



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:59 am BST

PDB ID : 5FRR
Title : Structure of the Pds5-Scc1 complex and implications for cohesin function
Authors : Muir, K.W.; Kschonsak, M.; Li, Y.; Metz, J.; Haering, C.H.; Panne, D.
Deposited on : 2015-12-22
Resolution : 5.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

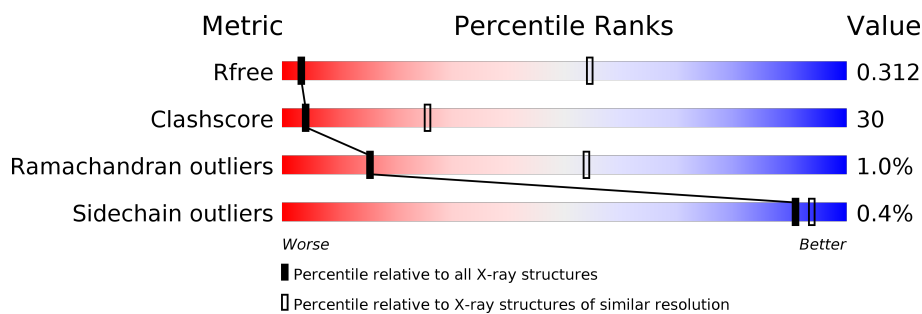
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1008 (7.70-3.86)
Clashscore	141614	1035 (7.70-3.90)
Ramachandran outliers	138981	1003 (7.70-3.86)
Sidechain outliers	138945	1006 (7.78-3.82)

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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	703	
1	B	703	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10858 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 SISTER CHROMATID COHESION PROTEIN PDS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	0	0	0
			5494	3526	914	1041	13			
1	B	660	Total	C	N	O	S	0	0	0
			5364	3455	889	1009	11			

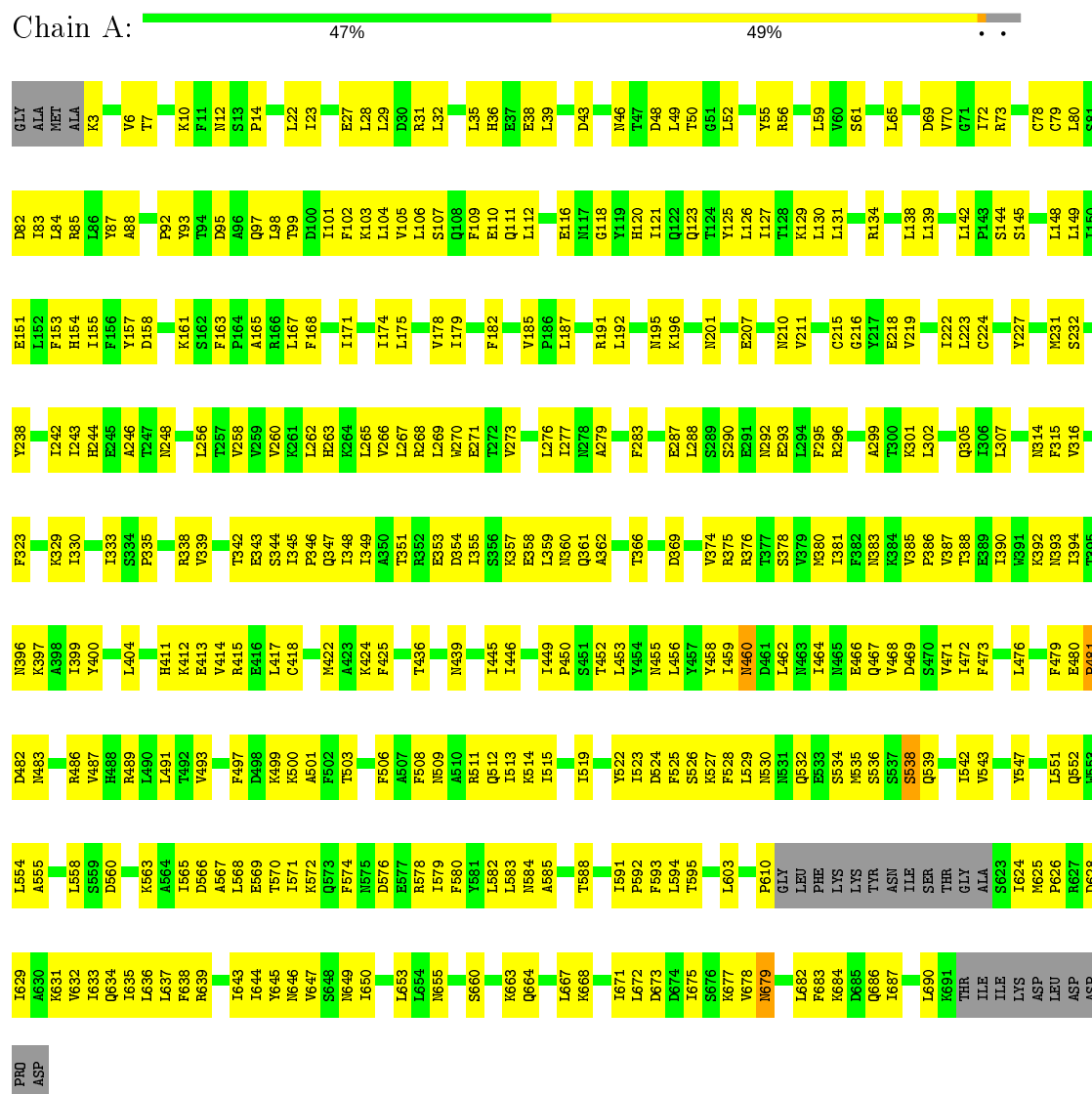
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q04264
A	0	ALA	-	expression tag	UNP Q04264
B	-1	GLY	-	expression tag	UNP Q04264
B	0	ALA	-	expression tag	UNP Q04264

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 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.

• Molecule 1: SISTER CHROMATID COHESION PROTEIN PDS5



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I633	E569	F502	L406	I330	I243	Y157	I83	GLY
Q634	T570	T503	H411	I333	D249	D158	L84	ALA
I635	I571	F506	K412	I333	D250	N160	Y87	MET
L636	K572		E413	V339	N251	K161	A88	ALA
L637			V414	E340		S162		K3
F638	K575						D95	V6
R639	ASP	N509	R415	W341	R254	F163		
	GLU	A510	E416	T342	L255	P164	A96	
P642	R578	R511	L417	E343	L256	A165	Q97	S17
I643	I579	Q512	C418	S344	R346	R166	L98	T18
I644	F580	Q513		S345	V258	L167	T99	
V645	E581	K514	M422	P346	V259	F168	D100	Q21
M646	L582	I515		Q347	V260		I101	L22
F647	S516	S516	F425	I348	K261	I171	F102	I23
S648	N584				L262		K103	T25
N649	A585	I519	L430	T351	H263	I174	L104	T26
F650	C586	S520	M431	R352	K264	L175	V105	N26
S651	V587	K521		E583	L265		L106	E27
V652	T588	Y522	I442	D354	V267	V178	E107	I28
L653	N589	I523	I442	I355	L267	L135	Q108	L29
L654	D590	F524	I446	S356	R268	F182	F109	D30
N655	I591	R525	T447	K357	L269	V185	E110	R31
	P592	D526	T448	D447	W270	V185	Q111	E32
S657	F593	K527	T449	S526	E271	P186		D33
ASN	L594	F528	P450	T452	L359	L87	E116	A34
ASN	T595	LEU	S451	A362	N360	E188	L35	L35
S660	K597	ASN	T453	A362	L276	V189	H120	R36
	N598	GLN	L453	L363	I277	R191	I121	E37
K663	C599	GLU	L456	T366		L192	Q122	E38
L667		SER			T283		Q123	L39
L603	L603	MET	D461	P372	I284	N195	T124	L42
V604	V604	SER	L462	R373			Y125	
		SER	N463	V374	E287	N201	L126	N46
L607	L607	SER	I464	R375	L288	P202	I127	N46
Q608	Q608	GLN		R376		N203	T47	T47
T609	T609	GLY	Q467	R377	N292	E204	K129	D48
PRO	PRO	PRO	V468	S378	E293	E204	L130	L49
	GLY	I542	D469	V379	L294	P206	L131	T50
LEU	LEU	V543	S470	M380	F295	E207	E132	G51
	PHE	M544	V471	I381	R296	C208	Y133	L52
LYS	LYS		I472			L209		R56
L682	L682	Y547	F473	V385	A299		I136	
F683	F683	TYR	L476	P386	T300	C215	V137	
K684	K684	ASN	L476	V387	K301	L139	L139	L59
	ILE	Q552			L302	E218		V60
SER	SER	L554	F479	I390	Q305	V219	L142	S61
THR	THR	L554	E480				P143	R62
	GLY	A555	P481	I394	T308	I222	S144	L65
ALA	ALA	S556	N483	T395	L223	C224	S145	K66
	SER		N396	N396	L233			
ILE	ILE	S559	D484	K397	N314	R230	L148	V70
MET	MET	D560	K485	K397	F315	E230	L149	G71
PRO	PRO		R486	I399	V316		I150	I72
	ARG	K563	V487	Y400	S320	T236	E151	R73
ASP	ASP	A564		T401		K237	L152	
	ASP	I639	L490	S402	L903	Y238	L152	
PRO	PRO	D566	L491	L403	K324	Y239	F153	C78
	ASP	K631	A567	L404			H154	C79
		L568		H405			I155	L80
			Y200	E406			F156	

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	283.69 Å 283.69 Å 172.79 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 5.80 49.19 – 5.79	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-5.80) 99.6 (49.19-5.79)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 5.73 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.311 0.251 , 0.312	Depositor DCC
R_{free} test set	518 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	383.9	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 403.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	10858	wwPDB-VP
Average B, all atoms (Å ²)	424.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.25	0/5600	0.42	0/7597
1	B	0.25	0/5464	0.41	0/7408
All	All	0.25	0/11064	0.41	0/15005

There are no bond length outliers.

There are no bond angle outliers.

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	5494	0	5551	334	0
1	B	5364	0	5435	324	1
All	All	10858	0	10986	647	1

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 30.

All (647) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ILE:HD12	1:B:333:ILE:H	1.29	0.97
1:A:98:LEU:HD23	1:A:142:LEU:HD21	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ARG:HA	1:B:376:ARG:HH12	1.36	0.91
1:B:98:LEU:HD23	1:B:142:LEU:HD21	1.52	0.89
1:B:462:LEU:HD13	1:B:559:SER:HA	1.53	0.88
1:A:333:ILE:H	1:A:333:ILE:HD12	1.39	0.86
1:A:483:ASN:HA	1:A:486:ARG:NH1	1.94	0.82
1:B:523:ILE:HD13	1:B:580:PHE:HA	1.63	0.81
1:A:70:VAL:HG12	1:A:73:ARG:HH21	1.46	0.80
1:B:372:PRO:HA	1:B:375:ARG:HE	1.49	0.78
1:B:70:VAL:HG12	1:B:73:ARG:HH21	1.47	0.78
1:B:396:ASN:HB3	1:B:399:ILE:HG12	1.65	0.78
1:A:342:THR:HA	1:A:345:ILE:HD13	1.65	0.78
1:B:308:THR:HA	1:B:351:THR:HG21	1.66	0.78
1:B:105:VAL:HG23	1:B:126:LEU:HD21	1.64	0.77
1:A:682:LEU:H	1:A:682:LEU:HD23	1.50	0.77
1:A:293:GLU:HA	1:A:296:ARG:HE	1.51	0.76
1:A:610:PRO:HG3	1:A:626:PRO:HG2	1.66	0.76
1:A:105:VAL:HG23	1:A:126:LEU:HD21	1.66	0.75
1:B:351:THR:HG22	1:B:352:ARG:HG3	1.67	0.75
1:B:111:GLN:HB2	1:B:123:GLN:HE22	1.53	0.73
1:A:396:ASN:HB3	1:A:399:ILE:HG12	1.70	0.73
1:B:483:ASN:HA	1:B:486:ARG:NH1	2.03	0.73
1:B:242:ILE:HG21	1:B:262:LEU:HD21	1.70	0.73
1:A:480:GLU:HB2	1:A:481:PRO:HA	1.70	0.72
1:A:69:ASP:HB3	1:A:72:ILE:HD13	1.72	0.72
1:A:330:ILE:HG21	1:A:362:ALA:HB1	1.70	0.72
1:A:121:ILE:HD12	1:A:121:ILE:H	1.54	0.71
1:A:154:HIS:HD2	1:A:192:LEU:HD22	1.55	0.70
1:B:633:ILE:HD12	1:B:634:GLN:N	2.07	0.70
1:B:512:GLN:HA	1:B:639:ARG:O	1.92	0.70
1:A:56:ARG:HD2	1:A:92:PRO:HB2	1.74	0.69
1:B:373:ARG:HA	1:B:376:ARG:NH1	2.07	0.69
1:A:380:MET:HA	1:A:383:ASN:HD22	1.55	0.69
1:A:111:GLN:HB2	1:A:123:GLN:HE22	1.57	0.69
1:A:381:ILE:O	1:A:385:VAL:HG12	1.91	0.69
1:B:522:TYR:OH	1:B:572:LYS:HG3	1.93	0.69
1:B:263:HIS:HB3	1:B:302:LEU:HD13	1.74	0.69
1:A:196:LYS:HE3	1:A:216:GLY:HA3	1.74	0.68
1:A:473:PHE:HB3	1:A:479:PHE:HE1	1.57	0.68
1:B:381:ILE:O	1:B:385:VAL:HG12	1.94	0.67
1:A:263:HIS:HB3	1:A:302:LEU:HD13	1.77	0.67
1:B:339:VAL:HG13	1:B:377:THR:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:ILE:HD12	1:B:514:LYS:N	2.10	0.67
1:A:52:LEU:HD23	1:A:52:LEU:O	1.95	0.66
1:A:201:ASN:ND2	1:A:268:ARG:HE	1.93	0.66
1:B:272:THR:HG23	1:B:273:VAL:HG22	1.76	0.66
1:A:513:ILE:HD12	1:A:514:LYS:N	2.09	0.66
1:B:522:TYR:OH	1:B:571:ILE:HG13	1.95	0.66
1:A:411:HIS:HE1	1:A:413:GLU:HB3	1.61	0.65
1:B:164:PRO:HG2	1:B:167:LEU:HD13	1.78	0.65
1:A:349:ILE:HG23	1:A:393:ASN:ND2	2.12	0.65
1:B:99:THR:HG22	1:B:142:LEU:HD13	1.79	0.65
1:B:522:TYR:CE1	1:B:568:LEU:HB3	2.32	0.65
1:B:330:ILE:HG21	1:B:362:ALA:HB1	1.79	0.65
1:A:539:GLN:O	1:A:543:VAL:HG12	1.97	0.64
1:B:604:VAL:O	1:B:608:GLN:HG3	1.98	0.64
1:A:687:ILE:HD13	1:B:687:ILE:HG12	1.78	0.64
1:A:482:ASP:CG	1:A:483:ASN:H	2.00	0.64
1:B:415:ARG:NH1	1:B:464:ILE:HD11	2.13	0.64
1:A:360:ASN:HB3	1:A:396:ASN:HB2	1.79	0.63
1:A:683:PHE:HZ	1:B:690:LEU:HB3	1.61	0.63
1:B:102:PHE:HA	1:B:105:VAL:HG12	1.80	0.63
1:A:333:ILE:HD12	1:A:333:ILE:N	2.13	0.63
1:A:683:PHE:CZ	1:B:690:LEU:HD13	2.33	0.63
1:A:79:CYS:O	1:A:83:ILE:HG12	1.98	0.63
1:A:509:ASN:OD1	1:A:644:ILE:HD11	1.99	0.63
1:B:490:LEU:O	1:B:490:LEU:HD23	1.99	0.63
1:A:551:LEU:HD12	1:A:552:GLN:N	2.14	0.63
1:B:201:ASN:O	1:B:204:GLU:HG2	1.99	0.63
1:B:267:LEU:O	1:B:271:GLU:HG3	1.99	0.63
1:B:522:TYR:HH	1:B:572:LYS:HG3	1.64	0.63
1:A:102:PHE:O	1:A:106:LEU:HG	1.99	0.62
1:B:572:LYS:NZ	1:B:572:LYS:HB3	2.14	0.62
1:B:635:ILE:HD12	1:B:636:LEU:N	2.14	0.62
1:B:449:ILE:O	1:B:453:LEU:HD13	1.99	0.62
1:A:165:ALA:HA	1:A:168:PHE:CD1	2.35	0.62
1:A:151:GLU:O	1:A:155:ILE:HG13	2.00	0.62
1:A:256:LEU:O	1:A:260:VAL:HG23	2.00	0.62
1:B:394:ILE:HD12	1:B:394:ILE:O	2.00	0.62
1:A:568:LEU:HD12	1:A:569:GLU:N	2.14	0.61
1:B:650:ILE:HD12	1:B:651:SER:N	2.14	0.61
1:A:412:LYS:HB3	1:A:412:LYS:NZ	2.15	0.61
1:A:583:LEU:HD13	1:A:633:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:PHE:O	1:A:287:GLU:HG3	1.99	0.61
1:A:333:ILE:CD1	1:A:333:ILE:H	2.13	0.61
1:A:394:ILE:HD12	1:A:394:ILE:O	2.00	0.61
1:B:462:LEU:HB3	1:B:559:SER:CB	2.30	0.61
1:B:18:THR:HG23	1:B:21:GLN:H	1.65	0.61
1:B:547:TYR:OH	1:B:572:LYS:HE3	2.00	0.61
1:A:686:GLN:O	1:A:690:LEU:HG	2.01	0.61
1:A:3:LYS:HB3	1:A:50:THR:HG21	1.82	0.61
1:A:387:VAL:HA	1:A:390:ILE:HD12	1.82	0.60
1:A:524:ASP:HA	1:A:527:LYS:HE2	1.83	0.60
1:B:80:LEU:HD13	1:B:101:ILE:HG23	1.83	0.60
1:A:415:ARG:NH1	1:A:464:ILE:HD11	2.16	0.60
1:B:513:ILE:HG22	1:B:589:ASN:HD21	1.65	0.60
1:A:483:ASN:HA	1:A:486:ARG:HH12	1.66	0.60
1:B:462:LEU:HB3	1:B:559:SER:HB3	1.83	0.60
1:A:201:ASN:HD22	1:A:268:ARG:HE	1.49	0.60
1:B:655:ASN:OD1	1:B:668:LYS:HD2	2.01	0.60
1:A:290:SER:O	1:A:296:ARG:HD3	2.01	0.60
1:A:288:LEU:HB3	1:A:329:LYS:HE3	1.83	0.60
1:B:151:GLU:O	1:B:155:ILE:HG13	2.02	0.60
1:B:554:LEU:HD12	1:B:555:ALA:N	2.17	0.60
1:A:635:ILE:HA	1:A:638:PHE:HD2	1.66	0.59
1:A:584:ASN:O	1:A:588:THR:HG23	2.01	0.59
1:B:355:ILE:HD12	1:B:355:ILE:N	2.17	0.59
1:B:467:GLN:O	1:B:471:VAL:HG23	2.03	0.59
1:B:628:ASP:O	1:B:631:LYS:HG2	2.01	0.59
1:A:489:ARG:O	1:A:493:VAL:HG23	2.02	0.59
1:B:648:SER:O	1:B:652:VAL:HG23	2.03	0.59
1:A:49:LEU:HD23	1:A:49:LEU:O	2.02	0.59
1:B:156:PHE:HA	1:B:163:PHE:CE2	2.38	0.59
1:B:333:ILE:H	1:B:333:ILE:CD1	2.07	0.59
1:A:418:CYS:O	1:A:422:MET:HG2	2.02	0.59
1:A:635:ILE:HA	1:A:638:PHE:CD2	2.38	0.59
1:B:70:VAL:HG12	1:B:73:ARG:NH2	2.16	0.59
1:A:673:ASP:OD1	1:A:677:LYS:HE2	2.03	0.59
1:A:70:VAL:HG12	1:A:73:ARG:NH2	2.16	0.59
1:B:676:SER:HA	1:B:682:LEU:HD11	1.84	0.59
1:B:49:LEU:O	1:B:49:LEU:HD23	2.03	0.59
1:A:456:LEU:O	1:A:459:ILE:HG13	2.02	0.59
1:B:254:ARG:O	1:B:258:VAL:HG23	2.03	0.58
1:B:95:ASP:O	1:B:99:THR:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ILE:HG13	1:A:645:TYR:CD1	2.38	0.58
1:B:523:ILE:HD11	1:B:583:LEU:HD23	1.85	0.58
1:A:121:ILE:HD12	1:A:121:ILE:N	2.17	0.58
1:B:288:LEU:HB3	1:B:329:LYS:CE	2.33	0.58
1:B:314:ASN:OD1	1:B:316:VAL:HG22	2.03	0.58
1:A:110:GLU:HG3	1:A:161:LYS:NZ	2.18	0.58
1:B:288:LEU:HB3	1:B:329:LYS:HE3	1.84	0.58
1:B:139:LEU:HD23	1:B:139:LEU:O	2.04	0.58
1:B:22:LEU:O	1:B:22:LEU:HD12	2.04	0.58
1:B:333:ILE:HD12	1:B:333:ILE:N	2.11	0.58
1:B:646:ASN:OD1	1:B:647:VAL:HG13	2.03	0.58
1:A:355:ILE:HD12	1:A:355:ILE:N	2.19	0.57
1:B:116:GLU:HA	1:B:120:HIS:CE1	2.39	0.57
1:B:186:PRO:HG2	1:B:189:VAL:HG23	1.86	0.57
1:B:256:LEU:O	1:B:260:VAL:HG23	2.04	0.57
1:B:355:ILE:HG22	1:B:359:LEU:HG	1.84	0.57
1:B:554:LEU:HD11	1:B:568:LEU:HD11	1.86	0.57
1:A:139:LEU:HD23	1:A:139:LEU:O	2.04	0.57
1:B:110:GLU:HG3	1:B:161:LYS:HZ1	1.69	0.57
1:B:523:ILE:HG21	1:B:580:PHE:HB3	1.85	0.57
1:B:251:ASN:HB3	1:B:254:ARG:HB2	1.85	0.57
1:A:624:ILE:HG12	1:A:625:MET:N	2.19	0.57
1:A:571:ILE:HA	1:A:574:PHE:CD2	2.39	0.57
1:B:519:ILE:O	1:B:522:TYR:HB3	2.04	0.57
1:B:481:PRO:HG2	1:B:482:ASP:H	1.70	0.57
1:A:288:LEU:HB3	1:A:329:LYS:CE	2.35	0.57
1:A:187:LEU:HG	1:A:191:ARG:NH1	2.20	0.57
1:B:509:ASN:HD21	1:B:644:ILE:HD11	1.69	0.57
1:A:293:GLU:HA	1:A:296:ARG:NE	2.19	0.56
1:A:449:ILE:N	1:A:450:PRO:HD2	2.19	0.56
1:A:376:ARG:O	1:A:380:MET:HG2	2.03	0.56
1:B:449:ILE:HB	1:B:450:PRO:HD3	1.87	0.56
1:B:633:ILE:O	1:B:637:LEU:HG	2.04	0.56
1:A:110:GLU:HG3	1:A:161:LYS:HZ1	1.69	0.56
1:A:446:ILE:HD12	1:A:446:ILE:N	2.21	0.56
1:B:645:TYR:CE2	1:B:678:VAL:HG21	2.41	0.56
1:B:175:LEU:HD12	1:B:219:VAL:HG11	1.88	0.56
1:B:513:ILE:HG22	1:B:589:ASN:ND2	2.21	0.56
1:B:686:GLN:O	1:B:690:LEU:HG	2.04	0.56
1:A:397:LYS:NZ	1:A:445:ILE:HD11	2.21	0.56
1:B:78:CYS:SG	1:B:122:GLN:HB3	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:SER:HA	1:B:23:ILE:HD13	1.88	0.56
1:B:579:ILE:HG23	1:B:603:LEU:HD11	1.87	0.56
1:A:560:ASP:OD1	1:A:563:LYS:HB2	2.06	0.56
1:B:62:ARG:NH1	1:B:66:LYS:HD2	2.21	0.56
1:B:187:LEU:O	1:B:187:LEU:HD23	2.06	0.56
1:B:273:VAL:HB	1:B:276:LEU:HD13	1.86	0.56
1:A:453:LEU:HA	1:A:456:LEU:HD13	1.86	0.55
1:B:23:ILE:HD12	1:B:23:ILE:N	2.22	0.55
1:A:14:PRO:HG2	1:A:31:ARG:NH1	2.21	0.55
1:B:110:GLU:HG3	1:B:161:LYS:NZ	2.21	0.55
1:B:584:ASN:HA	1:B:587:VAL:HG12	1.88	0.55
1:A:22:LEU:C	1:A:23:ILE:HD12	2.27	0.55
1:A:633:ILE:O	1:A:637:LEU:HG	2.07	0.55
1:B:386:PRO:O	1:B:390:ILE:HG13	2.06	0.55
1:A:459:ILE:HD12	1:A:460:ASN:N	2.21	0.55
1:A:95:ASP:O	1:A:99:THR:HG23	2.07	0.55
1:B:131:LEU:HB2	1:B:174:ILE:HD11	1.89	0.55
1:B:283:PHE:O	1:B:287:GLU:HG3	2.07	0.55
1:A:565:ILE:HG13	1:A:566:ASP:OD1	2.06	0.55
1:B:592:PRO:O	1:B:595:THR:HG22	2.07	0.55
1:A:568:LEU:HA	1:A:571:ILE:HD12	1.88	0.55
1:A:664:GLN:HG2	1:A:668:LYS:HE3	1.88	0.55
1:B:219:VAL:O	1:B:223:LEU:HD13	2.07	0.55
1:B:663:LYS:O	1:B:667:LEU:HD13	2.07	0.55
1:B:188:GLU:O	1:B:192:LEU:HG	2.08	0.54
1:A:270:TRP:HE3	1:A:277:ILE:HG13	1.73	0.54
1:B:102:PHE:O	1:B:106:LEU:HG	2.08	0.54
1:B:288:LEU:HD12	1:B:299:ALA:HB1	1.89	0.54
1:B:654:LEU:C	1:B:655:ASN:HD22	2.11	0.54
1:A:335:PRO:HA	1:A:338:ARG:HD2	1.90	0.54
1:A:628:ASP:O	1:A:632:VAL:HG23	2.07	0.54
1:B:372:PRO:HB3	1:B:375:ARG:HH21	1.71	0.54
1:A:219:VAL:O	1:A:223:LEU:HD13	2.08	0.54
1:B:102:PHE:O	1:B:105:VAL:HG12	2.08	0.54
1:B:238:TYR:O	1:B:242:ILE:HG12	2.07	0.54
1:B:418:CYS:O	1:B:422:MET:HG2	2.08	0.54
1:B:453:LEU:HD22	1:B:476:LEU:HD21	1.90	0.54
1:B:560:ASP:OD1	1:B:563:LYS:HG3	2.07	0.54
1:A:690:LEU:HD13	1:B:683:PHE:CE2	2.43	0.54
1:B:376:ARG:O	1:B:380:MET:HG2	2.08	0.54
1:A:668:LYS:O	1:A:672:LEU:HD13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:PHE:CZ	1:B:690:LEU:HB3	2.43	0.54
1:A:22:LEU:HD12	1:A:22:LEU:O	2.08	0.54
1:A:467:GLN:O	1:A:471:VAL:HG23	2.07	0.54
1:A:509:ASN:CG	1:A:644:ILE:HD11	2.29	0.53
1:B:165:ALA:HA	1:B:168:PHE:CD1	2.43	0.53
1:B:205:ILE:N	1:B:206:PRO:CD	2.71	0.53
1:B:316:VAL:HG11	1:B:355:ILE:HD11	1.90	0.53
1:A:157:TYR:HB2	1:A:192:LEU:HD21	1.89	0.53
1:A:585:ALA:O	1:A:591:ILE:HD13	2.07	0.53
1:B:396:ASN:HB3	1:B:399:ILE:CG1	2.37	0.53
1:B:411:HIS:HE1	1:B:413:GLU:HB3	1.72	0.53
1:A:23:ILE:N	1:A:23:ILE:HD12	2.23	0.53
1:A:84:LEU:O	1:A:88:ALA:HB2	2.08	0.53
1:A:635:ILE:HD12	1:A:636:LEU:N	2.24	0.53
1:B:156:PHE:HA	1:B:163:PHE:HE2	1.73	0.53
1:A:215:CYS:O	1:A:219:VAL:HG23	2.08	0.53
1:B:22:LEU:C	1:B:23:ILE:HD12	2.29	0.53
1:B:292:ASN:HB3	1:B:295:PHE:HD2	1.73	0.53
1:B:344:SER:O	1:B:348:ILE:HG13	2.09	0.53
1:B:516:SER:OG	1:B:587:VAL:HG22	2.09	0.53
1:A:154:HIS:O	1:A:158:ASP:HB2	2.09	0.53
1:A:646:ASN:OD1	1:A:647:VAL:HG13	2.09	0.53
1:B:479:PHE:HB3	1:B:597:LYS:HD3	1.90	0.53
1:A:571:ILE:HA	1:A:574:PHE:HD2	1.72	0.53
1:A:624:ILE:HG12	1:A:625:MET:H	1.73	0.53
1:B:205:ILE:O	1:B:207:GLU:HG2	2.09	0.53
1:A:380:MET:SD	1:A:417:LEU:HD21	2.49	0.52
1:A:411:HIS:CE1	1:A:413:GLU:HB3	2.43	0.52
1:A:673:ASP:O	1:A:677:LYS:HG3	2.09	0.52
1:B:566:ASP:O	1:B:570:THR:HG23	2.08	0.52
1:B:671:ILE:HG22	1:B:675:ILE:HD11	1.90	0.52
1:A:664:GLN:O	1:A:668:LYS:HG3	2.09	0.52
1:B:589:ASN:HA	1:B:642:PRO:HG3	1.91	0.52
1:B:84:LEU:O	1:B:88:ALA:HB2	2.10	0.52
1:A:339:VAL:O	1:A:343:GLU:HG3	2.09	0.52
1:A:449:ILE:O	1:A:453:LEU:HD13	2.09	0.52
1:A:551:LEU:HD22	1:A:568:LEU:HD11	1.91	0.52
1:B:254:ARG:HA	1:B:254:ARG:HE	1.74	0.52
1:B:643:ILE:HD12	1:B:643:ILE:N	2.25	0.52
1:A:644:ILE:HG13	1:A:645:TYR:HD1	1.75	0.52
1:A:72:ILE:N	1:A:72:ILE:HD12	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:LYS:HB3	1:B:525:PHE:CE2	2.44	0.52
1:B:380:MET:SD	1:B:417:LEU:HD21	2.50	0.52
1:B:3:LYS:HE3	1:B:50:THR:HG21	1.91	0.52
1:B:565:ILE:HG13	1:B:566:ASP:OD1	2.09	0.52
1:A:262:LEU:O	1:A:266:VAL:HG23	2.08	0.52
1:A:527:LYS:HA	1:A:530:ASN:OD1	2.10	0.52
1:A:121:ILE:CD1	1:A:121:ILE:H	2.20	0.52
1:A:238:TYR:O	1:A:242:ILE:HG12	2.10	0.52
1:A:396:ASN:HB3	1:A:399:ILE:CG1	2.40	0.52
1:A:99:THR:HG22	1:A:142:LEU:HD13	1.92	0.52
1:A:355:ILE:HG22	1:A:359:LEU:HG	1.92	0.51
1:A:27:GLU:O	1:A:31:ARG:HG3	2.10	0.51
1:A:523:ILE:HG23	1:A:580:PHE:HD2	1.75	0.51
1:B:649:ASN:O	1:B:653:LEU:HG	2.10	0.51
1:A:314:ASN:OD1	1:A:316:VAL:HG22	2.11	0.51
1:A:643:ILE:N	1:A:643:ILE:HD12	2.25	0.51
1:B:464:ILE:O	1:B:468:VAL:HG23	2.10	0.51
1:A:301:LYS:O	1:A:305:GLN:HG3	2.10	0.51
1:A:459:ILE:HD12	1:A:459:ILE:C	2.31	0.51
1:A:506:PHE:HA	1:A:509:ASN:HD22	1.74	0.51
1:B:215:CYS:O	1:B:219:VAL:HG23	2.11	0.51
1:B:607:LEU:HD23	1:B:633:ILE:HG12	1.92	0.51
1:B:693:ILE:HD12	1:B:694:ILE:N	2.26	0.51
1:A:87:TYR:HB3	1:A:92:PRO:HD3	1.92	0.51
1:A:265:LEU:O	1:A:269:LEU:HG	2.11	0.51
1:A:634:GLN:HG2	1:A:638:PHE:CE2	2.46	0.51
1:B:136:ILE:HG12	1:B:174:ILE:HG23	1.90	0.51
1:A:528:PHE:CE2	1:A:543:VAL:HG11	2.45	0.51
1:B:270:TRP:HE3	1:B:277:ILE:HG13	1.74	0.51
1:B:526:SER:CB	1:B:572:LYS:HE2	2.40	0.51
1:A:105:VAL:HG22	1:A:109:PHE:CE2	2.46	0.51
1:A:388:THR:O	1:A:392:LYS:HG2	2.10	0.51
1:A:576:ASP:OD2	1:A:578:ARG:HB3	2.10	0.51
1:B:415:ARG:HH11	1:B:464:ILE:HD11	1.74	0.51
1:A:663:LYS:O	1:A:667:LEU:HD13	2.11	0.51
1:B:360:ASN:HB3	1:B:396:ASN:HB2	1.92	0.51
1:B:397:LYS:HE3	1:B:401:THR:HG21	1.93	0.51
1:A:357:LYS:HB3	1:A:358:GLU:OE1	2.11	0.51
1:A:116:GLU:HG2	1:A:118:GLY:H	1.75	0.50
1:A:529:LEU:N	1:A:529:LEU:HD12	2.26	0.50
1:A:59:LEU:O	1:A:80:LEU:HD21	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:PHE:HA	1:A:593:PHE:HZ	1.75	0.50
1:A:523:ILE:HG23	1:A:580:PHE:CD2	2.46	0.50
1:A:56:ARG:HD3	1:A:87:TYR:CE2	2.45	0.50
1:B:97:GLN:O	1:B:101:ILE:HG13	2.11	0.50
1:A:273:VAL:HB	1:A:276:LEU:HD13	1.94	0.50
1:A:566:ASP:O	1:A:570:THR:HG23	2.12	0.50
1:A:650:ILE:HG21	1:B:650:ILE:HD13	1.93	0.50
1:B:339:VAL:O	1:B:343:GLU:HG3	2.11	0.50
1:B:430:LEU:HD12	1:B:431:ASN:OD1	2.11	0.50
1:B:578:ARG:NE	1:B:582:LEU:HD11	2.27	0.50
1:B:584:ASN:O	1:B:587:VAL:HG12	2.11	0.50
1:A:592:PRO:HB2	1:A:595:THR:HG22	1.93	0.50
1:A:366:THR:HG22	1:A:378:SER:OG	2.11	0.50
1:A:487:VAL:O	1:A:491:LEU:HG	2.12	0.50
1:A:211:VAL:O	1:A:211:VAL:HG22	2.12	0.50
1:B:51:GLY:C	1:B:52:LEU:HD12	2.32	0.50
1:A:387:VAL:HG23	1:A:425:PHE:CE1	2.47	0.50
1:A:72:ILE:HD12	1:A:72:ILE:H	1.77	0.50
1:A:635:ILE:HD12	1:A:635:ILE:C	2.32	0.50
1:B:209:LEU:N	1:B:209:LEU:HD12	2.26	0.50
1:B:262:LEU:O	1:B:266:VAL:HG23	2.12	0.50
1:A:468:VAL:O	1:A:472:ILE:HG13	2.12	0.50
1:B:105:VAL:HG22	1:B:109:PHE:CE2	2.47	0.50
1:B:167:LEU:O	1:B:171:ILE:HG13	2.12	0.50
1:B:354:ASP:HB3	1:B:355:ILE:HD12	1.94	0.50
1:B:690:LEU:O	1:B:694:ILE:HG13	2.12	0.50
1:A:134:ARG:HH11	1:A:134:ARG:HG2	1.76	0.49
1:A:390:ILE:O	1:A:394:ILE:HG13	2.11	0.49
1:A:526:SER:C	1:A:528:PHE:H	2.14	0.49
1:B:6:VAL:CG1	1:B:46:ASN:HD21	2.24	0.49
1:B:572:LYS:HB3	1:B:572:LYS:HZ3	1.77	0.49
1:A:102:PHE:HA	1:A:105:VAL:HG12	1.93	0.49
1:B:482:ASP:O	1:B:486:ARG:HG3	2.12	0.49
1:B:265:LEU:O	1:B:269:LEU:HG	2.11	0.49
1:A:683:PHE:HZ	1:B:690:LEU:HD13	1.78	0.49
1:A:508:PHE:HE1	1:A:639:ARG:HG2	1.77	0.49
1:B:154:HIS:O	1:B:158:ASP:HB2	2.11	0.49
1:B:366:THR:HG22	1:B:378:SER:OG	2.13	0.49
1:A:628:ASP:HA	1:A:631:LYS:HG2	1.94	0.49
1:A:97:GLN:O	1:A:101:ILE:HG13	2.12	0.49
1:A:102:PHE:HZ	1:A:138:LEU:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:SER:HB3	1:B:182:PHE:HZ	1.76	0.49
1:B:579:ILE:HG23	1:B:603:LEU:CD1	2.43	0.49
1:A:515:ILE:HD12	1:A:639:ARG:O	2.13	0.49
1:B:301:LYS:HD3	1:B:340:GLU:OE2	2.12	0.49
1:A:276:LEU:N	1:A:276:LEU:HD12	2.27	0.49
1:A:52:LEU:HD22	1:A:87:TYR:HE1	1.78	0.49
1:A:678:VAL:O	1:A:679:ASN:CB	2.61	0.49
1:A:687:ILE:HA	1:A:690:LEU:HD12	1.95	0.49
1:B:276:LEU:N	1:B:276:LEU:HD12	2.28	0.49
1:B:25:THR:O	1:B:29:LEU:HG	2.13	0.49
1:B:387:VAL:HG23	1:B:425:PHE:CE1	2.48	0.49
1:B:515:ILE:HG22	1:B:519:ILE:HD13	1.93	0.49
1:A:292:ASN:HB3	1:A:295:PHE:HD2	1.77	0.48
1:A:534:SER:OG	1:A:538:SER:HB3	2.13	0.48
1:B:461:ASP:HB3	1:B:464:ILE:HB	1.95	0.48
1:B:588:THR:O	1:B:588:THR:HG22	2.13	0.48
1:B:218:GLU:O	1:B:222:ILE:HG13	2.13	0.48
1:B:442:ILE:HG22	1:B:446:ILE:HD13	1.94	0.48
1:B:523:ILE:CD1	1:B:583:LEU:HD23	2.43	0.48
1:A:515:ILE:HG22	1:A:519:ILE:HD13	1.94	0.48
1:A:6:VAL:HG13	1:A:7:THR:HG23	1.94	0.48
1:B:452:THR:O	1:B:456:LEU:HG	2.14	0.48
1:B:582:LEU:HD23	1:B:599:CYS:O	2.13	0.48
1:A:266:VAL:HG13	1:A:277:ILE:HD12	1.96	0.48
1:B:144:SER:O	1:B:148:LEU:HD13	2.13	0.48
1:B:165:ALA:HA	1:B:168:PHE:CE1	2.48	0.48
1:A:357:LYS:HG2	1:A:361:GLN:HE21	1.77	0.48
1:A:473:PHE:CE2	1:A:638:PHE:HB3	2.49	0.48
1:B:166:ARG:HG3	1:B:167:LEU:CD1	2.43	0.48
1:B:56:ARG:HD3	1:B:87:TYR:CE2	2.48	0.48
1:A:354:ASP:HB3	1:A:355:ILE:HD12	1.96	0.48
1:A:511:ARG:O	1:A:515:ILE:HG13	2.14	0.48
1:A:102:PHE:CZ	1:A:138:LEU:HB2	2.48	0.48
1:A:131:LEU:HB2	1:A:174:ILE:HD11	1.95	0.48
1:A:523:ILE:CD1	1:A:584:ASN:HB2	2.44	0.48
1:B:515:ILE:O	1:B:519:ILE:HD13	2.13	0.48
1:B:468:VAL:O	1:B:472:ILE:HG13	2.13	0.48
1:B:513:ILE:HD12	1:B:513:ILE:C	2.34	0.48
1:B:681:THR:HA	1:B:684:LYS:HE3	1.96	0.48
1:A:104:LEU:HD23	1:A:104:LEU:C	2.34	0.48
1:A:104:LEU:O	1:A:104:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:THR:HA	1:A:455:ASN:HD22	1.79	0.48
1:A:109:PHE:HE1	1:A:127:ILE:HB	1.79	0.48
1:A:464:ILE:O	1:A:468:VAL:HG23	2.14	0.48
1:B:411:HIS:CE1	1:B:413:GLU:HB3	2.49	0.48
1:B:676:SER:CB	1:B:682:LEU:HD11	2.44	0.48
1:A:107:SER:O	1:A:111:GLN:HG3	2.14	0.47
1:B:153:PHE:CE1	1:B:175:LEU:HB3	2.49	0.47
1:B:293:GLU:HA	1:B:296:ARG:HD2	1.95	0.47
1:B:650:ILE:C	1:B:650:ILE:HD12	2.33	0.47
1:A:551:LEU:HB2	1:A:568:LEU:HD21	1.96	0.47
1:B:635:ILE:HD12	1:B:635:ILE:C	2.34	0.47
1:A:569:GLU:O	1:A:572:LYS:HB3	2.14	0.47
1:B:487:VAL:O	1:B:491:LEU:HG	2.15	0.47
1:B:509:ASN:ND2	1:B:644:ILE:HD11	2.28	0.47
1:A:436:THR:HG23	1:A:439:ASN:HD21	1.80	0.47
1:B:448:THR:O	1:B:452:THR:HG23	2.14	0.47
1:B:564:ALA:O	1:B:568:LEU:HG	2.15	0.47
1:B:402:SER:O	1:B:406:LEU:HG	2.15	0.47
1:B:582:LEU:H	1:B:582:LEU:HD12	1.79	0.47
1:A:565:ILE:O	1:A:569:GLU:HB2	2.15	0.47
1:B:149:LEU:HD22	1:B:182:PHE:CE2	2.50	0.47
1:B:131:LEU:HB2	1:B:174:ILE:CD1	2.45	0.47
1:B:314:ASN:HD21	1:B:352:ARG:HH22	1.63	0.47
1:A:682:LEU:H	1:A:682:LEU:CD2	2.25	0.47
1:B:201:ASN:ND2	1:B:268:ARG:HE	2.13	0.47
1:B:60:VAL:HA	1:B:65:LEU:HD11	1.96	0.47
1:A:567:ALA:O	1:A:571:ILE:HG13	2.15	0.47
1:B:404:LEU:N	1:B:404:LEU:HD12	2.29	0.47
1:B:48:ASP:C	1:B:50:THR:H	2.18	0.47
1:A:218:GLU:O	1:A:222:ILE:HG13	2.15	0.47
1:A:36:HIS:CE1	1:A:78:CYS:HB3	2.50	0.47
1:A:569:GLU:OE2	1:A:572:LYS:HD3	2.15	0.47
1:B:607:LEU:CD2	1:B:633:ILE:HG12	2.45	0.47
1:A:157:TYR:HB3	1:A:192:LEU:HD11	1.98	0.47
1:A:232:SER:OG	1:A:279:ALA:HB2	2.15	0.47
1:A:513:ILE:C	1:A:513:ILE:HD12	2.35	0.47
1:B:647:VAL:O	1:B:650:ILE:HG13	2.15	0.47
1:A:690:LEU:HD13	1:B:683:PHE:CD2	2.50	0.47
1:B:36:HIS:CE1	1:B:78:CYS:HB3	2.50	0.47
1:A:80:LEU:HD13	1:A:101:ILE:HG23	1.96	0.46
1:A:369:ASP:HB3	1:A:374:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:O	1:B:130:LEU:HG	2.15	0.46
1:B:416:GLU:HB3	1:B:467:GLN:HE22	1.80	0.46
1:B:594:LEU:HD13	1:B:594:LEU:C	2.35	0.46
1:A:112:LEU:HD21	1:A:167:LEU:HD13	1.97	0.46
1:A:386:PRO:O	1:A:390:ILE:HG13	2.14	0.46
1:A:592:PRO:O	1:A:595:THR:HG22	2.15	0.46
1:B:107:SER:O	1:B:111:GLN:HG3	2.14	0.46
1:B:630:ALA:O	1:B:634:GLN:HG3	2.15	0.46
1:B:59:LEU:O	1:B:80:LEU:HD21	2.15	0.46
1:A:462:LEU:HD13	1:A:558:LEU:O	2.15	0.46
1:B:109:PHE:HE1	1:B:127:ILE:HB	1.80	0.46
1:B:174:ILE:O	1:B:178:VAL:HG23	2.15	0.46
1:A:167:LEU:O	1:A:171:ILE:HG13	2.15	0.46
1:A:246:ALA:CB	1:A:258:VAL:HG21	2.46	0.46
1:A:243:ILE:HD11	1:A:262:LEU:HD12	1.97	0.46
1:A:539:GLN:C	1:A:543:VAL:HG12	2.36	0.46
1:A:678:VAL:HG23	1:A:679:ASN:N	2.30	0.46
1:B:104:LEU:C	1:B:104:LEU:HD23	2.36	0.46
1:B:582:LEU:N	1:B:582:LEU:HD12	2.30	0.46
1:A:153:PHE:HB3	1:A:192:LEU:HD23	1.95	0.46
1:A:267:LEU:O	1:A:271:GLU:HG3	2.16	0.46
1:A:10:LYS:HB2	1:A:38:GLU:OE2	2.15	0.46
1:B:102:PHE:HZ	1:B:138:LEU:HB2	1.80	0.46
1:B:345:ILE:HD13	1:B:363:LEU:HD21	1.97	0.46
1:B:357:LYS:O	1:B:361:GLN:HG3	2.15	0.46
1:A:404:LEU:N	1:A:404:LEU:HD12	2.30	0.46
1:B:476:LEU:HD12	1:B:476:LEU:N	2.29	0.46
1:B:526:SER:OG	1:B:572:LYS:HG2	2.15	0.46
1:B:687:ILE:HA	1:B:690:LEU:HD12	1.97	0.46
1:A:131:LEU:HB2	1:A:174:ILE:CD1	2.45	0.46
1:A:207:GLU:HG2	1:A:210:ASN:OD1	2.16	0.46
1:A:523:ILE:HD12	1:A:584:ASN:HB2	1.97	0.46
1:B:693:ILE:HD12	1:B:693:ILE:C	2.36	0.46
1:A:453:LEU:HD22	1:A:476:LEU:HD21	1.98	0.46
1:A:512:GLN:HA	1:A:639:ARG:O	2.16	0.46
1:B:166:ARG:NH1	1:B:167:LEU:HD11	2.31	0.46
1:A:288:LEU:HD12	1:A:299:ALA:HB1	1.97	0.45
1:A:532:GLN:HE22	1:A:535:MET:HB2	1.81	0.45
1:B:24:SER:HB3	1:B:27:GLU:HG3	1.98	0.45
1:A:125:TYR:CZ	1:A:129:LYS:HG3	2.51	0.45
1:A:168:PHE:CE2	1:A:215:CYS:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ASN:O	1:B:296:ARG:HG3	2.17	0.45
1:B:49:LEU:CA	1:B:52:LEU:HD13	2.46	0.45
1:A:390:ILE:HG22	1:A:394:ILE:HD11	1.97	0.45
1:A:476:LEU:N	1:A:476:LEU:HD12	2.31	0.45
1:A:542:ILE:HG13	1:A:543:VAL:N	2.31	0.45
1:A:83:ILE:HG21	1:A:93:TYR:OH	2.16	0.45
1:B:263:HIS:CG	1:B:302:LEU:HD22	2.51	0.45
1:A:145:SER:HB3	1:A:182:PHE:HZ	1.81	0.45
1:A:116:GLU:HA	1:A:120:HIS:NE2	2.32	0.45
1:A:629:ILE:O	1:A:633:ILE:HG22	2.16	0.45
1:A:165:ALA:HA	1:A:168:PHE:CE1	2.52	0.45
1:B:256:LEU:O	1:B:259:VAL:HG12	2.16	0.45
1:B:284:ILE:O	1:B:288:LEU:HD13	2.15	0.45
1:B:268:ARG:O	1:B:272:THR:HG22	2.16	0.45
1:B:586:CYS:HG	1:B:599:CYS:HG	1.63	0.45
1:B:635:ILE:HA	1:B:638:PHE:HD2	1.82	0.45
1:B:79:CYS:O	1:B:83:ILE:HD13	2.17	0.45
1:A:400:TYR:HB3	1:A:445:ILE:HG21	1.98	0.45
1:B:129:LYS:HD2	1:B:133:TYR:CE2	2.52	0.45
1:B:301:LYS:O	1:B:305:GLN:HG3	2.17	0.45
1:B:238:TYR:CE1	1:B:242:ILE:HD11	2.52	0.45
1:A:347:GLN:O	1:A:351:THR:HG23	2.17	0.44
1:A:411:HIS:CE1	1:A:414:VAL:HG23	2.52	0.44
1:A:519:ILE:O	1:A:522:TYR:HB3	2.17	0.44
1:A:558:LEU:HD13	1:A:632:VAL:HG13	2.00	0.44
1:A:149:LEU:HD22	1:A:182:PHE:CE2	2.52	0.44
1:A:191:ARG:HB3	1:A:195:ASN:HD21	1.82	0.44
1:A:594:LEU:HD13	1:A:594:LEU:C	2.37	0.44
1:B:243:ILE:HG23	1:B:255:LEU:HD11	1.99	0.44
1:B:61:SER:O	1:B:65:LEU:HD13	2.18	0.44
1:A:153:PHE:CE1	1:A:175:LEU:HB3	2.52	0.44
1:A:174:ILE:O	1:A:178:VAL:HG23	2.16	0.44
1:A:519:ILE:N	1:A:519:ILE:HD12	2.33	0.44
1:A:28:LEU:O	1:A:32:LEU:HG	2.18	0.44
1:A:345:ILE:HD12	1:A:345:ILE:N	2.32	0.44
1:B:345:ILE:HB	1:B:346:PRO:HD3	2.00	0.44
1:B:676:SER:CA	1:B:682:LEU:HD11	2.48	0.44
1:A:436:THR:OG1	1:A:439:ASN:ND2	2.51	0.44
1:A:52:LEU:HD22	1:A:87:TYR:CE1	2.52	0.44
1:B:387:VAL:HA	1:B:390:ILE:HD12	2.00	0.44
1:A:29:LEU:HD23	1:A:29:LEU:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASP:HB2	1:A:46:ASN:OD1	2.18	0.44
1:B:29:LEU:HD23	1:B:72:ILE:HD13	1.98	0.44
1:B:482:ASP:OD1	1:B:484:ASP:HB2	2.17	0.44
1:B:589:ASN:N	1:B:591:ILE:HD11	2.32	0.44
1:B:646:ASN:OD1	1:B:647:VAL:N	2.50	0.44
1:A:273:VAL:O	1:A:273:VAL:HG23	2.17	0.44
1:A:358:GLU:OE1	1:A:358:GLU:N	2.48	0.44
1:A:374:VAL:HG23	1:A:375:ARG:N	2.32	0.44
1:B:239:TYR:CE1	1:B:243:ILE:HD11	2.53	0.44
1:B:645:TYR:CD2	1:B:678:VAL:HG21	2.52	0.44
1:A:35:LEU:O	1:A:39:LEU:HG	2.18	0.44
1:A:646:ASN:OD1	1:A:647:VAL:N	2.51	0.44
1:A:683:PHE:CZ	1:B:690:LEU:HD22	2.52	0.44
1:B:551:LEU:C	1:B:551:LEU:HD23	2.37	0.44
1:A:506:PHE:HA	1:A:509:ASN:ND2	2.33	0.44
1:A:528:PHE:HB3	1:A:529:LEU:HD12	2.00	0.44
1:A:554:LEU:C	1:A:554:LEU:HD12	2.39	0.44
1:B:644:ILE:HG13	1:B:645:TYR:CD1	2.53	0.44
1:A:529:LEU:HD11	1:A:572:LYS:HE3	1.98	0.43
1:B:514:LYS:HE2	1:B:553:TRP:CZ2	2.53	0.43
1:A:139:LEU:C	1:A:139:LEU:HD23	2.38	0.43
1:B:201:ASN:OD1	1:B:203:ASN:ND2	2.51	0.43
1:B:446:ILE:HD12	1:B:446:ILE:N	2.33	0.43
1:A:227:TYR:O	1:A:231:MET:HG2	2.18	0.43
1:A:224:CYS:O	1:A:276:LEU:HD11	2.17	0.43
1:A:48:ASP:O	1:A:49:LEU:HB3	2.18	0.43
1:A:567:ALA:CB	1:A:629:ILE:HG12	2.48	0.43
1:B:522:TYR:CZ	1:B:568:LEU:HD22	2.53	0.43
1:B:544:MET:O	1:B:544:MET:HE3	2.19	0.43
1:B:672:LEU:N	1:B:672:LEU:HD12	2.33	0.43
1:A:582:LEU:N	1:A:582:LEU:HD12	2.34	0.43
1:B:35:LEU:O	1:B:39:LEU:HG	2.18	0.43
1:B:589:ASN:C	1:B:591:ILE:HD12	2.37	0.43
1:A:126:LEU:O	1:A:130:LEU:HG	2.18	0.43
1:B:341:TRP:CZ3	1:B:345:ILE:HD11	2.53	0.43
1:B:582:LEU:CD1	1:B:582:LEU:H	2.32	0.43
1:A:355:ILE:CG2	1:A:359:LEU:HG	2.49	0.43
1:A:72:ILE:H	1:A:72:ILE:CD1	2.31	0.43
1:B:104:LEU:O	1:B:104:LEU:HD23	2.17	0.43
1:B:499:LYS:O	1:B:503:THR:HG23	2.17	0.43
1:B:591:ILE:HD12	1:B:591:ILE:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TYR:CD2	1:A:192:LEU:HG	2.54	0.43
1:B:33:LYS:O	1:B:37:GLU:HG3	2.19	0.43
1:B:442:ILE:O	1:B:446:ILE:HD13	2.19	0.43
1:B:593:PHE:O	1:B:596:PHE:HB3	2.19	0.43
1:A:99:THR:O	1:A:103:LYS:HB2	2.18	0.43
1:A:116:GLU:HA	1:A:120:HIS:CD2	2.54	0.43
1:A:263:HIS:CG	1:A:302:LEU:HD22	2.54	0.43
1:A:482:ASP:CG	1:A:483:ASN:N	2.70	0.43
1:A:567:ALA:HB1	1:A:629:ILE:HG23	2.00	0.43
1:A:82:ASP:O	1:A:85:ARG:HB3	2.18	0.43
1:B:249:ASP:C	1:B:251:ASN:H	2.22	0.43
1:B:355:ILE:CG2	1:B:359:LEU:HG	2.47	0.43
1:B:139:LEU:C	1:B:139:LEU:HD23	2.38	0.42
1:B:273:VAL:HG23	1:B:273:VAL:O	2.18	0.42
1:B:686:GLN:N	1:B:686:GLN:OE1	2.47	0.42
1:B:80:LEU:O	1:B:84:LEU:HG	2.19	0.42
1:A:179:ILE:HG13	1:A:185:VAL:HG21	2.01	0.42
1:A:667:LEU:O	1:A:671:ILE:HG13	2.19	0.42
1:B:320:SER:O	1:B:324:LYS:HG3	2.19	0.42
1:A:48:ASP:C	1:A:50:THR:H	2.22	0.42
1:A:508:PHE:O	1:A:512:GLN:HG3	2.20	0.42
1:A:522:TYR:OH	1:A:568:LEU:HB2	2.18	0.42
1:A:671:ILE:HG22	1:A:675:ILE:HD11	2.02	0.42
1:B:292:ASN:HB3	1:B:295:PHE:CD2	2.51	0.42
1:A:383:ASN:OD1	1:A:424:LYS:HE2	2.19	0.42
1:A:480:GLU:HB2	1:A:481:PRO:CA	2.46	0.42
1:B:52:LEU:HD12	1:B:52:LEU:N	2.34	0.42
1:A:650:ILE:HD13	1:B:650:ILE:HB	2.01	0.42
1:B:249:ASP:O	1:B:250:ASP:HB3	2.20	0.42
1:B:554:LEU:C	1:B:554:LEU:HD12	2.39	0.42
1:A:307:LEU:HD21	1:A:315:PHE:HD2	1.84	0.42
1:A:539:GLN:HB3	1:A:542:ILE:HG13	2.01	0.42
1:B:652:VAL:HG12	1:B:672:LEU:HD11	2.02	0.42
1:A:497:PHE:CD2	1:A:501:ALA:HB1	2.55	0.42
1:A:525:PHE:O	1:A:528:PHE:HB2	2.19	0.42
1:B:481:PRO:HG2	1:B:482:ASP:N	2.33	0.42
1:B:49:LEU:C	1:B:49:LEU:HD23	2.40	0.42
1:A:112:LEU:HD21	1:A:167:LEU:CD1	2.49	0.42
1:A:292:ASN:HB3	1:A:295:PHE:CD2	2.54	0.42
1:A:462:LEU:O	1:A:466:GLU:HG3	2.19	0.42
1:A:499:LYS:O	1:A:503:THR:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:VAL:O	1:A:679:ASN:HB2	2.19	0.42
1:B:376:ARG:HB3	1:B:376:ARG:NH1	2.35	0.42
1:A:345:ILE:HB	1:A:346:PRO:HD3	2.02	0.42
1:A:568:LEU:C	1:A:568:LEU:HD12	2.40	0.42
1:A:671:ILE:O	1:A:675:ILE:HG13	2.20	0.42
1:A:678:VAL:O	1:A:679:ASN:ND2	2.52	0.42
1:B:154:HIS:CD2	1:B:192:LEU:HD11	2.54	0.42
1:B:509:ASN:O	1:B:512:GLN:HB3	2.19	0.42
1:B:511:ARG:HG2	1:B:515:ILE:HG13	2.00	0.42
1:A:191:ARG:HB3	1:A:195:ASN:ND2	2.34	0.42
1:A:376:ARG:HG2	1:A:376:ARG:HH11	1.85	0.41
1:A:671:ILE:HG22	1:A:675:ILE:CD1	2.49	0.41
1:B:224:CYS:O	1:B:276:LEU:HD11	2.20	0.41
1:B:48:ASP:O	1:B:49:LEU:HB3	2.20	0.41
1:B:125:TYR:CZ	1:B:129:LYS:HG3	2.55	0.41
1:B:164:PRO:CG	1:B:167:LEU:HD13	2.46	0.41
1:B:191:ARG:HB2	1:B:195:ASN:ND2	2.35	0.41
1:B:230:ARG:HH11	1:B:230:ARG:HG3	1.85	0.41
1:B:49:LEU:HA	1:B:52:LEU:HD13	2.01	0.41
1:A:3:LYS:HB3	1:A:50:THR:CG2	2.48	0.41
1:A:411:HIS:ND1	1:A:414:VAL:HG23	2.36	0.41
1:A:529:LEU:CD1	1:A:572:LYS:HE3	2.50	0.41
1:A:591:ILE:H	1:A:646:ASN:HD21	1.67	0.41
1:B:185:VAL:HG13	1:B:186:PRO:HD2	2.01	0.41
1:B:270:TRP:HB2	1:B:277:ILE:HG13	2.01	0.41
1:B:236:THR:HG23	1:B:283:PHE:CE2	2.56	0.41
1:B:523:ILE:HD13	1:B:580:PHE:CA	2.43	0.41
1:A:394:ILE:HD12	1:A:394:ILE:C	2.41	0.41
1:A:458:TYR:CE2	1:A:500:LYS:HB3	2.55	0.41
1:A:649:ASN:O	1:A:653:LEU:HB2	2.19	0.41
1:B:145:SER:HB3	1:B:182:PHE:CZ	2.54	0.41
1:B:157:TYR:O	1:B:159:PRO:HD3	2.21	0.41
1:B:523:ILE:CD1	1:B:580:PHE:HA	2.40	0.41
1:A:154:HIS:CD2	1:A:192:LEU:HD22	2.44	0.41
1:A:92:PRO:HG2	1:A:93:TYR:H	1.86	0.41
1:B:588:THR:O	1:B:589:ASN:HB2	2.20	0.41
1:B:65:LEU:O	1:B:73:ARG:HG2	2.21	0.41
1:B:390:ILE:CG2	1:B:394:ILE:HD11	2.51	0.41
1:A:144:SER:O	1:A:148:LEU:HG	2.21	0.41
1:A:161:LYS:HB3	1:A:163:PHE:CE1	2.56	0.41
1:A:335:PRO:HA	1:A:338:ARG:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:TYR:OH	1:B:568:LEU:O	2.37	0.41
1:A:353:GLU:O	1:A:353:GLU:HG2	2.19	0.41
1:A:49:LEU:C	1:A:49:LEU:HD23	2.41	0.41
1:A:579:ILE:HG23	1:A:603:LEU:HD11	2.01	0.41
1:A:686:GLN:CD	1:A:686:GLN:H	2.24	0.41
1:B:671:ILE:O	1:B:675:ILE:HG13	2.21	0.41
1:A:46:ASN:O	1:A:46:ASN:OD1	2.39	0.41
1:A:61:SER:O	1:A:65:LEU:HD13	2.21	0.41
1:B:348:ILE:O	1:B:351:THR:HB	2.21	0.41
1:B:38:GLU:O	1:B:42:LEU:HG	2.21	0.41
1:A:316:VAL:HG12	1:A:323:PHE:CD1	2.55	0.40
1:A:554:LEU:HD12	1:A:555:ALA:N	2.36	0.40
1:B:166:ARG:C	1:B:167:LEU:HD12	2.42	0.40
1:B:27:GLU:O	1:B:31:ARG:HG3	2.20	0.40
1:B:502:PHE:HB3	1:B:506:PHE:CE2	2.56	0.40
1:A:12:ASN:HA	1:A:55:TYR:OH	2.21	0.40
1:A:347:GLN:H	1:A:347:GLN:CD	2.24	0.40
1:B:416:GLU:CB	1:B:467:GLN:HE22	2.34	0.40
1:A:647:VAL:HG12	1:B:654:LEU:HD13	2.04	0.40
1:A:145:SER:HB3	1:A:182:PHE:CZ	2.56	0.40
1:A:244:HIS:CE1	1:A:248:ASN:ND2	2.90	0.40
1:A:344:SER:O	1:A:348:ILE:HG13	2.21	0.40
1:A:412:LYS:HZ2	1:A:412:LYS:HB3	1.86	0.40
1:B:272:THR:HG23	1:B:273:VAL:N	2.36	0.40
1:B:551:LEU:O	1:B:551:LEU:HD23	2.21	0.40
1:A:385:VAL:CG2	1:A:386:PRO:HD2	2.51	0.40
1:A:385:VAL:HG23	1:A:386:PRO:HD2	2.04	0.40
1:B:584:ASN:HA	1:B:587:VAL:CG1	2.50	0.40
1:B:473:PHE:CE2	1:B:638:PHE:HB3	2.56	0.40
1:A:560:ASP:CG	1:A:563:LYS:HB2	2.42	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	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:SER:CB	1:B:556:SER:CB[7_555]	2.12	0.08

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	673/703 (96%)	601 (89%)	64 (10%)	8 (1%)	13	49
1	B	650/703 (92%)	582 (90%)	63 (10%)	5 (1%)	19	60
All	All	1323/1406 (94%)	1183 (89%)	127 (10%)	13 (1%)	15	54

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	536	SER
1	A	538	SER
1	A	679	ASN
1	B	682	LEU
1	A	655	ASN
1	A	460	ASN
1	A	660	SER
1	A	684	LYS
1	B	481	PRO
1	B	589	ASN
1	B	587	VAL
1	B	202	PRO
1	A	481	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	629/650 (97%)	627 (100%)	2 (0%)	92	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	611/650 (94%)	608 (100%)	3 (0%)	88	93
All	All	1240/1300 (95%)	1235 (100%)	5 (0%)	91	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	469	ASP
1	A	547	TYR
1	B	120	HIS
1	B	469	ASP
1	B	547	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	123	GLN
1	A	154	HIS
1	A	195	ASN
1	A	201	ASN
1	A	244	HIS
1	A	248	ASN
1	A	252	ASN
1	A	347	GLN
1	A	361	GLN
1	A	393	ASN
1	A	428	ASN
1	A	439	ASN
1	A	455	ASN
1	A	509	ASN
1	A	549	GLN
1	A	575	ASN
1	A	598	ASN
1	A	655	ASN
1	B	36	HIS
1	B	117	ASN
1	B	123	GLN
1	B	154	HIS
1	B	195	ASN
1	B	244	HIS
1	B	460	ASN

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Mol	Chain	Res	Type
1	B	467	GLN
1	B	509	ASN
1	B	589	ASN

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 carbohydrates 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.