



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:28 AM UTC

PDB ID : 1M2V / pdb_00001m2v
Title : Crystal Structure of the yeast Sec23/24 heterodimer
Authors : Bi, X.; Corpina, R.A.; Goldberg, J.
Deposited on : 2002-06-25
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

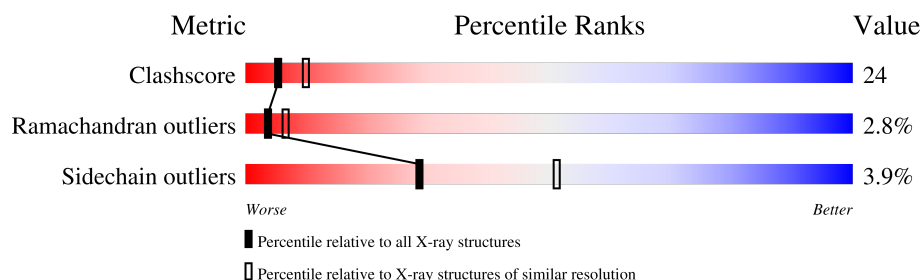
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	768	
2	B	926	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11577 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 protein transport protein SEC23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	705	Total	C	N	O	S	0	0	0
			5574	3560	933	1059	22			

- Molecule 2 is a protein called protein transport protein SEC24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	748	Total	C	N	O	S	0	0	0
			5932	3772	1018	1104	38			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is water.

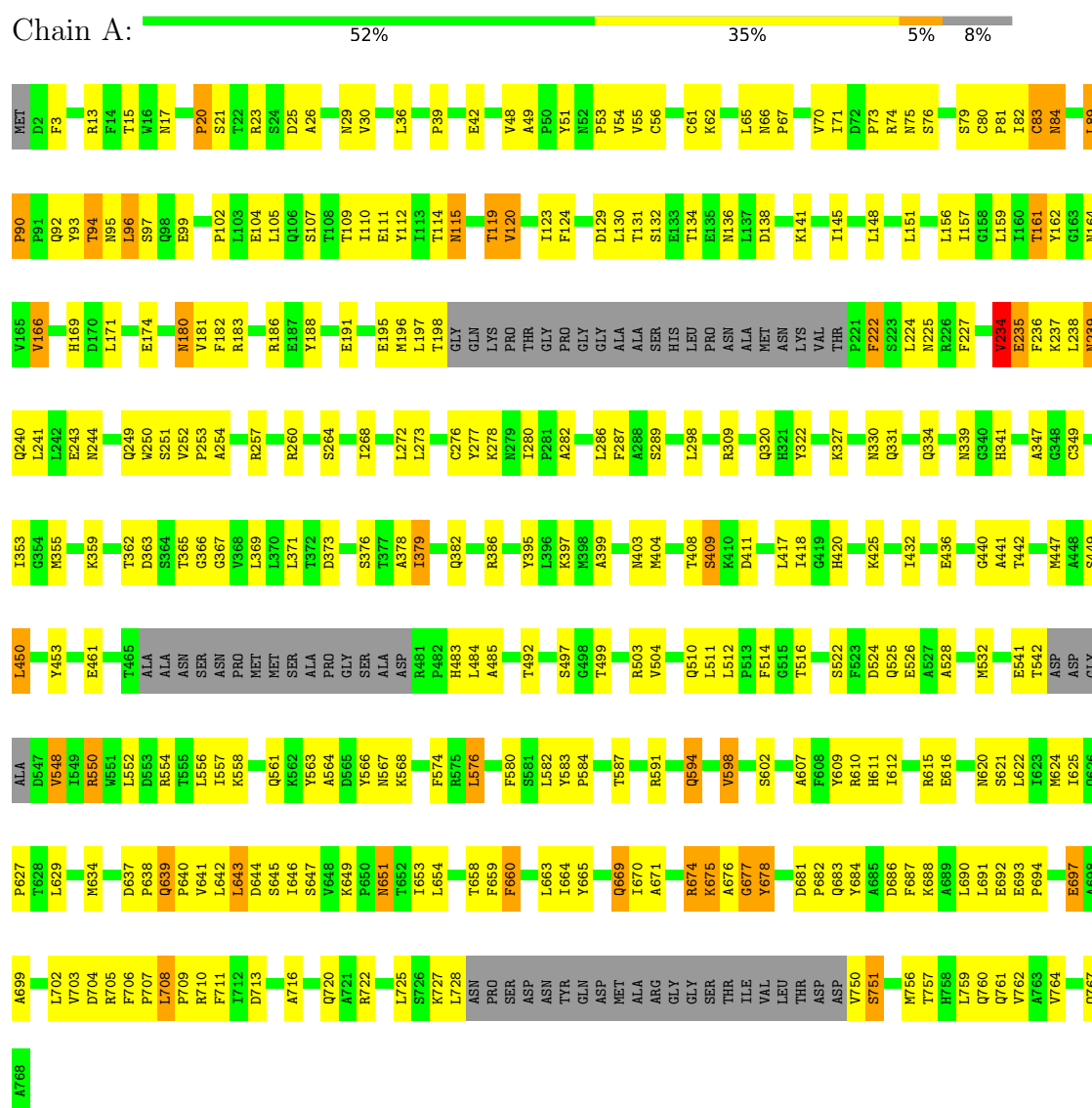
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	35	Total	O	0	0
			35	35		

3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: protein transport protein SEC23



- Molecule 2: protein transport protein SEC24



HIS	ALA	SER	PHE	D761	D681	S563	GLY	M376	T297	V214	SER	R61	MET
ALA	SER	THR	GLY	M762	K687	R567	VAL	D377	L296	D216	ALA	L62	SER
A888	THR	GLN	THR	A763	K687	M568	VAL	I378	R299	D216	ALA	L62	HIS
	ASP	ASP	ASP	E765	V692	M568	N467	F386	Q300	I217	MET	Q66	HIS
	ILE	ILE	ILE	A766	V692	F571	N467	T468	P302	D218	GLY	E87	LYS
	PHE	PHE	PHE	G767	A896	R578	S469	P387	P302	P219	GLN	Q68	LYS
	ASP	ASP	ASP	L768	G897	S579	Q479	R388	P303		ASN		ARG
	ILE	ILE	ILE	P769	G898	S579	I488	P389	L309	N223	MET	Q72	VAL
	PRO	PRO	PRO	VAL	A699	S580	T488	M392	V312	E224	R133	I73	TYR
	ILE	ILE	ILE	GLN	P700	D581	V493	V393	Q313	G226	P134	ASP	PRO
	GLY	GLY	GLY	THR	L701	L582	Q494	V394	Q314	L227	M135	GLN	GLN
	LYS	LYS	LYS	GLU	R702		M409	N402		L228	L138	ALA	ALA
	GLN	GLN	GLN	ASP	L703	T587	I495	I403	T325	V229		THR	LEU
	GLU	GLU	GLU	GLY	C704	M588	T496	C399	K318	R230	D142	THR	GLN
	ILE	ILE	ILE	GLU		P589	V497	R400	K318		L143	MET	TYR
	PRO	PRO	PRO	ALA	R707	R590	V497	Q401	G320	R236	L144	ASP	GLY
	VAL	VAL	VAL	THR	R708		L499	Q401	G320	S236	T145	ASN	GLN
	GLU	GLU	GLU		M709	S593	E504	N402	T325	Y237	E146	MET	ASN
	ASN	ASN	ASN		F710	F596	D505	I403	T325	N238	L147	HIS	ALA
	SER	SER	SER		P711		Y506	L406	L329	M239	P148	LEU	THR
	GLU	GLU	GLU		M714	N599	M507	L406	L329	P241	P150	ASN	PRO
	F848	F848	F848		H715	V600	D508	K409	L333	V242	I151	VAL	GLN
	N849	N849	N849		S716	D601	D508	I410	L333	T243	T152	PRO	GLN
	Q850	Q850	Q850		L717	E802	S516	P411	T336		D153	LEU	PRO
	R851	R851	R851		T718	S603		Q412	P337	G248	L154	VAL	ALA
	V852	V852	V852		K719	I604	T519	F414	N338	R249		ASP	ALA
	N853	N853	N853		R720		I413	Q415	N338	R250	V162	GLN	PHE
	I855	I855	I855		A722	Y610	A520	Q415	E341	N251	I163	ASN	MET
	R856	R856	R856		R723	V611	Q522	S416	R342	R259	P164	ALA	PRO
	R857	R857	R857		S725	Q612	T523	N417	T343	C253	P165	TYR	PRO
	Q858	Q858	Q858			L617	H524	L418	T345	N254	E166	GLN	GLN
	L859	L859	L859		V728	S618	F525	T420	C256	F255	R167	ASP	PRO
	R860	R860	R860		P729	L619	Y526	N421	S346	C256	M168	PRO	PRO
	H861	H861	H861		S730	N620	P527	F422		R257	L169	GLN	ALA
	D862	D862	D862		D731		S530	A423	V350		V170	VAL	ALA
	D863	D863	D863		H732	Q623	G531	L424	D351	N260		PRO	ALA
	V864	V864	V864		R733	R624	K532	L424	N352	D261	S175	VAL	GLY
	I865	I865	I865		R625	R625	N533	L428	A353	V262	N176	GLN	MET
	T867	T867	T867		L737	M633	P534	K429	Y356		A177	GLY	SER
	Y868	Y868	Y868		N739	P634	N535	S430		P271	I182	THR	GLY
	Q869	Q869	Q869		L740	T635	D536	K441	T359	N272		PRO	GLY
	S870	S870	S870		E741		I537	V445	P360	D273	T185	LEU	MET
	L871	L871	L871		L743	E641	K539	V445	L361	P274	N187	GLN	GLY
	Y872	Y872	Y872		S742		E543	T448	D362		A188	GLN	PRO
	I873	I873	I873		P744	V660	E543	L449	SER	R277	V189	GLN	PRO
	V874	V874	V874		L745		K546	P450	ASN	D279	P190	GLN	GLY
	R875	R875	R875		K750	S667	K546	N451	GLU		K191	PRO	GLY
	ALA	ALA	ALA		N751	L668	F552	L452	GLU	K284	N192	ALA	ALA
	SER	SER	SER		D670	D669	C553	G453	SER	C285	L205	VAL	VAL
	LEU	LEU	LEU		A671	A671	V557	I454	ALA		R208	PRO	SER
	SER	SER	SER		D755	R672	M558	R453	ASP	Y290	P209	ALA	MET
	GLU	GLU	GLU		V758		M558	R453	ASP	N291	T209	TYR	GLY
	PRO	PRO	PRO		F822		R559	R453	ASP	A292		GLY	GLY
	VAL	VAL	VAL		L759	K677	A560	E462	N374		H212	GLN	GLN
	ASN	ASN	ASN		H760	Q680		SER	M375	Y296	L213	PRO	GLN

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.31Å 126.37Å 180.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.75	Depositor
% Data completeness (in resolution range)	91.2 (19.96-2.75)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11577	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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:
ZN

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	0.46	0/5706	1.00	29/7765 (0.4%)
2	B	0.48	0/6054	1.04	44/8214 (0.5%)
All	All	0.47	0/11760	1.02	73/15979 (0.5%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	189	VAL	N-CA-C	9.15	116.50	108.63
1	A	649	LYS	CA-C-N	8.38	127.96	119.24
1	A	649	LYS	C-N-CA	8.38	127.96	119.24
1	A	320	GLN	N-CA-C	8.30	121.25	111.71
2	B	394	VAL	N-CA-C	7.50	120.72	109.17
2	B	454	ILE	N-CA-C	7.47	118.20	110.36
1	A	548	VAL	N-CA-C	-7.27	101.69	111.44
1	A	677	GLY	N-CA-C	7.27	130.42	113.18
1	A	249	GLN	N-CA-C	6.89	121.36	112.26
2	B	578	ARG	N-CA-C	-6.88	106.08	114.75
2	B	386	LEU	CA-C-N	6.84	126.08	118.97
2	B	386	LEU	C-N-CA	6.84	126.08	118.97
2	B	152	THR	N-CA-C	-6.78	103.68	112.23
2	B	298	LEU	N-CA-C	-6.66	102.57	111.96
1	A	257	ARG	N-CA-C	-6.62	101.49	110.36
2	B	670	ASP	N-CA-C	-6.59	104.14	111.71
1	A	639	GLN	CA-C-N	6.41	126.75	119.83
1	A	639	GLN	C-N-CA	6.41	126.75	119.83
2	B	270	ASP	CA-C-N	6.29	127.70	119.84
2	B	270	ASP	C-N-CA	6.29	127.70	119.84
2	B	783	LEU	CA-C-N	6.24	126.20	120.03
2	B	783	LEU	C-N-CA	6.24	126.20	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	GLY	N-CA-C	6.21	120.49	112.54
2	B	291	MET	N-CA-C	-6.16	97.67	108.20
2	B	702	ARG	N-CA-C	6.12	119.34	110.28
2	B	218	ASP	CA-C-N	-6.03	115.32	119.66
2	B	218	ASP	C-N-CA	-6.03	115.32	119.66
2	B	147	LEU	CA-C-N	-6.02	114.18	120.38
2	B	147	LEU	C-N-CA	-6.02	114.18	120.38
2	B	224	GLU	N-CA-C	-5.96	105.74	114.39
2	B	350	VAL	N-CA-C	5.91	117.27	108.46
2	B	185	THR	N-CA-C	-5.86	105.40	112.54
1	A	697	GLU	N-CA-C	-5.85	104.90	111.28
2	B	218	ASP	N-CA-C	5.82	122.67	109.81
1	A	252	VAL	CA-C-N	5.82	127.11	119.84
1	A	252	VAL	C-N-CA	5.82	127.11	119.84
2	B	239	ASN	N-CA-C	5.78	113.42	108.22
1	A	563	TYR	N-CA-C	5.71	120.31	113.23
1	A	550	ARG	N-CA-C	-5.70	105.15	111.36
2	B	208	ARG	CA-C-N	5.68	125.79	119.32
2	B	208	ARG	C-N-CA	5.68	125.79	119.32
1	A	580	PHE	N-CA-C	-5.65	107.02	114.31
1	A	89	LEU	N-CA-C	-5.61	101.40	109.48
2	B	582	LEU	N-CA-C	5.48	117.35	108.26
2	B	903	VAL	N-CA-C	5.48	120.73	109.34
1	A	90	PRO	CA-C-N	5.47	126.68	119.84
1	A	90	PRO	C-N-CA	5.47	126.68	119.84
1	A	96	LEU	N-CA-C	5.47	117.14	108.67
1	A	378	ALA	N-CA-C	-5.39	105.57	111.82
1	A	20	PRO	N-CA-C	-5.38	103.34	111.41
1	A	235	GLU	N-CA-C	5.33	117.84	111.71
2	B	459	ARG	N-CA-C	-5.30	103.15	110.35
2	B	409	LYS	N-CA-C	5.29	117.86	111.40
1	A	602	SER	N-CA-C	-5.28	103.00	110.29
2	B	451	ASN	N-CA-C	5.28	120.20	113.55
2	B	692	VAL	N-CA-C	5.25	116.33	111.81
1	A	322	TYR	N-CA-C	5.22	119.98	111.37
2	B	617	LEU	N-CA-C	5.22	117.12	109.24
1	A	161	THR	N-CA-C	-5.21	101.38	109.72
2	B	302	PRO	N-CA-C	5.19	117.03	110.70
2	B	301	PRO	CA-C-N	5.15	125.68	120.38
2	B	301	PRO	C-N-CA	5.15	125.68	120.38
2	B	320	GLY	N-CA-C	-5.08	108.31	115.32
2	B	336	ILE	CA-C-N	5.07	125.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	336	ILE	C-N-CA	5.07	125.08	119.90
2	B	285	CYS	N-CA-C	5.07	117.66	109.40
2	B	602	GLU	N-CA-C	-5.06	105.34	112.12
1	A	660	PHE	N-CA-C	-5.05	106.63	112.89
1	A	376	SER	N-CA-C	-5.05	107.29	113.50
1	A	84	ASN	N-CA-C	5.03	121.52	110.80
2	B	745	LEU	N-CA-C	5.03	117.15	111.11
2	B	392	MET	N-CA-C	-5.03	106.49	113.18
2	B	725	SER	N-CA-C	-5.03	100.54	108.73

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	5574	0	5475	244	0
2	B	5932	0	5958	311	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	34	0	0	5	0
4	B	35	0	0	3	0
All	All	11577	0	11433	553	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (553) 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)
2:B:907:ILE:HG22	2:B:908:LEU:HG	1.35	1.08
2:B:147:LEU:HB3	2:B:148:PRO:HD2	1.16	1.08
2:B:147:LEU:CB	2:B:148:PRO:HD2	1.97	0.95
1:A:651:ASN:H	1:A:651:ASN:HD22	0.96	0.94
1:A:359:LYS:HD2	1:A:607:ALA:HB1	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:GLN:HE21	1:A:669:GLN:HA	1.33	0.92
1:A:399:ALA:HB3	1:A:450:LEU:HD13	1.52	0.90
2:B:441:LYS:HE2	2:B:498:ASP:OD2	1.72	0.89
2:B:154:LEU:HG	2:B:709:MET:HE2	1.55	0.88
2:B:147:LEU:HB3	2:B:148:PRO:CD	2.02	0.88
2:B:459:ARG:HH11	2:B:459:ARG:HG2	1.39	0.87
1:A:379:ILE:HD12	1:A:379:ILE:H	1.42	0.84
2:B:333:LEU:HB2	2:B:400:ARG:NH2	1.93	0.83
2:B:147:LEU:O	2:B:148:PRO:C	2.21	0.83
2:B:352:ASN:HD22	2:B:353:ALA:N	1.75	0.82
1:A:651:ASN:H	1:A:651:ASN:ND2	1.75	0.82
1:A:70:VAL:HB	1:A:79:SER:HB2	1.59	0.82
1:A:485:ALA:HB2	1:A:511:LEU:HD11	1.60	0.81
2:B:133:ARG:HH21	2:B:135:MET:HE2	1.44	0.81
1:A:119:THR:HG21	1:A:280:ILE:HD12	1.61	0.80
2:B:375:MET:HE1	2:B:413:ILE:HG21	1.64	0.80
2:B:147:LEU:HD13	2:B:914:ARG:NH1	1.97	0.79
1:A:157:ILE:HG21	1:A:238:LEU:HD11	1.65	0.79
2:B:151:ILE:HD13	2:B:709:MET:HE1	1.64	0.79
1:A:550:ARG:CD	1:A:554:ARG:HH21	1.95	0.79
2:B:680:GLN:HG3	2:B:920:MET:HE1	1.65	0.78
2:B:142:ASP:CG	2:B:700:PRO:HB3	2.08	0.78
1:A:96:LEU:HD22	1:A:102:PRO:HD3	1.65	0.77
2:B:919:ILE:O	2:B:923:ARG:HG3	1.83	0.77
2:B:759:LEU:HD22	2:B:762:MET:HE2	1.66	0.76
2:B:296:TYR:O	2:B:624:ARG:NH1	2.19	0.76
1:A:703:VAL:O	1:A:704:ASP:HB2	1.85	0.76
1:A:651:ASN:HD22	1:A:651:ASN:N	1.78	0.76
1:A:750:VAL:HG12	1:A:751:SER:H	1.49	0.76
1:A:15:THR:HG22	1:A:528:ALA:HA	1.68	0.75
1:A:239:ASN:O	1:A:243:GLU:HG3	1.87	0.75
2:B:209:PRO:HG3	2:B:558:MET:HE1	1.69	0.75
2:B:660:VAL:HG11	2:B:741:GLU:HB3	1.68	0.74
1:A:432:ILE:HD13	1:A:442:THR:HA	1.69	0.73
2:B:567:ARG:HH21	2:B:599:ASN:HD22	1.36	0.72
1:A:665:TYR:OH	1:A:716:ALA:HB2	1.90	0.72
2:B:226:GLY:O	2:B:293:PRO:HG3	1.90	0.72
2:B:557:VAL:HG13	2:B:582:LEU:HD11	1.70	0.71
2:B:225:ASP:OD1	2:B:227:LEU:HB3	1.90	0.71
1:A:688:LYS:O	1:A:692:GLU:HG2	1.91	0.71
2:B:142:ASP:O	2:B:146:GLU:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ASN:HB3	1:A:492:THR:HG23	1.74	0.70
2:B:696:ALA:HB2	2:B:702:ARG:HH21	1.57	0.70
2:B:801:LEU:HD11	2:B:808:LEU:HD22	1.74	0.70
2:B:493:VAL:HG23	2:B:495:ILE:HG13	1.73	0.70
1:A:557:ILE:O	1:A:561:GLN:HG3	1.92	0.69
1:A:681:ASP:HB3	1:A:684:TYR:HD1	1.55	0.69
1:A:669:GLN:HE21	1:A:669:GLN:CA	2.04	0.69
2:B:699:ALA:HB1	2:B:921:LYS:NZ	2.08	0.69
1:A:80:CYS:O	1:A:84:ASN:HA	1.93	0.69
2:B:279:ASP:HA	2:B:284:LYS:HE3	1.74	0.69
1:A:30:VAL:HG22	1:A:558:LYS:HD3	1.74	0.68
2:B:817:VAL:C	2:B:819:ALA:H	2.01	0.68
2:B:768:LEU:HG	2:B:769:PRO:HD2	1.73	0.68
2:B:818:PRO:C	2:B:820:LEU:H	2.00	0.68
1:A:188:TYR:CD2	1:A:196:MET:HE1	2.28	0.68
1:A:550:ARG:CG	1:A:554:ARG:HH21	2.07	0.68
1:A:102:PRO:HD2	1:A:105:LEU:HD12	1.75	0.68
2:B:459:ARG:HG2	2:B:459:ARG:NH1	2.07	0.67
1:A:395:TYR:CD2	1:A:497:SER:HA	2.29	0.67
2:B:764:ASP:HA	2:B:851:ARG:HH22	1.60	0.67
2:B:766:ALA:O	2:B:768:LEU:N	2.26	0.67
2:B:154:LEU:CG	2:B:709:MET:HE2	2.24	0.67
1:A:669:GLN:HA	1:A:669:GLN:NE2	2.09	0.67
2:B:312:VAL:HG11	2:B:414:PHE:CD2	2.30	0.67
1:A:359:LYS:HD2	1:A:607:ALA:CB	2.25	0.66
1:A:512:LEU:HD13	1:A:516:THR:HG21	1.77	0.66
2:B:303:PRO:HG3	2:B:342:ARG:CZ	2.25	0.66
1:A:74:ARG:HG3	1:A:75:ASN:H	1.61	0.66
2:B:209:PRO:CG	2:B:558:MET:HE1	2.26	0.66
2:B:312:VAL:HG11	2:B:414:PHE:CG	2.31	0.66
2:B:799:LEU:HD13	2:B:812:MET:HE3	1.77	0.65
2:B:362:ASP:OD1	2:B:401:GLN:HB2	1.95	0.65
2:B:812:MET:SD	2:B:820:LEU:HD22	2.36	0.65
2:B:750:LYS:HE3	2:B:805:GLY:HA2	1.77	0.65
2:B:920:MET:HE3	2:B:920:MET:HA	1.77	0.65
2:B:399:CYS:O	2:B:403:ILE:HG13	1.97	0.65
2:B:672:ARG:HH11	2:B:725:SER:HB3	1.62	0.65
2:B:297:THR:HG22	2:B:624:ARG:HD3	1.79	0.65
2:B:422:PHE:H	2:B:451:ASN:HB3	1.61	0.65
2:B:525:PHE:CE2	2:B:527:PRO:HG3	2.33	0.64
1:A:616:GLU:HG3	1:A:620:ASN:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:PRO:O	2:B:151:ILE:HG12	1.97	0.64
1:A:171:LEU:HA	1:A:237:LYS:HE2	1.80	0.64
1:A:541:GLU:OE1	1:A:610:ARG:HD3	1.98	0.64
1:A:671:ALA:O	1:A:675:LYS:HB2	1.96	0.64
2:B:856:ILE:HD13	2:B:871:LEU:HD22	1.79	0.64
1:A:699:ALA:O	1:A:703:VAL:HG23	1.98	0.64
1:A:612:ILE:HG12	4:A:826:HOH:O	1.97	0.64
2:B:914:ARG:O	2:B:918:GLN:HG2	1.98	0.64
2:B:133:ARG:NH2	2:B:135:MET:HE2	2.13	0.64
2:B:789:ALA:O	2:B:904:GLU:HB2	1.98	0.64
1:A:450:LEU:N	1:A:450:LEU:HD12	2.12	0.63
2:B:147:LEU:HD13	2:B:914:ARG:HH12	1.61	0.63
2:B:255:PHE:CZ	2:B:612:GLN:HB2	2.33	0.63
1:A:379:ILE:HD12	1:A:379:ILE:N	2.10	0.63
2:B:312:VAL:HG12	2:B:312:VAL:O	1.99	0.63
1:A:278:LYS:HE3	1:A:339:ASN:ND2	2.14	0.62
2:B:750:LYS:HD2	2:B:803:ASP:OD2	1.98	0.62
2:B:352:ASN:HD22	2:B:353:ALA:H	1.47	0.62
1:A:132:SER:HB3	1:A:289:SER:OG	2.00	0.62
1:A:379:ILE:H	1:A:379:ILE:CD1	2.10	0.62
2:B:808:LEU:O	2:B:871:LEU:HD12	1.98	0.61
2:B:449:LEU:HD12	2:B:450:PRO:HD2	1.81	0.61
2:B:539:LYS:HA	2:B:868:TYR:CD2	2.34	0.61
1:A:550:ARG:HG2	1:A:554:ARG:HH21	1.66	0.61
1:A:188:TYR:CE2	1:A:196:MET:HE1	2.35	0.61
1:A:767:GLN:HB3	4:A:815:HOH:O	2.01	0.61
1:A:225:ASN:OD1	1:A:276:CYS:HB2	2.00	0.61
2:B:424:LEU:HG	2:B:428:LEU:HD22	1.81	0.61
1:A:250:TRP:CE3	2:B:389:PRO:HB3	2.36	0.60
2:B:680:GLN:CG	2:B:920:MET:HE1	2.30	0.60
2:B:668:LEU:HG	2:B:672:ARG:HH21	1.67	0.60
2:B:539:LYS:HE3	2:B:543:GLU:OE2	2.02	0.60
2:B:687:LYS:NZ	2:B:925:SER:HA	2.15	0.60
2:B:375:MET:CE	2:B:413:ILE:HG21	2.31	0.60
2:B:524:HIS:CE1	2:B:866:ILE:HD11	2.37	0.60
2:B:209:PRO:HG3	2:B:558:MET:CE	2.32	0.60
1:A:182:PHE:HZ	1:A:197:LEU:HD21	1.67	0.59
1:A:653:ILE:HD11	1:A:691:LEU:HD23	1.83	0.59
1:A:114:THR:O	1:A:115:ASN:O	2.21	0.59
2:B:270:ASP:HB2	2:B:273:ASP:HB3	1.83	0.59
2:B:205:LEU:HD13	2:B:611:VAL:HG11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:ARG:NH2	2:B:635:THR:O	2.36	0.59
2:B:333:LEU:HB2	2:B:400:ARG:CZ	2.32	0.59
2:B:352:ASN:ND2	2:B:353:ALA:N	2.49	0.59
2:B:711:PRO:HD2	4:B:976:HOH:O	2.00	0.59
2:B:915:GLU:O	2:B:919:ILE:HG13	2.02	0.59
1:A:157:ILE:HG21	1:A:238:LEU:CD1	2.32	0.59
1:A:417:LEU:HD23	1:A:418:ILE:N	2.18	0.59
2:B:205:LEU:HD12	2:B:568:MET:HE1	1.84	0.59
2:B:667:SER:HB3	2:B:670:ASP:HB2	1.85	0.59
1:A:525:GLN:OE1	1:A:582:LEU:HB2	2.03	0.59
1:A:634:MET:HE1	1:A:686:ASP:HB3	1.85	0.59
2:B:764:ASP:HA	2:B:851:ARG:NH2	2.17	0.59
1:A:330:ASN:O	1:A:334:GLN:HG3	2.03	0.58
1:A:74:ARG:HG3	1:A:75:ASN:N	2.16	0.58
2:B:272:ASN:O	2:B:274:PRO:HD3	2.04	0.58
2:B:228:ILE:HD13	2:B:290:TYR:CD2	2.38	0.58
2:B:728:VAL:HG21	2:B:733:ARG:NH2	2.18	0.58
2:B:135:MET:HE1	2:B:634:PRO:HB2	1.86	0.58
2:B:147:LEU:CB	2:B:148:PRO:CD	2.74	0.58
2:B:729:PRO:HB2	2:B:732:HIS:HD2	1.68	0.58
2:B:378:ILE:HD11	2:B:387:PRO:HG3	1.86	0.58
1:A:703:VAL:O	1:A:704:ASP:CB	2.50	0.57
2:B:593:SER:HB2	2:B:744:PRO:HA	1.86	0.57
2:B:872:TYR:CE2	2:B:897:TRP:HZ3	2.23	0.57
2:B:849:ASN:OD1	2:B:853:ARG:HD3	2.04	0.57
1:A:557:ILE:HD13	1:A:762:VAL:HG11	1.86	0.57
2:B:563:SER:HB3	2:B:610:TYR:H	1.68	0.57
1:A:129:ASP:OD2	1:A:260:ARG:HD3	2.05	0.57
2:B:138:LEU:HD22	2:B:704:CYS:HB3	1.85	0.57
2:B:672:ARG:NH1	2:B:725:SER:HB3	2.19	0.57
2:B:303:PRO:HG3	2:B:342:ARG:NH1	2.19	0.57
1:A:25:ASP:OD1	1:A:514:PHE:HB2	2.05	0.57
1:A:159:LEU:HG	1:A:169:HIS:HD2	1.69	0.57
2:B:147:LEU:HD13	2:B:914:ARG:CZ	2.34	0.57
2:B:696:ALA:CB	2:B:702:ARG:HH21	2.18	0.57
1:A:61:CYS:SG	1:A:83:CYS:HB3	2.45	0.56
1:A:616:GLU:CG	1:A:620:ASN:HB2	2.35	0.56
1:A:417:LEU:HD23	1:A:417:LEU:C	2.30	0.56
2:B:802:ILE:O	2:B:808:LEU:HD23	2.05	0.56
2:B:498:ASP:C	2:B:499:LEU:HD12	2.30	0.56
1:A:132:SER:HB3	1:A:289:SER:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ALA:HB2	1:A:353:ILE:HD13	1.87	0.56
1:A:659:PHE:O	1:A:709:PRO:HB3	2.06	0.56
2:B:225:ASP:HB3	4:B:984:HOH:O	2.06	0.56
1:A:166:VAL:HG22	1:A:182:PHE:HB2	1.87	0.55
2:B:817:VAL:C	2:B:819:ALA:N	2.64	0.55
1:A:526:GLU:HB3	1:A:622:LEU:HD11	1.87	0.55
2:B:516:SER:HB2	2:B:521:GLY:C	2.31	0.55
2:B:677:LYS:HG2	2:B:681:ASP:OD2	2.07	0.55
1:A:131:THR:OG1	1:A:260:ARG:NH1	2.38	0.55
2:B:809:PHE:CD2	2:B:898:ALA:HB2	2.42	0.55
1:A:240:GLN:O	1:A:244:ASN:ND2	2.40	0.54
1:A:399:ALA:HB3	1:A:450:LEU:CD1	2.29	0.54
1:A:757:THR:O	1:A:761:GLN:HG3	2.07	0.54
2:B:568:MET:HE3	2:B:596:PHE:HB3	1.88	0.54
2:B:162:VAL:O	2:B:634:PRO:HG3	2.08	0.54
2:B:488:ILE:HD11	2:B:578:ARG:HH22	1.71	0.54
2:B:801:LEU:HD12	2:B:809:PHE:O	2.07	0.54
2:B:822:PHE:CD1	2:B:822:PHE:N	2.74	0.54
1:A:681:ASP:HB3	1:A:684:TYR:CD1	2.39	0.54
1:A:327:LYS:O	1:A:331:GLN:HG3	2.07	0.54
2:B:216:ASP:O	2:B:219:PRO:HD3	2.07	0.54
2:B:818:PRO:C	2:B:820:LEU:N	2.66	0.54
2:B:277:ARG:O	2:B:279:ASP:N	2.41	0.54
1:A:120:VAL:HG21	1:A:277:TYR:CE2	2.43	0.54
1:A:420:HIS:CE1	1:A:615:ARG:HB2	2.43	0.54
2:B:410:ILE:HB	2:B:411:PRO:HD3	1.89	0.54
1:A:224:LEU:HD22	1:A:272:LEU:CD1	2.38	0.54
2:B:191:LYS:HE3	2:B:604:ILE:O	2.08	0.54
2:B:352:ASN:HA	2:B:452:LEU:HD23	1.90	0.54
2:B:361:LEU:HD22	2:B:398:ALA:HB1	1.90	0.54
1:A:17:ASN:HB2	1:A:522:SER:HB2	1.90	0.54
1:A:528:ALA:O	1:A:532:MET:HG2	2.08	0.54
2:B:146:GLU:O	2:B:147:LEU:O	2.26	0.54
1:A:725:LEU:C	1:A:727:LYS:H	2.16	0.54
1:A:132:SER:HB2	1:A:136:ASN:HD22	1.72	0.53
1:A:159:LEU:HG	1:A:169:HIS:CD2	2.43	0.53
1:A:164:ASN:HB2	1:A:250:TRP:CD1	2.43	0.53
1:A:23:ARG:HH21	1:A:461:GLU:CD	2.16	0.53
1:A:42:GLU:OE2	1:A:397:LYS:HE2	2.09	0.53
1:A:432:ILE:CD1	1:A:442:THR:HA	2.37	0.53
2:B:429:LYS:HD2	2:B:454:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:ASP:OD1	2:B:602:GLU:N	2.41	0.53
1:A:612:ILE:HD12	1:A:660:PHE:CE2	2.43	0.53
2:B:496:THR:HA	2:B:519:THR:HB	1.89	0.53
2:B:699:ALA:N	2:B:700:PRO:HD3	2.24	0.53
2:B:250:ARG:HB3	2:B:260:ASN:O	2.09	0.53
2:B:819:ALA:HA	2:B:822:PHE:CE1	2.44	0.53
1:A:90:PRO:HG2	1:A:93:TYR:CD2	2.44	0.53
2:B:346:SER:OG	2:B:393:VAL:HG22	2.09	0.53
2:B:754:PRO:HG3	2:B:901:THR:O	2.09	0.53
1:A:693:GLU:O	1:A:697:GLU:HG2	2.09	0.52
2:B:303:PRO:HG3	2:B:342:ARG:NH2	2.24	0.52
1:A:71:ILE:O	1:A:73:PRO:HD3	2.09	0.52
2:B:699:ALA:HB1	2:B:921:LYS:HZ1	1.74	0.52
2:B:714:MET:HE2	2:B:714:MET:HA	1.89	0.52
2:B:822:PHE:N	2:B:822:PHE:HD1	2.08	0.52
2:B:142:ASP:OD2	2:B:700:PRO:HB3	2.08	0.52
2:B:406:LEU:O	2:B:410:ILE:HG13	2.10	0.52
2:B:795:GLU:C	2:B:797:TYR:H	2.17	0.52
1:A:550:ARG:HG3	1:A:550:ARG:HH11	1.74	0.52
2:B:277:ARG:C	2:B:279:ASP:H	2.18	0.52
1:A:591:ARG:HG3	1:A:591:ARG:HH11	1.75	0.52
2:B:533:ASN:HB3	2:B:536:ASP:OD2	2.10	0.52
1:A:48:VAL:HA	1:A:111:GLU:O	2.10	0.52
1:A:109:THR:HA	1:A:504:VAL:O	2.10	0.52
2:B:135:MET:HE3	2:B:641:GLU:OE1	2.09	0.52
1:A:550:ARG:CD	1:A:554:ARG:NH2	2.71	0.52
1:A:574:PHE:CE2	1:A:576:LEU:HD22	2.44	0.52
2:B:715:HIS:HB2	2:B:916:PHE:CE2	2.45	0.52
2:B:722:ALA:HB1	2:B:737:LEU:HD23	1.92	0.52
1:A:403:ASN:HB3	1:A:492:THR:CG2	2.40	0.51
2:B:352:ASN:ND2	2:B:352:ASN:C	2.67	0.51
2:B:817:VAL:O	2:B:819:ALA:N	2.42	0.51
2:B:279:ASP:CA	2:B:284:LYS:HE3	2.39	0.51
2:B:420:THR:HG22	2:B:420:THR:O	2.10	0.51
2:B:759:LEU:O	2:B:762:MET:HE3	2.10	0.51
2:B:906:LYS:O	2:B:907:ILE:HD13	2.10	0.51
1:A:550:ARG:HD3	1:A:554:ARG:HH21	1.74	0.51
1:A:235:GLU:O	1:A:239:ASN:HB2	2.11	0.51
2:B:162:VAL:O	2:B:163:ILE:HD13	2.10	0.51
2:B:519:THR:O	2:B:520:ALA:HB3	2.10	0.51
1:A:273:LEU:HB3	1:A:341:HIS:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:THR:HG22	1:A:222:PHE:O	2.11	0.51
1:A:366:GLY:HA3	1:A:449:SER:O	2.11	0.51
2:B:722:ALA:HB1	2:B:737:LEU:CD2	2.41	0.51
1:A:674:ARG:O	1:A:676:ALA:N	2.44	0.51
2:B:704:CYS:SG	2:B:707:LEU:HD12	2.50	0.51
2:B:417:ASN:OD1	2:B:419:ILE:N	2.41	0.50
2:B:516:SER:HB2	2:B:522:GLN:N	2.26	0.50
2:B:860:ARG:HG2	2:B:869:GLN:HB2	1.93	0.50
2:B:250:ARG:HA	2:B:262:VAL:HG23	1.93	0.50
2:B:352:ASN:HD22	2:B:352:ASN:C	2.11	0.50
2:B:448:THR:HG22	2:B:449:LEU:O	2.11	0.50
2:B:768:LEU:CG	2:B:769:PRO:HD2	2.40	0.50
1:A:3:PHE:CE1	1:A:524:ASP:HA	2.46	0.50
1:A:395:TYR:CE2	1:A:497:SER:HA	2.46	0.50
2:B:710:PHE:HB3	2:B:711:PRO:HD3	1.94	0.50
1:A:707:PRO:HD3	4:A:826:HOH:O	2.12	0.50
1:A:94:THR:HG22	1:A:94:THR:O	2.12	0.50
2:B:248:GLY:O	2:B:277:ARG:NH2	2.33	0.50
2:B:149:PRO:O	2:B:150:PRO:C	2.53	0.50
2:B:715:HIS:CE1	2:B:719:LYS:HE3	2.46	0.50
1:A:97:SER:OG	1:A:99:GLU:HG2	2.12	0.50
1:A:120:VAL:HG21	1:A:277:TYR:HE2	1.76	0.50
2:B:499:LEU:HD12	2:B:499:LEU:N	2.27	0.49
1:A:264:SER:O	1:A:268:ILE:HG12	2.12	0.49
1:A:550:ARG:HG2	1:A:554:ARG:HE	1.76	0.49
2:B:372:GLN:HG2	2:B:373:ILE:N	2.26	0.49
1:A:371:LEU:O	1:A:710:ARG:NH2	2.44	0.49
2:B:163:ILE:HG22	2:B:168:MET:HE2	1.95	0.49
2:B:504:GLU:OE2	2:B:530:SER:HB3	2.12	0.49
1:A:693:GLU:N	1:A:694:PRO:HD2	2.27	0.49
2:B:794:PHE:HA	2:B:800:TYR:CZ	2.48	0.49
1:A:615:ARG:NH1	4:A:826:HOH:O	2.45	0.49
1:A:664:ILE:HD12	1:A:711:PHE:CZ	2.47	0.49
1:A:53:PRO:HG3	1:A:112:TYR:CG	2.48	0.49
2:B:300:GLN:O	2:B:301:PRO:C	2.56	0.49
2:B:309:LEU:HD12	2:B:309:LEU:C	2.38	0.49
2:B:855:ILE:O	2:B:858:GLN:HB3	2.12	0.49
2:B:150:PRO:HG2	2:B:708:ARG:HH11	1.77	0.49
2:B:423:ALA:HA	2:B:452:LEU:O	2.13	0.49
2:B:589:PRO:O	2:B:590:ARG:HD3	2.13	0.49
2:B:907:ILE:HG22	2:B:908:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:908:LEU:C	2:B:910:ASN:H	2.21	0.49
2:B:911:GLU:HG3	2:B:919:ILE:HD11	1.94	0.49
2:B:920:MET:HE3	2:B:920:MET:CA	2.39	0.49
2:B:279:ASP:C	2:B:284:LYS:HE3	2.36	0.48
2:B:338:ASN:OD1	2:B:341:GLU:HA	2.13	0.48
1:A:54:VAL:HG21	1:A:93:TYR:HE2	1.78	0.48
1:A:659:PHE:HA	1:A:705:ARG:NH1	2.29	0.48
1:A:110:ILE:HG12	1:A:111:GLU:N	2.29	0.48
1:A:484:LEU:HD23	1:A:510:GLN:HA	1.94	0.48
2:B:356:TYR:OH	2:B:430:SER:HB3	2.13	0.48
2:B:667:SER:HB3	2:B:670:ASP:CB	2.44	0.48
2:B:488:ILE:HD11	2:B:578:ARG:NH2	2.28	0.48
2:B:703:LEU:HG	2:B:704:CYS:H	1.78	0.48
2:B:215:ASP:O	2:B:219:PRO:HG3	2.13	0.48
1:A:567:ASN:O	1:A:568:LYS:C	2.57	0.48
2:B:764:ASP:CA	2:B:851:ARG:HH22	2.24	0.48
1:A:286:LEU:HD12	1:A:287:PHE:N	2.28	0.48
1:A:556:LEU:HD22	1:A:587:THR:HG21	1.95	0.48
1:A:664:ILE:HD12	1:A:711:PHE:HZ	1.78	0.48
2:B:796:ARG:NH1	2:B:815:ASP:OD2	2.47	0.48
1:A:624:MET:HG2	1:A:660:PHE:CE1	2.48	0.48
2:B:192:ASN:HA	2:B:603:SER:HA	1.96	0.48
2:B:312:VAL:O	2:B:312:VAL:CG1	2.61	0.48
2:B:352:ASN:HD22	2:B:352:ASN:N	2.11	0.48
2:B:791:SER:H	2:B:905:ASP:CG	2.21	0.48
1:A:251:SER:O	1:A:253:PRO:HD3	2.14	0.47
1:A:674:ARG:C	1:A:676:ALA:H	2.22	0.47
2:B:230:ARG:HD3	2:B:237:TYR:CD2	2.49	0.47
2:B:133:ARG:NE	2:B:135:MET:SD	2.87	0.47
2:B:168:MET:SD	2:B:175:SER:OG	2.69	0.47
2:B:534:PRO:O	2:B:538:VAL:HG23	2.13	0.47
1:A:542:THR:HG22	1:A:542:THR:O	2.15	0.47
1:A:612:ILE:HD12	1:A:660:PHE:HE2	1.79	0.47
1:A:759:LEU:O	1:A:759:LEU:HD12	2.15	0.47
2:B:715:HIS:NE2	2:B:719:LYS:HE3	2.30	0.47
2:B:795:GLU:HB3	2:B:797:TYR:CE2	2.49	0.47
2:B:177:ALA:HB1	2:B:182:ILE:HG22	1.96	0.47
2:B:378:ILE:CD1	2:B:387:PRO:HG3	2.44	0.47
1:A:61:CYS:O	1:A:62:LYS:HB2	2.15	0.47
1:A:425:LYS:NZ	1:A:441:ALA:HB3	2.29	0.47
1:A:222:PHE:CD1	1:A:222:PHE:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HD22	1:A:272:LEU:HD12	1.95	0.47
1:A:665:TYR:C	1:A:665:TYR:CD2	2.92	0.47
2:B:249:ARG:O	2:B:250:ARG:HG2	2.15	0.47
2:B:325:THR:OG1	2:B:445:VAL:HG11	2.15	0.47
2:B:848:PHE:O	2:B:851:ARG:HB2	2.15	0.47
1:A:663:LEU:C	1:A:663:LEU:HD23	2.40	0.47
2:B:205:LEU:CD1	2:B:611:VAL:HG11	2.44	0.47
1:A:347:ALA:HB2	1:A:355:MET:HE3	1.97	0.47
2:B:699:ALA:HB1	2:B:921:LYS:HZ2	1.80	0.47
2:B:687:LYS:HZ2	2:B:925:SER:HA	1.80	0.46
1:A:702:LEU:CD2	1:A:709:PRO:HD2	2.45	0.46
2:B:388:ARG:HB2	2:B:389:PRO:HD2	1.97	0.46
1:A:362:THR:O	1:A:365:THR:O	2.32	0.46
1:A:485:ALA:HB2	1:A:511:LEU:CD1	2.39	0.46
2:B:224:GLU:HA	2:B:291:MET:HG3	1.96	0.46
2:B:314:GLN:CG	2:B:318:LYS:HE3	2.46	0.46
1:A:411:ASP:OD1	1:A:483:HIS:NE2	2.49	0.46
1:A:440:GLY:O	1:A:442:THR:HG22	2.16	0.46
1:A:566:TYR:CD1	1:A:764:VAL:HG12	2.50	0.46
1:A:674:ARG:C	1:A:676:ALA:N	2.72	0.46
1:A:681:ASP:O	1:A:684:TYR:N	2.45	0.46
2:B:150:PRO:HG2	2:B:708:ARG:HD3	1.97	0.46
2:B:170:VAL:O	2:B:170:VAL:HG12	2.16	0.46
2:B:580:SER:O	2:B:581:ASP:HB2	2.14	0.46
1:A:180:ASN:HD22	1:A:180:ASN:N	2.14	0.46
2:B:600:VAL:HG13	2:B:604:ILE:HD11	1.96	0.46
1:A:238:LEU:C	1:A:238:LEU:HD23	2.41	0.46
1:A:594:GLN:HE21	1:A:594:GLN:HB3	1.65	0.46
2:B:230:ARG:HD2	2:B:235:ARG:O	2.15	0.46
2:B:761:ASP:O	2:B:762:MET:O	2.33	0.46
1:A:93:TYR:O	1:A:96:LEU:HG	2.15	0.46
2:B:362:ASP:CG	2:B:401:GLN:HB2	2.41	0.46
2:B:795:GLU:O	2:B:797:TYR:N	2.49	0.46
1:A:197:LEU:HD13	1:A:227:PHE:CE1	2.51	0.46
1:A:725:LEU:HD23	1:A:728:LEU:HD12	1.98	0.46
2:B:277:ARG:C	2:B:279:ASP:N	2.74	0.46
1:A:564:ALA:HB2	1:A:576:LEU:HD13	1.98	0.46
1:A:637:ASP:O	1:A:638:PRO:C	2.56	0.46
1:A:756:MET:O	1:A:760:GLN:HG3	2.15	0.46
1:A:134:THR:HG22	1:A:138:ASP:OD2	2.16	0.45
1:A:629:LEU:HG	1:A:641:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:ARG:HG3	2:B:135:MET:HG2	1.97	0.45
2:B:378:ILE:HD13	2:B:385:PHE:CZ	2.51	0.45
1:A:450:LEU:HD12	1:A:450:LEU:H	1.80	0.45
1:A:687:PHE:O	1:A:690:LEU:HB3	2.16	0.45
2:B:144:LEU:HD22	2:B:918:GLN:NE2	2.31	0.45
2:B:212:HIS:O	2:B:590:ARG:HB3	2.16	0.45
2:B:292:ALA:HA	2:B:293:PRO:HD3	1.83	0.45
2:B:668:LEU:HD21	2:B:733:ARG:NH1	2.31	0.45
1:A:111:GLU:OE2	1:A:503:ARG:NH1	2.49	0.45
1:A:183:ARG:NH2	1:A:186:ARG:HD2	2.31	0.45
2:B:291:MET:HE1	2:B:623:GLN:NE2	2.31	0.45
2:B:820:LEU:C	2:B:822:PHE:N	2.74	0.45
1:A:20:PRO:HG3	1:A:29:ASN:ND2	2.31	0.45
1:A:241:LEU:HD23	1:A:241:LEU:O	2.16	0.45
1:A:583:TYR:HB3	1:A:584:PRO:HD3	1.97	0.45
2:B:151:ILE:CD1	2:B:709:MET:HE1	2.39	0.45
2:B:822:PHE:HD1	2:B:822:PHE:H	1.63	0.45
1:A:627:PRO:O	1:A:643:LEU:HD11	2.17	0.45
1:A:369:LEU:HD23	1:A:611:HIS:HB2	1.98	0.45
2:B:217:ILE:C	2:B:219:PRO:HD3	2.41	0.45
1:A:92:GLN:OE1	1:A:92:GLN:N	2.41	0.45
2:B:62:LEU:HA	2:B:66:GLN:OE1	2.17	0.45
2:B:313:SER:O	2:B:317:ILE:HG12	2.16	0.45
1:A:236:PHE:HB3	4:A:820:HOH:O	2.16	0.45
1:A:645:SER:O	1:A:646:ILE:C	2.60	0.45
2:B:417:ASN:HD21	2:B:419:ILE:HD12	1.81	0.45
2:B:756:VAL:O	2:B:786:PRO:HA	2.17	0.45
1:A:119:THR:O	1:A:120:VAL:O	2.34	0.44
2:B:145:THR:C	2:B:147:LEU:H	2.25	0.44
2:B:552:PHE:CD1	2:B:552:PHE:C	2.95	0.44
1:A:550:ARG:CZ	1:A:550:ARG:HB2	2.47	0.44
1:A:705:ARG:HD2	1:A:709:PRO:HD3	1.99	0.44
2:B:223:ASN:O	2:B:291:MET:HG2	2.17	0.44
2:B:750:LYS:HE3	2:B:805:GLY:CA	2.46	0.44
2:B:424:LEU:O	2:B:428:LEU:HB2	2.17	0.44
1:A:238:LEU:HD23	1:A:238:LEU:O	2.17	0.44
2:B:419:ILE:HG22	2:B:421:ASN:H	1.82	0.44
2:B:571:PHE:HD2	2:B:596:PHE:CE1	2.35	0.44
2:B:672:ARG:NH1	2:B:725:SER:HA	2.32	0.44
2:B:900:SER:HA	2:B:907:ILE:HG21	1.97	0.44
2:B:148:PRO:O	2:B:149:PRO:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ILE:HD13	2:B:634:PRO:HG3	2.00	0.44
2:B:253:CYS:SG	2:B:255:PHE:HB2	2.58	0.44
2:B:506:TYR:CE2	2:B:508:ASP:HB2	2.52	0.44
2:B:579:SER:O	2:B:580:SER:C	2.60	0.44
2:B:668:LEU:O	2:B:671:ALA:HB3	2.18	0.44
1:A:355:MET:O	1:A:359:LYS:HB2	2.17	0.44
1:A:598:VAL:HG23	1:A:598:VAL:O	2.17	0.44
2:B:147:LEU:O	2:B:149:PRO:N	2.50	0.44
2:B:723:PHE:O	2:B:724:ARG:C	2.60	0.44
2:B:68:GLN:O	2:B:72:GLN:HG3	2.17	0.44
2:B:150:PRO:O	2:B:151:ILE:HB	2.18	0.44
2:B:462:GLU:CD	2:B:730:SER:HB2	2.43	0.44
1:A:234:VAL:O	1:A:234:VAL:HG13	2.18	0.43
1:A:359:LYS:HG2	1:A:363:ASP:OD2	2.18	0.43
2:B:680:GLN:CB	2:B:920:MET:HE1	2.48	0.43
1:A:145:ILE:HA	1:A:148:LEU:HD12	2.00	0.43
1:A:182:PHE:CZ	1:A:197:LEU:HD21	2.51	0.43
2:B:242:VAL:CG1	2:B:251:TRP:HB2	2.48	0.43
2:B:729:PRO:O	2:B:730:SER:C	2.60	0.43
2:B:908:LEU:C	2:B:910:ASN:N	2.77	0.43
1:A:13:ARG:HH21	1:A:524:ASP:CG	2.26	0.43
1:A:119:THR:CG2	1:A:120:VAL:N	2.81	0.43
2:B:302:PRO:HA	2:B:303:PRO:HD3	1.73	0.43
1:A:55:VAL:HG12	1:A:56:CYS:N	2.33	0.43
2:B:535:ASN:O	2:B:536:ASP:C	2.59	0.43
2:B:729:PRO:HB2	2:B:732:HIS:CD2	2.52	0.43
2:B:919:ILE:HG22	2:B:923:ARG:HD2	1.99	0.43
1:A:138:ASP:HA	1:A:141:LYS:HD3	2.01	0.43
1:A:382:GLN:HB3	1:A:708:LEU:HD11	1.99	0.43
1:A:587:THR:O	1:A:591:ARG:HG2	2.18	0.43
2:B:761:ASP:O	2:B:762:MET:C	2.61	0.43
1:A:65:LEU:HD23	1:A:104:GLU:HG3	2.00	0.43
2:B:147:LEU:HD23	2:B:147:LEU:HA	1.74	0.43
2:B:224:GLU:HA	2:B:291:MET:CG	2.49	0.43
2:B:459:ARG:NH1	2:B:459:ARG:CG	2.79	0.43
1:A:166:VAL:HG21	1:A:268:ILE:HG13	2.01	0.43
1:A:309:ARG:H	1:A:309:ARG:HD3	1.84	0.43
2:B:783:LEU:HA	2:B:784:PRO:HD3	1.81	0.43
1:A:564:ALA:HB2	1:A:576:LEU:CD1	2.49	0.43
1:A:629:LEU:HD11	1:A:654:LEU:HB3	2.00	0.43
1:A:670:ILE:HD13	1:A:690:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:MET:HG2	2:B:241:PHE:CE2	2.53	0.43
1:A:20:PRO:HB3	1:A:25:ASP:CB	2.49	0.42
2:B:600:VAL:O	2:B:601:ASP:C	2.61	0.42
2:B:764:ASP:O	2:B:851:ARG:NH2	2.51	0.42
2:B:789:ALA:HB1	2:B:902:LEU:HA	2.01	0.42
1:A:93:TYR:CE1	1:A:102:PRO:HB3	2.54	0.42
1:A:670:ILE:CD1	1:A:690:LEU:HD21	2.49	0.42
2:B:144:LEU:HD22	2:B:918:GLN:HE22	1.84	0.42
1:A:20:PRO:HG2	1:A:26:ALA:HA	2.00	0.42
1:A:80:CYS:HA	1:A:81:PRO:HD3	1.86	0.42
1:A:708:LEU:HD23	1:A:708:LEU:N	2.33	0.42
2:B:361:LEU:HD23	2:B:399:CYS:SG	2.58	0.42
1:A:720:GLN:C	1:A:722:ARG:N	2.76	0.42
2:B:344:ARG:HA	2:B:394:VAL:O	2.18	0.42
2:B:497:VAL:HG12	2:B:499:LEU:HD11	2.01	0.42
2:B:802:ILE:HB	2:B:809:PHE:HB2	2.01	0.42
1:A:39:PRO:O	1:A:503:ARG:HG2	2.20	0.42
1:A:191:GLU:O	1:A:195:GLU:HG3	2.19	0.42
1:A:725:LEU:C	1:A:727:LYS:N	2.78	0.42
2:B:250:ARG:HD2	2:B:260:ASN:O	2.18	0.42
2:B:864:ASP:OD1	2:B:864:ASP:N	2.53	0.42
1:A:20:PRO:HB3	1:A:25:ASP:HB3	2.02	0.42
1:A:39:PRO:HG3	1:A:404:MET:HE1	2.02	0.42
1:A:386:ARG:NH1	1:A:705:ARG:O	2.49	0.42
1:A:625:ILE:O	1:A:627:PRO:HD3	2.19	0.42
1:A:706:PHE:CD2	1:A:706:PHE:C	2.97	0.42
2:B:242:VAL:CG1	2:B:243:THR:N	2.83	0.42
2:B:253:CYS:O	2:B:257:ARG:HA	2.19	0.42
2:B:359:ILE:HD11	2:B:406:LEU:HD23	2.01	0.42
1:A:93:TYR:C	1:A:95:ASN:H	2.27	0.42
1:A:129:ASP:HB2	1:A:162:TYR:CZ	2.55	0.42
1:A:671:ALA:O	1:A:675:LYS:N	2.42	0.42
2:B:138:LEU:HB2	4:B:953:HOH:O	2.20	0.42
2:B:546:LYS:NZ	2:B:862:HIS:O	2.52	0.42
1:A:130:LEU:HD11	1:A:161:THR:HB	2.00	0.42
1:A:447:MET:SD	1:A:447:MET:N	2.93	0.42
2:B:333:LEU:HD12	2:B:400:ARG:NE	2.35	0.42
1:A:49:ALA:HB1	1:A:51:TYR:CZ	2.55	0.41
1:A:66:ASN:HB2	1:A:67:PRO:CD	2.50	0.41
1:A:124:PHE:CE1	1:A:151:LEU:HD22	2.55	0.41
1:A:130:LEU:CD1	1:A:161:THR:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:THR:HG22	1:A:591:ARG:HD2	2.02	0.41
2:B:553:CYS:O	2:B:587:THR:HA	2.19	0.41
2:B:212:HIS:CD2	2:B:217:ILE:HB	2.55	0.41
1:A:750:VAL:HG12	1:A:751:SER:N	2.27	0.41
2:B:601:ASP:CG	2:B:602:GLU:N	2.75	0.41
2:B:187:ASN:O	2:B:634:PRO:HD2	2.20	0.41
2:B:717:LEU:HD12	2:B:717:LEU:HA	1.83	0.41
1:A:75:ASN:O	1:A:76:SER:C	2.63	0.41
1:A:408:THR:C	1:A:409:SER:O	2.61	0.41
1:A:642:LEU:O	1:A:644:ASP:N	2.47	0.41
1:A:674:ARG:HH22	1:A:713:ASP:CG	2.25	0.41
1:A:89:LEU:HD12	1:A:90:PRO:HD2	2.03	0.41
1:A:349:CYS:HA	1:A:373:ASP:O	2.21	0.41
1:A:609:TYR:HA	1:A:660:PHE:CE2	2.54	0.41
2:B:146:GLU:C	2:B:147:LEU:O	2.62	0.41
2:B:205:LEU:CD1	2:B:568:MET:HE1	2.50	0.41
2:B:249:ARG:C	2:B:250:ARG:HG2	2.46	0.41
2:B:781:ILE:HB	2:B:858:GLN:OE1	2.21	0.41
1:A:21:SER:HA	1:A:511:LEU:HD23	2.02	0.41
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.89	0.41
1:A:594:GLN:OE1	1:A:727:LYS:NZ	2.49	0.41
1:A:658:THR:O	1:A:659:PHE:HB3	2.21	0.41
2:B:279:ASP:HA	2:B:284:LYS:CE	2.48	0.41
2:B:496:THR:OG1	2:B:587:THR:HG23	2.20	0.41
2:B:530:SER:C	2:B:532:LYS:H	2.29	0.41
1:A:93:TYR:CD1	1:A:102:PRO:HG3	2.56	0.41
1:A:574:PHE:CD2	1:A:760:GLN:HG2	2.56	0.41
1:A:639:GLN:HA	1:A:640:PRO:HD3	1.81	0.41
2:B:270:ASP:CB	2:B:273:ASP:HB3	2.50	0.41
2:B:351:ASP:C	2:B:353:ALA:N	2.79	0.41
2:B:680:GLN:HA	2:B:920:MET:HE2	2.03	0.41
1:A:369:LEU:HB3	1:A:611:HIS:CD2	2.56	0.41
2:B:242:VAL:HG12	2:B:243:THR:N	2.34	0.41
2:B:560:ALA:HA	2:B:612:GLN:O	2.21	0.41
1:A:282:ALA:HB3	1:A:341:HIS:CD2	2.56	0.40
1:A:621:SER:HA	1:A:624:MET:HE3	2.03	0.40
2:B:147:LEU:C	2:B:149:PRO:N	2.79	0.40
2:B:163:ILE:HA	2:B:164:PRO:HD3	1.90	0.40
1:A:123:ILE:HG12	1:A:156:LEU:HB2	2.02	0.40
1:A:591:ARG:HG3	1:A:591:ARG:NH1	2.35	0.40
2:B:373:ILE:C	2:B:374:ASN:ND2	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:633:MET:HA	2:B:634:PRO:HD3	1.89	0.40
1:A:309:ARG:HD3	1:A:309:ARG:N	2.36	0.40
1:A:677:GLY:O	1:A:678:TYR:C	2.65	0.40
2:B:301:PRO:HA	2:B:302:PRO:HD3	1.68	0.40
2:B:336:ILE:HA	2:B:337:PRO:HD3	1.91	0.40
2:B:696:ALA:O	2:B:697:GLY:C	2.63	0.40
1:A:453:TYR:CE2	1:A:704:ASP:O	2.75	0.40
1:A:594:GLN:OE1	1:A:658:THR:HG21	2.21	0.40
2:B:329:LEU:O	2:B:333:LEU:HD23	2.22	0.40
2:B:441:LYS:HD2	2:B:552:PHE:CE2	2.57	0.40
2:B:872:TYR:CE2	2:B:897:TRP:CZ3	3.06	0.40
1:A:181:VAL:HB	2:B:378:ILE:HG12	2.04	0.40
2:B:623:GLN:OE1	2:B:625:ARG:NH2	2.54	0.40
2:B:698:GLY:O	2:B:699:ALA:C	2.64	0.40
2:B:799:LEU:HD13	2:B:812:MET:CE	2.50	0.40

There are no symmetry-related clashes.

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	695/768 (90%)	631 (91%)	52 (8%)	12 (2%)	7	14
2	B	734/926 (79%)	651 (89%)	55 (8%)	28 (4%)	2	4
All	All	1429/1694 (84%)	1282 (90%)	107 (8%)	40 (3%)	4	6

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	120	VAL
1	A	234	VAL

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Mol	Chain	Res	Type
1	A	254	ALA
1	A	678	TYR
2	B	147	LEU
2	B	148	PRO
2	B	151	ILE
2	B	601	ASP
2	B	762	MET
2	B	766	ALA
2	B	767	GLY
2	B	796	ARG
1	A	409	SER
1	A	643	LEU
1	A	675	LYS
2	B	278	TYR
2	B	313	SER
2	B	415	GLN
2	B	469	SER
2	B	580	SER
2	B	697	GLY
2	B	867	THR
2	B	903	VAL
2	B	479	GLN
2	B	530	SER
2	B	620	ASN
2	B	724	ARG
2	B	793	LEU
1	A	751	SER
2	B	149	PRO
1	A	94	THR
2	B	818	PRO
2	B	859	LEU
2	B	146	GLU
2	B	215	ASP
2	B	271	PRO
2	B	763	ALA
1	A	82	ILE
1	A	598	VAL

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	621/668 (93%)	596 (96%)	25 (4%)	28	50
2	B	672/819 (82%)	647 (96%)	25 (4%)	30	54
All	All	1293/1487 (87%)	1243 (96%)	50 (4%)	28	51

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	CYS
1	A	107	SER
1	A	119	THR
1	A	166	VAL
1	A	174	GLU
1	A	180	ASN
1	A	222	PHE
1	A	234	VAL
1	A	239	ASN
1	A	298	LEU
1	A	379	ILE
1	A	436	GLU
1	A	450	LEU
1	A	499	THR
1	A	548	VAL
1	A	552	LEU
1	A	576	LEU
1	A	594	GLN
1	A	647	SER
1	A	651	ASN
1	A	669	GLN
1	A	674	ARG
1	A	682	PRO
1	A	683	GLN
1	A	708	LEU
2	B	138	LEU
2	B	149	PRO
2	B	150	PRO
2	B	152	THR
2	B	166	GLU
2	B	213	LEU

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Mol	Chain	Res	Type
2	B	228	ILE
2	B	270	ASP
2	B	285	CYS
2	B	309	LEU
2	B	352	ASN
2	B	374	ASN
2	B	377	ASP
2	B	428	LEU
2	B	459	ARG
2	B	557	VAL
2	B	611	VAL
2	B	618	SER
2	B	739	ASN
2	B	743	LEU
2	B	751	ASN
2	B	761	ASP
2	B	822	PHE
2	B	870	SER
2	B	874	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	A	169	HIS
1	A	180	ASN
1	A	233	GLN
1	A	244	ASN
1	A	256	HIS
1	A	274	GLN
1	A	301	ASN
1	A	318	HIS
1	A	330	ASN
1	A	339	ASN
1	A	360	GLN
1	A	382	GLN
1	A	494	GLN
1	A	626	GLN
1	A	651	ASN
1	A	669	GLN
1	A	760	GLN
2	B	265	GLN

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Mol	Chain	Res	Type
2	B	352	ASN
2	B	372	GLN
2	B	374	ASN
2	B	421	ASN
2	B	479	GLN
2	B	485	ASN
2	B	514	ASN
2	B	533	ASN
2	B	535	ASN
2	B	599	ASN
2	B	676	ASN
2	B	732	HIS
2	B	739	ASN
2	B	918	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.