B:313:PHE:C	1:B:313:PHE:CD2	2.78	0.55
1:B:70:ALA:HB2	1:B:339:MET:SD	2.47	0.55
1:B:182:ILE:O	1:B:192:PRO:HA	2.07	0.55
1:A:41:ALA:O	1:A:258:ASN:HA	2.07	0.55
1:B:94:VAL:HG12	1:B:95:CYS:N	2.21	0.55
1:B:339:MET:HA	1:B:343:VAL:HB	1.89	0.55
1:B:86:ALA:C	1:B:88:LEU:H	2.09	0.55
1:B:446:SER:O	1:B:450:LYS:HG3	2.07	0.55
1:A:143:LEU:HD23	1:A:166:TRP:CE2	2.43	0.54
1:B:212:ALA:O	1:B:286:ILE:HG23	2.06	0.54
1:B:318:CYS:SG	1:B:323:PHE:HB2	2.47	0.54
1:B:516:VAL:HG12	1:B:516:VAL:O	2.07	0.54
1:B:335:ARG:HD3	1:B:348:LEU:HB3	1.89	0.54
1:B:88:LEU:HD21	1:B:420:LEU:HD11	1.90	0.54
1:A:353:LEU:H	1:A:353:LEU:CD1	2.19	0.54
1:B:523:ARG:NH1	1:B:525:ILE:HD11	2.21	0.54
1:B:149:ASN:O	1:B:153:GLN:HG2	2.08	0.54
1:B:150:HIS:CE1	1:B:157:LEU:H	2.26	0.54
1:A:158:ASN:O	1:A:230:THR:HA	2.07	0.54
1:B:84:ALA:HB2	1:B:416:GLY:O	2.07	0.54
1:B:152:GLN:OE1	1:B:190:GLY:HA2	2.08	0.54
1:B:61:LEU:HD13	1:B:313:PHE:CE1	2.43	0.54
1:A:36:TYR:HE1	1:A:42:LYS:HG3	1.72	0.54
1:B:509:PHE:HD1	1:B:510:THR:N	2.05	0.54
1:A:143:LEU:CD2	1:A:225:ILE:HD13	2.38	0.54
1:B:277:ASN:HB3	1:B:304:PHE:CE2	2.42	0.54
1:B:220:GLU:OE2	1:B:224:ARG:NH1	2.40	0.54
1:B:326:ASP:O	1:B:376:PRO:HD2	2.08	0.54
1:B:354:GLU:O	1:B:357:ARG:HB3	2.08	0.54
1:B:219:LYS:HE3	4:B:621:HOH:O	2.05	0.54
1:B:451:ILE:HD12	1:B:466:TYR:OH	2.08	0.54
1:A:412:TRP:CD2	2:A:565:SO4:O4	2.60	0.54
1:B:370:ILE:HG21	1:B:377:ALA:HB2	1.90	0.54
1:A:125:ILE:HA	1:A:129:PHE:CD1	2.42	0.54
1:A:301:GLU:OE1	4:A:714:HOH:O	2.18	0.54
1:A:49:ARG:CZ	4:A:692:HOH:O	2.55	0.54
1:A:341:GLY:HA3	1:A:355:ALA:O	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:405:GLU:HB2	1:B:422:LEU:CD1	2.38	0.54
1:B:75:THR:HA	1:B:301:GLU:OE2	2.08	0.53
1:B:488:VAL:HG23	1:B:523:ARG:HD3	1.91	0.53
1:B:121:PRO:HG2	1:B:124:ASP:HB2	1.89	0.53
1:A:488:VAL:HG23	1:A:523:ARG:HD3	1.88	0.53
1:B:459:TYR:HA	1:B:496:PHE:HB3	1.90	0.53
1:B:50:ARG:HG3	1:B:51:LEU:N	2.23	0.53
1:B:375:VAL:HA	1:B:435:SER:CB	2.39	0.53
1:B:8:ILE:HG13	1:B:11:ALA:HB2	1.90	0.53
1:B:167:ARG:NH1	1:B:198:ASP:OD1	2.42	0.53
1:A:47:VAL:HA	1:A:50:ARG:HH12	1.72	0.53
1:A:529:THR:OG1	1:A:530:GLY:N	2.39	0.53
1:B:22:LEU:HD11	1:B:261:GLN:CD	2.28	0.53
1:B:141:ASN:O	1:B:144:ALA:HB3	2.09	0.53
1:B:23:ALA:CA	1:B:28:ILE:HD12	2.36	0.53
1:B:20:MET:HE1	1:B:30:GLU:HA	1.91	0.53
1:B:408:LEU:HD13	1:B:414:LYS:HE3	1.91	0.53
1:A:459:TYR:CD1	1:A:459:TYR:N	2.75	0.53
1:A:167:ARG:NH1	1:A:198:ASP:OD1	2.42	0.52
1:A:169:VAL:CG2	1:A:170:ILE:N	2.71	0.52
1:B:515:GLU:HG2	1:B:516:VAL:H	1.74	0.52
1:B:335:ARG:HH21	1:B:349:ALA:HA	1.71	0.52
1:A:515:GLU:HB3	1:A:527:PRO:HG2	1.92	0.52
1:A:466:TYR:HD2	1:A:513:VAL:HG22	1.74	0.52
1:B:80:GLY:N	1:B:117:ALA:HB1	2.25	0.52
1:A:31:ASP:OD2	1:A:32:GLU:HG3	2.10	0.52
1:B:51:LEU:O	1:B:293:LYS:HG2	2.09	0.52
1:B:325:PRO:HD2	1:B:437:PHE:CD2	2.44	0.52
1:B:143:LEU:HD23	1:B:166:TRP:CZ2	2.45	0.52
1:A:378:VAL:HG11	1:A:405:GLU:OE2	2.09	0.52
1:B:441:TYR:CE2	1:B:454:ILE:HD11	2.44	0.52
1:A:49:ARG:NE	4:A:692:HOH:O	2.42	0.52
1:B:36:TYR:CE2	1:B:130:THR:HB	2.45	0.52
1:A:530:GLY:C	1:A:532:ILE:N	2.61	0.52
1:B:91:ARG:HB3	1:B:296:ASP:CG	2.31	0.52
1:B:315:ASP:O	1:B:319:ARG:HD2	2.10	0.52
1:A:111:ALA:O	1:A:113:GLY:N	2.43	0.52
1:A:440:LEU:HD22	1:A:458:ILE:HD11	1.91	0.52
1:B:58:LYS:HA	1:B:326:ASP:OD2	2.09	0.52
1:B:363:LEU:HD23	1:B:395:LEU:HD11	1.92	0.52
1:B:472:LYS:O	1:B:476:ARG:HG3	2.10	0.52
1:A:66:THR:HB	1:A:340:HIS:CE1	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:379:VAL:HB	1:B:404:ALA:HA	1.91	0.51
1:B:399:CYS:O	1:B:401:LYS:N	2.43	0.51
1:B:210:CYS:CA	1:B:284:SER:HA	2.40	0.51
1:B:79:VAL:HB	1:B:117:ALA:O	2.10	0.51
1:A:175:ARG:HG2	1:A:178:ARG:CZ	2.40	0.51
1:B:285:ILE:O	1:B:287:ALA:N	2.43	0.51
1:B:277:ASN:HD22	1:B:277:ASN:N	2.09	0.51
1:B:9:GLU:OE2	1:B:111:ALA:HB3	2.11	0.51
1:A:533:MET:CE	1:A:536:PRO:HA	2.41	0.51
1:A:83:ASP:OD2	1:A:262:THR:HG21	2.10	0.51
1:B:150:HIS:CE1	1:B:156:VAL:N	2.78	0.51
1:A:181:VAL:HG13	1:A:193:ARG:O	2.09	0.51
1:A:319:ARG:NH2	1:A:441:TYR:O	2.42	0.51
1:B:275:PHE:HD2	1:B:277:ASN:HD21	1.57	0.51
1:B:550:ASP:O	1:B:552:ASP:N	2.43	0.51
1:A:66:THR:CB	1:A:362:ASN:HD21	2.22	0.51
1:B:75:THR:CB	1:B:113:GLY:HA2	2.41	0.51
1:A:118:GLN:HG3	1:A:263:LEU:HD21	1.91	0.51
1:A:389:GLU:HB3	1:A:393:ASN:ND2	2.25	0.51
1:A:459:TYR:HB3	1:A:496:PHE:O	2.10	0.51
1:B:303:GLY:HA2	2:B:560:SO4:O1	2.11	0.51
1:B:487:VAL:HG12	1:B:489:MET:HE2	1.92	0.51
1:B:514:ARG:HD2	1:B:528:ILE:O	2.10	0.51
1:B:420:LEU:O	1:B:423:ALA:HB3	2.11	0.51
1:A:175:ARG:NH1	1:A:537:GLY:HA3	2.26	0.51
1:B:323:PHE:CD2	1:B:323:PHE:N	2.77	0.51
1:B:10:ILE:HA	1:B:122:MET:CE	2.41	0.51
1:A:515:GLU:O	1:A:527:PRO:HD2	2.11	0.51
1:B:221:ARG:HG2	1:B:221:ARG:HH21	1.76	0.51
1:B:497:SER:HA	1:B:511:ILE:HD11	1.93	0.51
1:B:58:LYS:HG2	1:B:297:TYR:HD1	1.77	0.50
1:B:75:THR:HG23	1:B:301:GLU:OE1	2.11	0.50
1:B:257:PRO:HD3	1:B:286:ILE:HD13	1.93	0.50
1:B:275:PHE:O	1:B:279:ALA:HB3	2.11	0.50
1:A:540:LYS:C	1:A:542:PRO:HD3	2.31	0.50
1:A:459:TYR:OH	4:A:741:HOH:O	2.13	0.50
1:B:329:VAL:HG12	1:B:330:ILE:N	2.27	0.50
1:B:448:LYS:HD3	1:B:466:TYR:CZ	2.46	0.50
1:B:150:HIS:HE1	1:B:157:LEU:H	1.57	0.50
1:A:512:THR:O	1:A:528:ILE:HG23	2.11	0.50
1:A:440:LEU:HD11	1:A:457:GLU:OE1	2.11	0.50
1:B:60:ILE:HD12	1:B:299:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:277:ASN:N	1:B:304:PHE:HE2	2.10	0.50
1:B:443:LEU:HG	1:B:484:ASN:O	2.12	0.50
1:B:229:TYR:CD1	1:B:229:TYR:N	2.79	0.50
1:B:42:LYS:NZ	1:B:132:ASP:OD2	2.38	0.50
1:B:556:THR:O	1:B:556:THR:CG2	2.60	0.50
1:B:451:ILE:HG12	1:B:489:MET:CE	2.38	0.50
1:B:159:ILE:HA	1:B:230:THR:HA	1.93	0.50
1:B:350:THR:CG2	1:B:351:GLU:N	2.75	0.50
1:B:398:LEU:C	1:B:400:ALA:H	2.15	0.50
1:B:42:LYS:NZ	1:B:254:ALA:HA	2.26	0.50
1:A:42:LYS:NZ	1:A:132:ASP:OD2	2.44	0.49
1:A:17:LYS:N	1:A:261:GLN:NE2	2.55	0.49
1:B:152:GLN:NE2	1:B:187:LYS:O	2.38	0.49
1:B:486:PRO:HD2	1:B:523:ARG:HB3	1.94	0.49
1:A:92:VAL:HG23	1:A:297:TYR:C	2.33	0.49
1:A:529:THR:C	1:A:531:ALA:H	2.14	0.49
1:A:530:GLY:O	1:A:532:ILE:N	2.45	0.49
1:B:472:LYS:HD3	1:B:476:ARG:HH21	1.74	0.49
1:A:143:LEU:O	1:A:147:VAL:HG23	2.12	0.49
1:B:43:ILE:HD12	1:B:269:PHE:CE1	2.47	0.49
1:A:36:TYR:O	1:A:40:LYS:NZ	2.40	0.49
1:B:335:ARG:HB3	1:B:348:LEU:HD22	1.93	0.49
1:B:487:VAL:HG11	1:B:489:MET:HE2	1.93	0.49
1:B:12:GLN:NE2	1:B:263:LEU:CD1	2.74	0.49
1:A:150:HIS:NE2	1:A:157:LEU:HD12	2.27	0.49
1:A:343:VAL:HG23	1:A:355:ALA:CB	2.42	0.49
1:A:72:GLU:HA	1:A:333:THR:HG23	1.94	0.49
1:B:327:ALA:HB2	1:B:430:LEU:HD13	1.94	0.49
1:A:112:ALA:O	1:A:118:GLN:HA	2.12	0.49
1:B:150:HIS:HE2	1:B:157:LEU:HG	1.78	0.49
1:A:120:VAL:O	1:A:260:VAL:HB	2.11	0.49
1:A:353:LEU:N	1:A:353:LEU:HD12	2.26	0.49
1:B:389:GLU:O	1:B:393:ASN:ND2	2.45	0.49
1:A:461:ALA:HB2	1:A:509:PHE:CE1	2.48	0.49
1:B:125:ILE:HG12	1:B:129:PHE:CE1	2.46	0.49
1:B:258:ASN:O	1:B:269:PHE:CD1	2.64	0.49
1:B:429:THR:O	1:B:433:ARG:HB3	2.13	0.49
1:B:377:ALA:O	1:B:378:VAL:HG23	2.12	0.49
1:B:288:THR:O	1:B:292:LEU:HG	2.13	0.49
1:B:494:TYR:O	1:B:495:SER:HB2	2.13	0.49
1:A:340:HIS:ND1	1:A:504:GLY:N	2.53	0.49
1:B:47:VAL:CG1	1:B:294:LEU:HD21	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:133:ILE:O	1:B:134:HIS:C	2.51	0.49
1:B:519:SER:C	1:B:521:GLY:H	2.16	0.49
1:A:147:VAL:HG11	1:A:164:ILE:HD13	1.93	0.49
1:B:61:LEU:O	1:B:328:THR:HA	2.13	0.49
1:B:276:ALA:CA	1:B:281:GLY:HA3	2.42	0.49
1:B:277:ASN:ND2	1:B:278:ILE:HD13	2.28	0.49
1:B:477:TYR:CE2	1:B:516:VAL:HG12	2.40	0.49
1:A:401:LYS:CB	4:A:748:HOH:O	2.48	0.49
1:A:230:THR:C	1:A:232:ASP:N	2.66	0.49
1:A:344:PRO:O	1:A:348:LEU:HG	2.13	0.49
1:B:339:MET:C	1:B:341:GLY:H	2.16	0.49
1:A:140:HIS:HE1	1:A:167:ARG:O	1.96	0.48
1:B:63:THR:O	1:B:331:VAL:HG23	2.13	0.48
1:A:277:ASN:ND2	1:A:278:ILE:N	2.60	0.48
1:B:49:ARG:HD3	1:B:49:ARG:C	2.33	0.48
1:B:225:ILE:O	1:B:225:ILE:HG23	2.13	0.48
1:B:36:TYR:CB	1:B:40:LYS:NZ	2.76	0.48
1:B:193:ARG:NH2	1:B:195:THR:OG1	2.45	0.48
1:A:426:VAL:O	1:A:430:LEU:HB2	2.12	0.48
1:B:8:ILE:HG13	1:B:11:ALA:CB	2.43	0.48
1:A:133:ILE:HG21	1:A:171:ASP:OD1	2.13	0.48
1:B:65:ILE:HB	1:B:66:THR:H	1.44	0.48
1:B:417:GLU:O	1:B:419:GLY:N	2.46	0.48
1:B:157:LEU:O	1:B:230:THR:CG2	2.61	0.48
1:A:149:ASN:OD1	1:A:153:GLN:HG2	2.13	0.48
1:B:304:PHE:CE1	1:B:493:GLN:NE2	2.81	0.48
1:A:543:ALA:O	1:A:547:ILE:HG12	2.14	0.48
1:B:164:ILE:HD12	1:B:193:ARG:NE	2.28	0.48
1:A:20:MET:CE	1:A:33:VAL:HB	2.43	0.48
1:B:94:VAL:HG12	1:B:95:CYS:H	1.79	0.48
1:B:420:LEU:O	1:B:421:GLU:C	2.52	0.48
1:A:182:ILE:HG23	1:A:183:GLY:N	2.26	0.48
1:B:393:ASN:HB3	4:B:597:HOH:O	2.14	0.48
1:B:440:LEU:CD2	1:B:458:ILE:HD11	2.43	0.48
1:B:492:THR:O	1:B:492:THR:HG23	2.14	0.48
1:A:65:ILE:O	1:A:66:THR:C	2.52	0.48
1:B:417:GLU:C	1:B:419:GLY:H	2.17	0.48
1:A:35:LEU:HD23	1:A:40:LYS:O	2.13	0.48
1:B:276:ALA:HB2	1:B:303:GLY:HA3	1.95	0.48
1:A:92:VAL:HG22	1:A:93:MET:N	2.27	0.48
1:B:35:LEU:HD23	1:B:41:ALA:HB2	1.95	0.48
1:B:388:THR:O	1:B:392:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:497:SER:C	1:A:499:ASP:H	2.17	0.48
1:A:140:HIS:HD2	1:A:203:SER:HG	1.56	0.48
1:A:204:GLU:O	1:A:207:ALA:HB3	2.14	0.48
1:B:461:ALA:HA	1:B:509:PHE:CE1	2.48	0.48
1:A:446:SER:HB3	1:A:449:ASP:CB	2.41	0.48
1:A:211:LEU:HA	1:A:285:ILE:HD12	1.96	0.48
1:B:555:ILE:O	1:B:556:THR:CB	2.55	0.48
1:A:136:VAL:HG13	1:A:205:VAL:HG12	1.95	0.48
1:A:400:ALA:O	1:A:401:LYS:HB2	2.12	0.48
1:A:221:ARG:HA	1:A:224:ARG:HG3	1.94	0.48
1:B:414:LYS:O	1:B:417:GLU:HB3	2.14	0.48
1:A:332:ALA:O	1:A:381:ILE:HA	2.13	0.48
1:A:106:GLY:CA	1:A:538:LEU:HD22	2.44	0.48
1:B:313:PHE:CE2	1:B:318:CYS:SG	3.06	0.47
1:B:351:GLU:OE2	1:B:353:LEU:HD11	2.14	0.47
1:A:533:MET:CB	2:A:561:SO4:O2	2.61	0.47
1:B:241:LEU:O	1:B:242:GLU:HB2	2.14	0.47
1:B:244:GLN:CD	1:B:244:GLN:H	2.17	0.47
1:B:20:MET:HE3	1:B:30:GLU:CG	2.44	0.47
1:A:288:THR:O	1:A:291:ALA:N	2.47	0.47
1:A:463:GLY:O	1:A:510:THR:HG23	2.14	0.47
1:B:247:MET:HA	1:B:250:LEU:HD23	1.96	0.47
1:A:399:CYS:O	1:A:401:LYS:N	2.47	0.47
1:B:466:TYR:HA	1:B:513:VAL:HG13	1.97	0.47
1:B:144:ALA:HB1	1:B:168:ARG:NH2	2.28	0.47
1:B:175:ARG:HG2	1:B:178:ARG:CZ	2.45	0.47
1:A:360:PHE:CE2	1:A:364:GLU:HB2	2.50	0.47
1:B:169:VAL:HG12	1:B:200:SER:OG	2.15	0.47
1:A:107:ILE:O	1:A:108:LYS:HB2	2.13	0.47
1:A:225:ILE:HG23	1:A:238:ALA:HB2	1.96	0.47
1:A:61:LEU:HD13	1:A:313:PHE:CE2	2.50	0.47
1:B:450:LYS:O	1:B:454:ILE:HG13	2.14	0.47
1:A:288:THR:HG22	1:A:292:LEU:HD12	1.95	0.47
1:A:140:HIS:CE1	1:A:166:TRP:CZ2	3.02	0.47
1:B:304:PHE:CD1	1:B:493:GLN:HG3	2.50	0.47
1:B:459:TYR:HE2	1:B:489:MET:HG3	1.80	0.47
1:A:87:ARG:NH1	1:A:264:GLU:OE1	2.48	0.47
1:B:83:ASP:O	4:B:612:HOH:O	2.21	0.47
1:B:408:LEU:CD2	1:B:408:LEU:O	2.63	0.47
1:B:304:PHE:HE1	1:B:493:GLN:HE21	1.60	0.47
1:B:523:ARG:H	1:B:523:ARG:HE	1.51	0.47
1:A:533:MET:HA	2:A:561:SO4:O2	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:303:GLY:O	1:B:309:GLY:HA3	2.14	0.47
1:A:9:GLU:OE1	1:A:114:GLY:HA3	2.14	0.47
1:A:32:GLU:OE1	1:A:47:VAL:HG22	2.15	0.47
1:B:215:LEU:HD21	1:B:255:ILE:HB	1.97	0.47
1:B:384:PHE:CD1	1:B:385:PRO:HD2	2.50	0.47
1:A:459:TYR:O	1:A:509:PHE:HZ	1.98	0.47
1:A:54:LYS:HB3	1:A:55:PRO:HD2	1.97	0.47
1:B:42:LYS:HE2	1:B:258:ASN:OD1	2.15	0.46
1:B:375:VAL:HA	1:B:435:SER:HB2	1.97	0.46
1:B:353:LEU:CD1	1:B:353:LEU:N	2.77	0.46
1:A:43:ILE:CD1	1:A:43:ILE:N	2.78	0.46
1:A:550:ASP:C	1:A:552:ASP:H	2.17	0.46
1:B:140:HIS:HE1	1:B:167:ARG:O	1.97	0.46
1:A:42:LYS:HZ3	1:A:254:ALA:HA	1.80	0.46
1:B:491:LYS:HB3	1:B:528:ILE:HG13	1.95	0.46
1:B:338:LYS:O	1:B:341:GLY:N	2.44	0.46
1:B:75:THR:O	1:B:76:THR:C	2.53	0.46
1:A:259:LEU:O	1:A:260:VAL:HG13	2.15	0.46
1:A:143:LEU:HD23	1:A:166:TRP:CZ2	2.50	0.46
1:A:144:ALA:HB1	1:A:168:ARG:HE	1.81	0.46
1:B:515:GLU:O	1:B:516:VAL:HG23	2.15	0.46
1:B:333:THR:HB	1:B:382:ASN:HB3	1.97	0.46
1:A:417:GLU:O	1:A:420:LEU:HD23	2.15	0.46
1:B:86:ALA:HA	1:B:90:LYS:HB2	1.96	0.46
1:B:357:ARG:O	1:B:360:PHE:CB	2.61	0.46
1:B:335:ARG:HH21	1:B:386:THR:HG21	1.80	0.46
1:B:31:ASP:OD2	1:B:32:GLU:HG3	2.16	0.46
1:B:12:GLN:HE22	1:B:263:LEU:HD13	1.76	0.46
1:A:150:HIS:CE1	1:A:157:LEU:HB2	2.51	0.46
1:A:550:ASP:C	1:A:552:ASP:N	2.69	0.46
1:A:97:ARG:HB3	1:A:273:GLY:HA3	1.98	0.46
1:B:323:PHE:O	1:B:324:LYS:HG3	2.15	0.46
1:B:515:GLU:O	1:B:527:PRO:HD2	2.14	0.46
1:A:526:VAL:O	1:A:526:VAL:HG22	2.15	0.46
1:B:323:PHE:N	1:B:323:PHE:HD2	2.14	0.46
1:B:440:LEU:HD22	1:B:458:ILE:HD11	1.96	0.46
1:A:394:LEU:O	1:A:398:LEU:HB2	2.16	0.46
1:A:476:ARG:HD2	4:A:610:HOH:O	2.11	0.46
1:A:374:GLY:HA3	1:A:436:ASN:O	2.16	0.46
1:A:39:TYR:O	1:A:40:LYS:HG3	2.16	0.46
1:A:346:SER:HB3	4:A:732:HOH:O	2.16	0.46
1:A:90:LYS:HD2	1:A:297:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:144:ALA:CB	1:B:168:ARG:HE	2.29	0.46
1:B:146:MET:SD	1:B:243:ALA:HB2	2.55	0.46
1:B:83:ASP:HB3	1:B:416:GLY:CA	2.45	0.46
1:B:393:ASN:O	1:B:397:GLU:HG2	2.16	0.46
1:B:314:TYR:OH	1:B:328:THR:HG21	2.16	0.45
1:B:66:THR:O	1:B:68:THR:HG23	2.15	0.45
1:B:51:LEU:HD12	1:B:294:LEU:HD23	1.97	0.45
1:B:239:GLY:HA2	1:B:244:GLN:NE2	2.30	0.45
1:B:373:PHE:CE2	1:B:440:LEU:HB2	2.51	0.45
1:A:51:LEU:O	1:A:53:ASP:N	2.49	0.45
1:A:337:LEU:HA	1:A:337:LEU:HD12	1.75	0.45
1:B:66:THR:HB	1:B:362:ASN:HD21	1.81	0.45
1:B:69:PRO:HG2	1:B:339:MET:CE	2.46	0.45
1:B:50:ARG:C	1:B:52:LYS:H	2.18	0.45
1:B:116:TYR:HB2	1:B:415:GLY:CA	2.45	0.45
1:B:75:THR:CG2	1:B:113:GLY:HA2	2.46	0.45
1:A:315:ASP:O	1:A:319:ARG:HD2	2.15	0.45
1:A:353:LEU:H	1:A:353:LEU:HD12	1.82	0.45
1:B:280:HIS:HA	1:B:312:LYS:HD3	1.97	0.45
1:B:447:ILE:HD12	1:B:478:GLU:HG3	1.98	0.45
1:A:215:LEU:HD11	1:A:252:LYS:HA	1.98	0.45
1:A:505:ARG:HG2	1:A:507:ARG:NH2	2.31	0.45
1:B:61:LEU:HD22	1:B:313:PHE:CZ	2.52	0.45
1:B:95:CYS:HB3	1:B:283:ASN:ND2	2.32	0.45
1:B:463:GLY:O	1:B:510:THR:HG23	2.15	0.45
1:B:408:LEU:HD23	1:B:408:LEU:O	2.17	0.45
1:B:505:ARG:HG2	1:B:505:ARG:O	2.16	0.45
1:B:40:LYS:HD3	1:B:124:ASP:OD2	2.17	0.45
1:A:105:PHE:CD1	1:A:105:PHE:N	2.84	0.45
1:A:245:GLY:O	1:A:248:ALA:HB3	2.17	0.45
1:B:150:HIS:NE2	1:B:157:LEU:HG	2.32	0.45
1:A:311:GLU:HG3	1:A:312:LYS:N	2.32	0.45
1:A:353:LEU:N	1:A:353:LEU:CD1	2.79	0.45
1:B:312:LYS:HE2	1:B:488:VAL:HG13	1.99	0.45
1:B:509:PHE:CD1	1:B:510:THR:N	2.84	0.45
1:B:127:LEU:HB3	1:B:128:HIS:H	1.55	0.45
1:B:125:ILE:HA	1:B:129:PHE:CD1	2.52	0.45
1:B:22:LEU:HD11	1:B:261:GLN:NE2	2.32	0.45
1:A:227:VAL:HG22	1:A:236:VAL:O	2.16	0.45
1:A:520:ALA:C	1:A:522:GLY:H	2.21	0.45
1:A:20:MET:CE	1:A:30:GLU:HA	2.46	0.45
1:B:175:ARG:O	1:B:178:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:541:ARG:N	1:B:542:PRO:HD3	2.32	0.45
1:B:93:MET:HB3	1:B:94:VAL:H	1.55	0.45
1:B:18:PRO:O	1:B:22:LEU:HG	2.16	0.45
1:B:74:LYS:CB	1:B:74:LYS:NZ	2.76	0.45
1:B:10:ILE:HG23	1:B:11:ALA:N	2.32	0.44
1:B:8:ILE:CG1	1:B:11:ALA:HB2	2.47	0.44
1:A:182:ILE:HG22	1:A:183:GLY:N	2.31	0.44
1:B:160:ASP:HB3	1:B:163:THR:HG23	1.97	0.44
1:A:225:ILE:CG2	1:A:238:ALA:HB3	2.46	0.44
1:B:287:ALA:O	1:B:291:ALA:HB2	2.17	0.44
1:B:405:GLU:HG3	1:B:425:LYS:HB2	1.98	0.44
1:B:174:ASP:OD1	1:B:177:LEU:CG	2.63	0.44
1:A:476:ARG:HG2	1:A:476:ARG:HH11	1.81	0.44
1:B:20:MET:CE	1:B:30:GLU:HA	2.46	0.44
1:A:343:VAL:HG23	1:A:355:ALA:HB1	1.99	0.44
1:B:166:TRP:HZ3	1:B:225:ILE:CG1	2.27	0.44
1:B:285:ILE:O	1:B:286:ILE:C	2.55	0.44
1:B:8:ILE:HB	1:B:10:ILE:HG22	2.00	0.44
1:B:12:GLN:HE21	1:B:263:LEU:HD13	1.79	0.44
1:A:140:HIS:CE1	1:A:166:TRP:CE2	3.04	0.44
1:B:329:VAL:HG12	1:B:330:ILE:H	1.82	0.44
1:A:523:ARG:HH11	1:A:525:ILE:HD11	1.79	0.44
1:B:215:LEU:CG	1:B:255:ILE:HG21	2.47	0.44
1:B:276:ALA:O	1:B:279:ALA:O	2.36	0.44
1:B:277:ASN:HB3	1:B:304:PHE:HE2	1.82	0.44
1:A:446:SER:CB	1:A:449:ASP:HB2	2.45	0.44
1:B:157:LEU:O	1:B:230:THR:HG21	2.17	0.44
1:B:100:SER:O	1:B:103:PRO:HD2	2.17	0.44
1:A:334:VAL:HG21	1:A:392:LEU:HD23	2.00	0.44
1:B:288:THR:HA	1:B:291:ALA:HB3	2.00	0.44
1:B:274:PRO:HG2	1:B:281:GLY:HA2	2.00	0.44
1:B:515:GLU:HB3	1:B:527:PRO:HG3	1.99	0.44
1:B:339:MET:CG	1:B:348:LEU:HD21	2.47	0.44
1:B:245:GLY:O	1:B:248:ALA:HB3	2.18	0.44
1:B:160:ASP:OD1	1:B:162:ARG:HB2	2.18	0.44
1:B:210:CYS:HA	1:B:284:SER:CA	2.47	0.44
1:B:202:ALA:HB2	1:B:275:PHE:CE1	2.52	0.44
1:B:522:GLY:HA3	1:B:523:ARG:HH21	1.83	0.44
1:A:363:LEU:HD11	1:A:379:VAL:HG22	2.00	0.44
1:A:82:THR:CG2	1:A:266:THR:HG21	2.45	0.44
1:B:285:ILE:O	1:B:288:THR:N	2.51	0.44
1:B:367:ILE:O	1:B:370:ILE:HB	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:417:GLU:C	1:B:419:GLY:N	2.71	0.44
1:B:420:LEU:HD12	1:B:424:ARG:HH12	1.82	0.44
1:A:143:LEU:HD21	1:A:225:ILE:HD13	1.99	0.44
1:B:97:ARG:HB3	1:B:273:GLY:HA2	2.00	0.44
1:B:178:ARG:HD3	1:B:535:MET:O	2.17	0.44
1:A:90:LYS:HB3	1:A:297:TYR:CD2	2.53	0.44
1:A:369:ASN:O	1:A:372:LYS:N	2.48	0.44
1:B:12:GLN:HE21	1:B:263:LEU:CD1	2.31	0.44
1:A:175:ARG:O	1:A:177:LEU:N	2.51	0.43
1:B:488:VAL:HG23	1:B:523:ARG:CG	2.47	0.43
1:B:65:ILE:CG2	1:B:332:ALA:HB2	2.48	0.43
1:A:556:THR:HG22	1:A:556:THR:O	2.18	0.43
1:A:36:TYR:HB3	1:A:40:LYS:HZ3	1.83	0.43
1:B:493:GLN:CD	1:B:494:TYR:CE1	2.92	0.43
1:B:523:ARG:HB2	1:B:524:LEU:H	1.41	0.43
1:B:29:GLN:HB2	1:B:31:ASP:OD2	2.18	0.43
1:A:160:ASP:OD2	1:A:162:ARG:NH2	2.43	0.43
1:A:311:GLU:HG2	4:A:741:HOH:O	2.17	0.43
1:B:42:LYS:HE2	1:B:130:THR:OG1	2.18	0.43
1:B:353:LEU:H	1:B:353:LEU:CD1	2.32	0.43
1:A:555:ILE:O	1:A:556:THR:CB	2.67	0.43
1:B:9:GLU:HG3	1:B:118:GLN:NE2	2.29	0.43
1:A:262:THR:CG2	1:A:263:LEU:N	2.79	0.43
1:B:99:PRO:HD2	1:B:125:ILE:HG22	2.01	0.43
1:B:466:TYR:N	1:B:466:TYR:CD1	2.87	0.43
1:A:246:SER:O	1:A:250:LEU:HD23	2.17	0.43
1:B:257:PRO:CA	1:B:271:HIS:ND1	2.81	0.43
1:B:286:ILE:HD12	1:B:286:ILE:C	2.37	0.43
1:B:277:ASN:HD22	1:B:277:ASN:H	1.65	0.43
1:B:320:TYR:CD2	1:B:320:TYR:N	2.86	0.43
1:A:447:ILE:HA	1:A:450:LYS:HD2	2.01	0.43
1:B:150:HIS:O	1:B:151:LEU:C	2.56	0.43
1:B:221:ARG:NH2	1:B:221:ARG:HG2	2.34	0.43
1:A:97:ARG:HG2	1:A:273:GLY:HA2	1.99	0.43
1:A:226:VAL:HG23	4:A:760:HOH:O	2.18	0.43
1:B:286:ILE:CA	1:B:289:LYS:HG2	2.44	0.43
1:A:16:MET:HB2	1:A:39:TYR:CD2	2.54	0.43
1:B:481:GLY:C	1:B:483:GLY:H	2.21	0.43
1:B:32:GLU:O	1:B:33:VAL:HG23	2.19	0.43
1:A:381:ILE:HD12	1:A:395:LEU:CD2	2.47	0.43
1:A:48:TYR:O	1:A:51:LEU:N	2.34	0.43
1:B:285:ILE:HG22	1:B:286:ILE:N	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:332:ALA:HB1	1:B:337:LEU:HD11	2.01	0.43
1:A:87:ARG:HD2	1:A:416:GLY:HA3	2.00	0.43
1:B:384:PHE:CG	1:B:385:PRO:HD2	2.54	0.43
1:A:453:LYS:HA	4:A:658:HOH:O	2.18	0.43
1:A:246:SER:O	1:A:250:LEU:CD2	2.67	0.43
1:A:23:ALA:HB1	1:A:28:ILE:HB	2.00	0.43
1:B:358:GLU:O	1:B:359:GLY:C	2.57	0.43
1:B:280:HIS:CD2	1:B:282:CYS:SG	3.12	0.42
1:B:215:LEU:HA	1:B:215:LEU:HD23	1.88	0.42
1:A:412:TRP:CB	2:A:565:SO4:O4	2.67	0.42
1:B:440:LEU:O	1:B:440:LEU:HG	2.18	0.42
1:B:111:ALA:HA	1:B:122:MET:HG3	2.00	0.42
1:A:8:ILE:HG13	1:A:11:ALA:HB2	2.01	0.42
1:A:388:THR:HG23	1:A:391:GLU:OE1	2.19	0.42
1:B:212:ALA:O	1:B:286:ILE:CG2	2.66	0.42
1:B:488:VAL:HG23	1:B:523:ARG:CD	2.49	0.42
1:B:333:THR:O	1:B:337:LEU:HD13	2.19	0.42
1:B:491:LYS:HB3	1:B:528:ILE:HG12	2.00	0.42
1:B:232:ASP:HB2	4:B:610:HOH:O	2.20	0.42
1:B:164:ILE:HD12	1:B:193:ARG:CD	2.49	0.42
1:B:337:LEU:O	1:B:359:GLY:HA3	2.19	0.42
1:B:332:ALA:O	1:B:381:ILE:HA	2.20	0.42
1:B:172:LEU:O	1:B:535:MET:CE	2.68	0.42
1:B:335:ARG:HA	1:B:338:LYS:HE3	2.01	0.42
1:B:455:ALA:HA	1:B:459:TYR:HD2	1.85	0.42
1:B:442:ASN:OD1	1:B:443:LEU:N	2.51	0.42
1:B:61:LEU:HD22	1:B:313:PHE:CD2	2.53	0.42
1:B:51:LEU:O	1:B:293:LYS:CG	2.67	0.42
1:A:151:LEU:HA	1:A:155:ASN:HB2	2.01	0.42
1:B:339:MET:HG2	1:B:348:LEU:HD21	2.02	0.42
1:B:555:ILE:O	1:B:555:ILE:CG2	2.67	0.42
1:A:278:ILE:HG23	1:A:278:ILE:O	2.19	0.42
1:B:35:LEU:HD23	1:B:41:ALA:CB	2.49	0.42
1:B:83:ASP:HB3	1:B:416:GLY:HA3	2.02	0.42
1:A:75:THR:O	1:A:76:THR:C	2.58	0.42
1:B:207:ALA:O	1:B:208:CYS:C	2.57	0.42
1:B:199:ILE:CD1	4:B:609:HOH:O	2.67	0.42
1:A:278:ILE:HD12	1:A:278:ILE:HA	1.79	0.42
1:B:507:ARG:C	1:B:509:PHE:H	2.23	0.42
1:B:47:VAL:HG13	1:B:294:LEU:HD21	2.01	0.42
1:B:150:HIS:O	1:B:153:GLN:N	2.48	0.42
1:B:357:ARG:O	1:B:358:GLU:C	2.58	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:405:GLU:CD	1:A:425:LYS:HB2	2.40	0.42
1:A:60:ILE:HD13	1:A:426:VAL:HG11	2.01	0.42
1:A:105:PHE:O	1:A:544:ALA:N	2.52	0.42
1:A:244:GLN:O	1:A:248:ALA:HB2	2.18	0.42
1:A:20:MET:HE1	1:A:33:VAL:HB	2.02	0.42
1:B:517:ARG:NH2	1:B:532:ILE:HG13	2.22	0.42
1:B:86:ALA:C	1:B:88:LEU:N	2.72	0.42
1:A:75:THR:HA	1:A:301:GLU:OE2	2.20	0.42
1:B:402:ALA:O	1:B:403:GLY:C	2.58	0.42
1:B:97:ARG:NH1	1:B:281:GLY:O	2.53	0.41
1:A:297:TYR:HE1	1:A:430:LEU:HD23	1.85	0.41
1:A:367:ILE:HG21	1:A:401:LYS:HD3	2.02	0.41
1:B:459:TYR:OH	1:B:489:MET:CB	2.68	0.41
1:A:343:VAL:HA	1:A:344:PRO:HD3	1.94	0.41
1:B:286:ILE:CD1	1:B:287:ALA:N	2.81	0.41
1:B:490:ALA:HB2	1:B:525:ILE:CG2	2.42	0.41
1:B:19:VAL:HA	1:B:22:LEU:HG	2.02	0.41
1:B:492:THR:HG21	1:B:498:ASP:O	2.20	0.41
1:A:440:LEU:O	1:A:453:LYS:HE2	2.20	0.41
1:A:280:HIS:CD2	1:A:282:CYS:HB2	2.55	0.41
1:B:101:LEU:HG	1:B:105:PHE:HE1	1.85	0.41
1:B:66:THR:CB	1:B:362:ASN:HD21	2.33	0.41
1:B:532:ILE:HD11	4:B:603:HOH:O	2.21	0.41
1:A:204:GLU:OE1	1:A:519:SER:HB3	2.20	0.41
1:A:48:TYR:HB2	1:A:290:THR:OG1	2.19	0.41
1:A:92:VAL:CG2	1:A:93:MET:N	2.83	0.41
1:B:554:VAL:HG12	1:B:555:ILE:N	2.34	0.41
1:A:29:GLN:HB2	1:A:32:GLU:HG3	2.02	0.41
1:B:448:LYS:HD3	1:B:466:TYR:CE2	2.54	0.41
1:A:369:ASN:O	1:A:372:LYS:HB2	2.20	0.41
1:B:408:LEU:HD13	1:B:414:LYS:NZ	2.35	0.41
1:A:292:LEU:HG	1:A:298:VAL:HG21	2.02	0.41
1:A:377:ALA:O	1:A:402:ALA:HB1	2.21	0.41
1:A:308:LEU:O	1:A:309:GLY:C	2.58	0.41
1:B:193:ARG:NE	4:B:605:HOH:O	2.22	0.41
1:B:190:GLY:O	1:B:192:PRO:HD3	2.19	0.41
1:A:225:ILE:HG22	1:A:238:ALA:HB3	2.02	0.41
1:B:324:LYS:O	1:B:326:ASP:N	2.53	0.41
1:A:519:SER:O	1:A:523:ARG:N	2.54	0.41
1:A:488:VAL:HB	1:A:525:ILE:HD12	2.02	0.41
1:B:352:ASN:O	1:B:356:LEU:HB2	2.21	0.41
1:B:144:ALA:HB1	1:B:168:ARG:HE	1.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:56:ASP:HB3	1:B:57:GLY:H	1.71	0.41
1:A:335:ARG:HH11	1:A:335:ARG:CB	2.34	0.41
1:B:370:ILE:CG2	1:B:377:ALA:HB2	2.50	0.41
1:B:426:VAL:O	1:B:430:LEU:CB	2.69	0.41
1:A:155:ASN:CG	1:A:155:ASN:O	2.59	0.41
1:A:10:ILE:C	1:A:12:GLN:H	2.23	0.41
1:B:124:ASP:O	1:B:129:PHE:CA	2.69	0.41
1:B:477:TYR:CZ	1:B:518:LEU:HB2	2.56	0.41
1:B:363:LEU:CD2	1:B:395:LEU:HD11	2.50	0.41
1:B:66:THR:HA	1:B:67:PRO:HD2	1.93	0.41
1:A:547:ILE:CD1	1:A:556:THR:O	2.68	0.41
1:A:515:GLU:OE2	1:A:517:ARG:HD3	2.21	0.41
1:B:62:VAL:HG21	1:B:78:SER:OG	2.20	0.41
1:B:311:GLU:OE1	1:B:315:ASP:OD1	2.39	0.41
1:A:170:ILE:HA	1:A:170:ILE:HD12	1.90	0.41
1:B:490:ALA:HB3	1:B:527:PRO:CA	2.49	0.41
1:B:308:LEU:O	1:B:312:LYS:HG3	2.20	0.41
1:B:65:ILE:HG21	1:B:337:LEU:HD11	2.03	0.41
1:B:367:ILE:HG21	1:B:401:LYS:HD3	2.02	0.41
1:A:533:MET:CA	2:A:561:SO4:O2	2.67	0.41
1:B:62:VAL:HG11	1:B:78:SER:CB	2.51	0.41
1:B:269:PHE:CD2	1:B:291:ALA:HB2	2.57	0.41
1:B:523:ARG:HH11	1:B:525:ILE:CD1	2.30	0.41
1:B:339:MET:C	1:B:341:GLY:N	2.75	0.41
1:A:360:PHE:CE2	1:A:398:LEU:HD12	2.55	0.41
1:A:106:GLY:HA3	1:A:538:LEU:HD22	2.03	0.41
1:A:67:PRO:O	1:A:494:TYR:HD2	2.03	0.41
1:A:368:GLU:CG	1:A:401:LYS:HE2	2.51	0.40
1:B:466:TYR:CG	1:B:513:VAL:CG1	3.04	0.40
1:A:159:ILE:O	1:A:161:PRO:CD	2.67	0.40
1:A:389:GLU:HB3	1:A:393:ASN:HD21	1.85	0.40
1:B:65:ILE:CD1	1:B:332:ALA:HA	2.51	0.40
1:B:17:LYS:O	1:B:261:GLN:NE2	2.51	0.40
1:A:517:ARG:HH12	1:A:532:ILE:HG13	1.86	0.40
1:A:149:ASN:O	1:A:153:GLN:HG2	2.21	0.40
1:B:393:ASN:CB	4:B:597:HOH:O	2.70	0.40
1:B:350:THR:CG2	1:B:351:GLU:H	2.34	0.40
1:A:159:ILE:HG12	1:A:236:VAL:HG21	2.04	0.40
1:B:107:ILE:HD12	1:B:107:ILE:O	2.21	0.40
1:B:319:ARG:HH21	1:B:443:LEU:HB2	1.86	0.40
1:B:539:PRO:O	1:B:542:PRO:HG3	2.22	0.40
1:B:540:LYS:C	1:B:542:PRO:HD3	2.42	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271:HIS:CD2	1:A:272:GLY:H	2.40	0.40
1:A:33:VAL:HG13	1:A:41:ALA:HB1	2.02	0.40
1:B:96:LEU:C	1:B:97:ARG:HG3	2.41	0.40
1:B:203:SER:OG	1:B:205:VAL:HB	2.21	0.40
1:A:311:GLU:OE1	1:A:315:ASP:OD1	2.39	0.40
1:A:124:ASP:N	1:A:124:ASP:OD1	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:187:LYS:NZ	4:B:572:HOH:O[4_555]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	547/557 (98%)	445 (81%)	84 (15%)	18 (3%)	6	32
1	B	546/557 (98%)	392 (72%)	109 (20%)	45 (8%)	1	6
All	All	1093/1114 (98%)	837 (77%)	193 (18%)	63 (6%)	3	15

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	52	LYS
1	A	352	ASN
1	A	556	THR
1	B	65	ILE
1	B	286	ILE
1	B	325	PRO
1	B	400	ALA
1	B	445	LEU
1	A	166	TRP

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Mol	Chain	Res	Type
1	A	176	ALA
1	A	317	LYS
1	A	401	LYS
1	A	531	ALA
1	A	533	MET
1	B	56	ASP
1	B	72	GLU
1	B	187	LYS
1	B	294	LEU
1	B	332	ALA
1	B	388	THR
1	B	401	LYS
1	B	412	TRP
1	B	509	PHE
1	B	556	THR
1	A	49	ARG
1	A	400	ALA
1	B	244	GLN
1	B	317	LYS
1	B	456	THR
1	B	495	SER
1	B	520	ALA
1	A	112	ALA
1	A	498	ASP
1	B	48	TYR
1	B	76	THR
1	B	100	SER
1	B	102	GLY
1	B	176	ALA
1	B	273	GLY
1	B	328	THR
1	B	399	CYS
1	B	403	GLY
1	B	418	GLY
1	B	551	ALA
1	B	554	VAL
1	A	26	LEU
1	B	12	GLN
1	B	49	ARG
1	B	285	ILE
1	B	319	ARG
1	B	334	VAL

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Mol	Chain	Res	Type
1	B	367	ILE
1	A	160	ASP
1	B	376	PRO
1	A	344	PRO
1	B	154	GLY
1	B	385	PRO
1	B	486	PRO
1	B	516	VAL
1	A	325	PRO
1	B	60	ILE
1	B	528	ILE

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	432/440 (98%)	399 (92%)	33 (8%)	19	57
1	B	431/440 (98%)	400 (93%)	31 (7%)	21	59
All	All	863/880 (98%)	799 (93%)	64 (7%)	20	58

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	MET
1	A	61	LEU
1	A	62	VAL
1	A	94	VAL
1	A	124	ASP
1	A	195	THR
1	A	224	ARG
1	A	226	VAL
1	A	232	ASP
1	A	244	GLN
1	A	277	ASN
1	A	278	ILE
1	A	286	ILE
1	A	311	GLU

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Mol	Chain	Res	Type
1	A	319	ARG
1	A	328	THR
1	A	330	ILE
1	A	337	LEU
1	A	346	SER
1	A	347	ASP
1	A	356	LEU
1	A	375	VAL
1	A	398	LEU
1	A	409	SER
1	A	443	LEU
1	A	456	THR
1	A	480	LEU
1	A	517	ARG
1	A	523	ARG
1	A	526	VAL
1	A	529	THR
1	A	533	MET
1	A	552	ASP
1	B	12	GLN
1	B	20	MET
1	B	72	GLU
1	B	85	LEU
1	B	124	ASP
1	B	148	ASP
1	B	193	ARG
1	B	222	PHE
1	B	229	TYR
1	B	244	GLN
1	B	265	ASN
1	B	266	THR
1	B	275	PHE
1	B	277	ASN
1	B	290	THR
1	B	311	GLU
1	B	313	PHE
1	B	333	THR
1	B	375	VAL
1	B	382	ASN
1	B	396	TYR
1	B	462	ASP
1	B	466	TYR

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Mol	Chain	Res	Type
1	B	480	LEU
1	B	503	LEU
1	B	523	ARG
1	B	526	VAL
1	B	529	THR
1	B	535	MET
1	B	549	ILE
1	B	552	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	126	ASN
1	A	140	HIS
1	A	150	HIS
1	A	189	ASN
1	A	244	GLN
1	A	277	ASN
1	A	362	ASN
1	A	382	ASN
1	A	393	ASN
1	A	465	ASN
1	A	484	ASN
1	A	546	ASN
1	B	12	GLN
1	B	29	GLN
1	B	118	GLN
1	B	140	HIS
1	B	150	HIS
1	B	153	GLN
1	B	189	ASN
1	B	244	GLN
1	B	265	ASN
1	B	277	ASN
1	B	280	HIS
1	B	362	ASN
1	B	369	ASN
1	B	382	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	560	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	A	561	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	A	562	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	A	563	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	A	564	-	4,4,4	1.65	1 (25%)	6,6,6	0.47	0
2	SO4	A	565	-	4,4,4	1.66	1 (25%)	6,6,6	0.47	0
2	SO4	A	566	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	B	560	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	B	561	1	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	B	562	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0
2	SO4	B	563	-	4,4,4	1.66	1 (25%)	6,6,6	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	560	-	-	0/0/0/0	0/0/0/0
2	SO4	A	561	-	-	0/0/0/0	0/0/0/0
2	SO4	A	562	-	-	0/0/0/0	0/0/0/0
2	SO4	A	563	-	-	0/0/0/0	0/0/0/0
2	SO4	A	564	-	-	0/0/0/0	0/0/0/0
2	SO4	A	565	-	-	0/0/0/0	0/0/0/0
2	SO4	A	566	-	-	0/0/0/0	0/0/0/0
2	SO4	B	560	-	-	0/0/0/0	0/0/0/0
2	SO4	B	561	1	-	0/0/0/0	0/0/0/0
2	SO4	B	562	-	-	0/0/0/0	0/0/0/0
2	SO4	B	563	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	566	SO4	O1-S	-2.28	1.39	1.47
2	B	563	SO4	O1-S	-2.28	1.39	1.47
2	A	565	SO4	O1-S	-2.28	1.39	1.47
2	B	561	SO4	O1-S	-2.27	1.39	1.47
2	A	563	SO4	O1-S	-2.27	1.39	1.47
2	A	562	SO4	O1-S	-2.27	1.39	1.47
2	B	560	SO4	O1-S	-2.26	1.39	1.47
2	A	564	SO4	O1-S	-2.26	1.39	1.47
2	B	562	SO4	O1-S	-2.26	1.39	1.47
2	A	561	SO4	O1-S	-2.24	1.39	1.47
2	A	560	SO4	O1-S	-2.25	1.39	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.