



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 01:49 pm GMT

PDB ID : 4RCN
Title : Structure and function of a single-chain, multi-domain long-chain acyl-coa carboxylase
Authors : Tran, T.H.; Tong, L.
Deposited on : 2014-09-16
Resolution : 3.01 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 : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

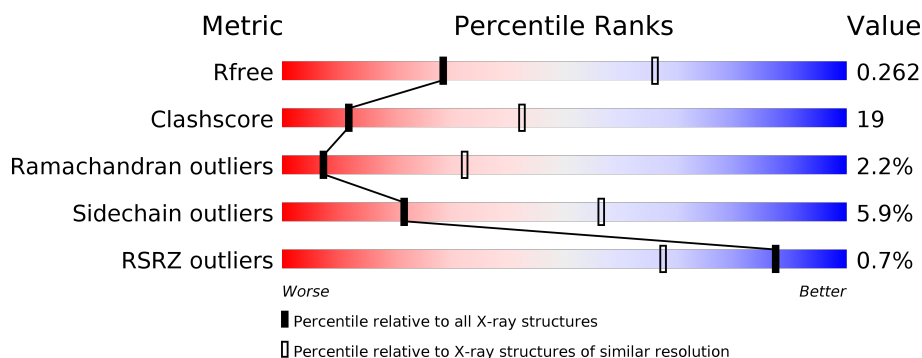
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.01 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}	111664	2110 (3.04-3.00)
Clashscore	122126	2436 (3.04-3.00)
Ramachandran outliers	120053	2362 (3.04-3.00)
Sidechain outliers	120020	2365 (3.04-3.00)
RSRZ outliers	108989	2001 (3.04-3.00)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1093	
1	B	1093	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14630 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 long-chain acyl-CoA carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	972	Total	C	N	O	S	0	0	0
			7211	4528	1319	1340	24			
1	B	1000	Total	C	N	O	S	0	0	0
			7419	4661	1354	1377	27			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1076	GLU	-	EXPRESSION TAG	UNP Q73VY8
A	1077	LEU	-	EXPRESSION TAG	UNP Q73VY8
A	1078	LEU	-	EXPRESSION TAG	UNP Q73VY8
A	1079	VAL	-	EXPRESSION TAG	UNP Q73VY8
A	1080	ASP	-	EXPRESSION TAG	UNP Q73VY8
A	1081	LYS	-	EXPRESSION TAG	UNP Q73VY8
A	1082	LEU	-	EXPRESSION TAG	UNP Q73VY8
A	1083	ALA	-	EXPRESSION TAG	UNP Q73VY8
A	1084	ALA	-	EXPRESSION TAG	UNP Q73VY8
A	1085	ALA	-	EXPRESSION TAG	UNP Q73VY8
A	1086	LEU	-	EXPRESSION TAG	UNP Q73VY8
A	1087	GLU	-	EXPRESSION TAG	UNP Q73VY8
A	1088	HIS	-	EXPRESSION TAG	UNP Q73VY8
A	1089	HIS	-	EXPRESSION TAG	UNP Q73VY8
A	1090	HIS	-	EXPRESSION TAG	UNP Q73VY8
A	1091	HIS	-	EXPRESSION TAG	UNP Q73VY8
A	1092	HIS	-	EXPRESSION TAG	UNP Q73VY8
A	1093	HIS	-	EXPRESSION TAG	UNP Q73VY8
B	1076	GLU	-	EXPRESSION TAG	UNP Q73VY8
B	1077	LEU	-	EXPRESSION TAG	UNP Q73VY8
B	1078	LEU	-	EXPRESSION TAG	UNP Q73VY8
B	1079	VAL	-	EXPRESSION TAG	UNP Q73VY8
B	1080	ASP	-	EXPRESSION TAG	UNP Q73VY8
B	1081	LYS	-	EXPRESSION TAG	UNP Q73VY8
B	1082	LEU	-	EXPRESSION TAG	UNP Q73VY8

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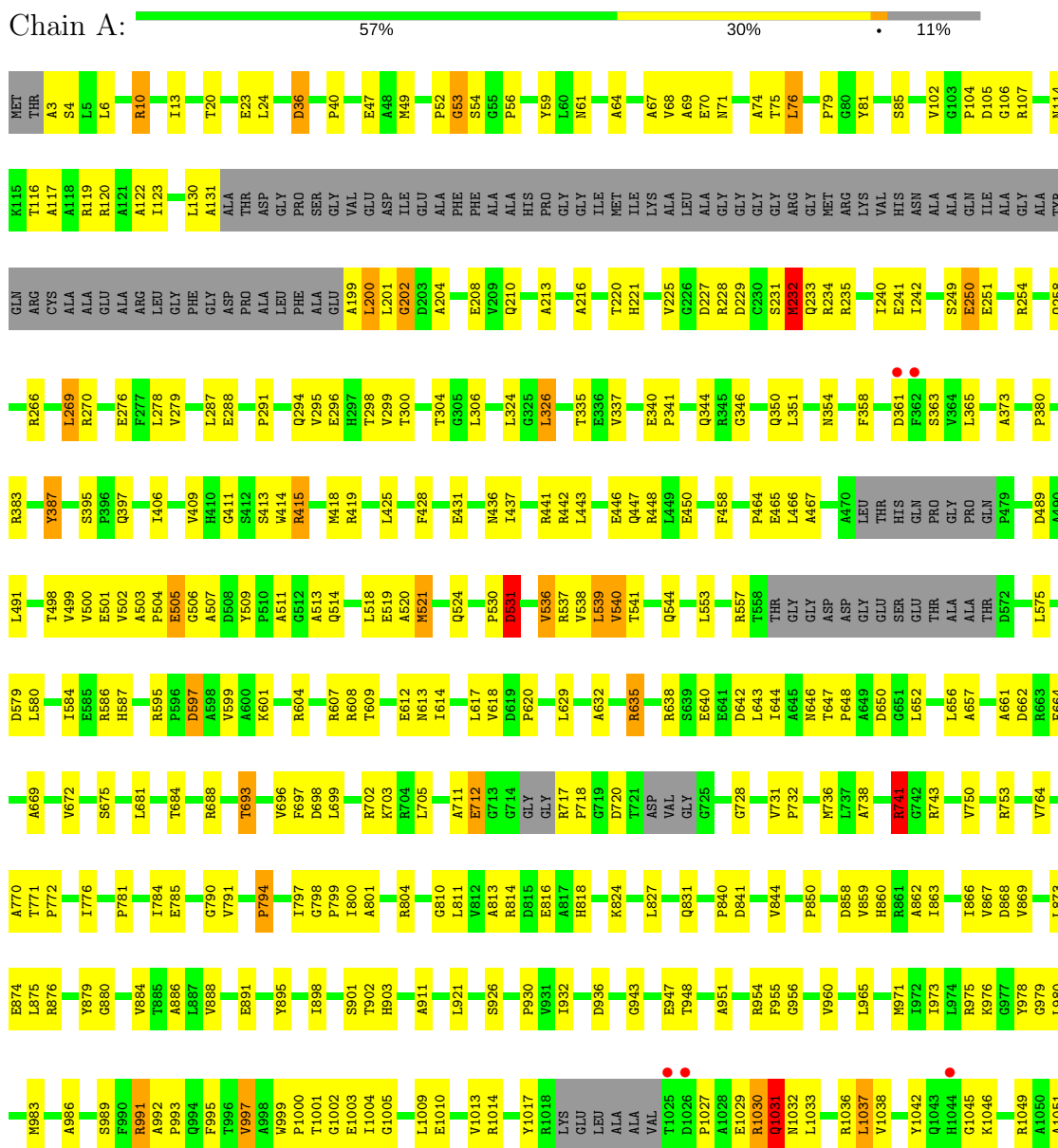
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1083	ALA	-	EXPRESSION TAG	UNP Q73VY8
B	1084	ALA	-	EXPRESSION TAG	UNP Q73VY8
B	1085	ALA	-	EXPRESSION TAG	UNP Q73VY8
B	1086	LEU	-	EXPRESSION TAG	UNP Q73VY8
B	1087	GLU	-	EXPRESSION TAG	UNP Q73VY8
B	1088	HIS	-	EXPRESSION TAG	UNP Q73VY8
B	1089	HIS	-	EXPRESSION TAG	UNP Q73VY8
B	1090	HIS	-	EXPRESSION TAG	UNP Q73VY8
B	1091	HIS	-	EXPRESSION TAG	UNP Q73VY8
B	1092	HIS	-	EXPRESSION TAG	UNP Q73VY8
B	1093	HIS	-	EXPRESSION TAG	UNP Q73VY8

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 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.

- Molecule 1: long-chain acyl-CoA carboxylase



T1052	T1053	F1054	E1055	D1056	D1057	D1058	V1059	T1060	D1061	P1062	T1069	T1070	R1071	L1072	S1073	GLY	GLY	GLU	LEU	LEU	VAL	ASP	LYS	LEU	ALA	ALA	ALA	ALA	GLU	HIS	HIS	HIS	HIS	HIS
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 1: long-chain acyl-CoA carboxylase



M1	L5	R10	G11	E12	I13	A14	L15	R16	R19	T20	E23	L24	G25	M26	V31	Y32	A33	A34	D35	D36	P40	M49	P50	L51	P52	G53	S54	G55	P56	Y59	L60	A64	L65	V68	L76	Y81	G82	F83	E86	K92	T100	P104	D105						
G106	R107	L111	N114	K115	T116	I113	A117	L118	A122	I123	V127	P128	T129	G130	T133	D134	A135	A136	D135	D136	P140	M149	P150	L151	P152	G153	S154	G155	P156	HIS	PRO	GLY	G152	I153	M154	I155	K156	ALA	LEU	ALA	G165	M166	R167	K168	V169	H170	ASN	P104	D105
ALA	GLN	ILE	ALA	GLY	ALA	TYR	GLN	ARG	CYS	ALA	ALA	GLU	ARG	LEU	PHE	GLY	ASP	PRO	L195	F196	A197	L200	L201	G202	D203	Q210	A216	ALA	HIS	PRO	GLY	G152	D229	C230	M231	M232	Q233	R234	R235	Y236	Q237	E241	I242	Q246	G247	L248	L252	R253	R254
A255	L256	H257	Q258	V261	R262	L263	V267	R270	G271	L272	A273	E275	V276	F277	L278	S280	R283	L287	E288	L290	M290	P291	R292	L293	Q294	V295	E296	V299	Q312	L315	E319	L324	G325	L326	V337	E340	F341	A342	G346	Q350	L351	R352							
A355	A360	S363	A373	P380	R383	G384	D385	T386	Y387	G388	L392	V393	Q397	D399	I406	V407	E408	V409	H410	Q411	R415	L425	S426	F427	F428	E431	G432	V433	T437	R441	R442	Q447	R448	T451	G452	W453	V454	M455	V459										
A468	A469	A470	LEU	THR	HIS	GLN	PRO	GLY	GLY	V482	G487	Q494	L495	T498	V499	V502	A503	P504	E505	A511	V516	V517	V518	E519	A520	M521	V526	P530	D531	A532	L533	V536	R537	V538	L539	V540	T541	P542	G543	Q544	V545	G547	D550						
T556	R557	T558	THR	GLY	GLY	ASP	ASP	GLY	GLU	SER	GLN	PRO	GLY	THR	ALA	THR	ASP	LEU	LEU	T576	D579	L580	R595	P596	D597	A598	V599	R602	R607	R608	T609	E612	N613	V618	D619	P620	F623	V624	E625	T631	A632	Q634	R635	R638	S639	E640	E641	D642	
L643	I644	A645	N646	T647	P648	A649	D650	G651	L652	A657	A671	S675	T679	A682	G683	T684	Q685	G686	M687	R688	N689	R690	A691	K692	A598	T693	K703	R704	L705	P706	F710	A711	E712	G713	R717	L718	T721	ASP	VAL	GLY	G725	V731	P732	T733	M736	R743	R843	V844	
S751	G752	R753	C754	F755	V764	C765	P772	G777	I784	Y791	Y792	P793	F794	E795	A796	I797	G798	P799	Q803	R804	R805	N806	G810	A813	R814	D815	E816	A817	R818	A819	V820	G821	L822	A823	K824	Q825	V826	L827	S828	Q831	W837	Q838	P839	P840	D841	P842	R843	V844	
A845	R846	H847	V848	V849	P850	R853	L854	R855	A862	D868	S871	V872	L873	R876	Y879	G880	V884	T885	R889	R890	E891	G896	L897	R898	H904	L905	A908	A914	D915	K916	A917	G918	L921	E925	L934	M941	V942	G943	E947	T948									
F955	N958	L961	L965	L969	G970	M971	L974	R975	A986	R991	A992	P993	V997	A998	W999	P1000	T1001	G1002	V997	E1010	R1014	Y1017	R1018	LYS	GLU	LEU	ALA	ALA	VAL	T1025	D1026	P1027	A1028	E1029	R1030	Q1031	N1032	L1033	R1036	L1037	V1038	A1039	T1052	D1057	D1058				
V1059	I1060	D1061	P1062	R1066	I1069	T1070	L1071	G1072	S1073	GLY	GLY	GLU	LEU	LEU	VAL	ASP	LYS	LEU	ALA	ALA	ALA	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	220.88Å 220.88Å 220.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 3.01 49.39 – 3.01	Depositor EDS
% Data completeness (in resolution range)	91.0 (49.39-3.01) 91.1 (49.39-3.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.01Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.209 , 0.262 0.209 , 0.262	Depositor DCC
R_{free} test set	3516 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14630	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.37	0/7339	0.66	0/9980
1	B	0.39	0/7550	0.66	1/10259 (0.0%)
All	All	0.38	0/14889	0.66	1/20239 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	896	GLY	N-CA-C	-5.05	100.47	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7211	0	7244	275	0
1	B	7419	0	7452	277	0
All	All	14630	0	14696	545	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 19.

All (545) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ALA:H	1:A:647:THR:HG21	1.27	1.00
1:A:504:PRO:HD2	1:A:509:TYR:OH	1.65	0.96
1:A:210:GLN:HE21	1:A:228:ARG:HH12	1.03	0.94
1:B:753:ARG:HG2	1:B:753:ARG:HH11	1.34	0.92
1:B:92:LYS:HE2	1:B:107:ARG:NH1	1.84	0.92
1:B:231:SER:O	1:B:233:GLN:HG2	1.71	0.91
1:B:326:LEU:HD12	1:B:326:LEU:H	1.36	0.91
1:B:608:ARG:HH11	1:B:613:ASN:HD22	1.18	0.91
1:B:499:VAL:HG21	1:B:540:VAL:HG11	1.54	0.90
1:B:92:LYS:HE2	1:B:107:ARG:HH11	1.36	0.88
1:A:632:ALA:N	1:A:647:THR:HG21	1.90	0.87
1:B:1033:LEU:O	1:B:1037:LEU:HD13	1.74	0.86
1:A:500:VAL:HG21	1:A:519:GLU:HG3	1.60	0.84
1:B:850:PRO:HG2	1:B:975:ARG:HH22	1.43	0.84
1:A:859:VAL:HG11	1:A:901:SER:HA	1.60	0.84
1:B:632:ALA:H	1:B:647:THR:HG21	1.44	0.83
1:B:373:ALA:HB3	1:B:431:GLU:HB3	1.61	0.83
1:B:814:ARG:H	1:B:818:HIS:HD2	1.25	0.82
1:A:210:GLN:NE2	1:A:228:ARG:HH12	1.78	0.82
1:B:425:LEU:HD22	1:B:437:ILE:HG23	1.63	0.81
1:B:711:ALA:O	1:B:712:GLU:HB2	1.80	0.81
1:B:426:SER:HB3	1:B:441:ARG:NH2	1.96	0.80
1:A:642:ASP:HB2	1:A:646:ASN:ND2	1.96	0.80
1:A:800:ILE:O	1:A:804:ARG:HB2	1.83	0.77
1:A:781:PRO:HG2	1:A:794:PRO:HG3	1.66	0.77
1:A:580:LEU:O	1:A:584:ILE:HG12	1.83	0.77
1:A:199:ALA:O	1:A:200:LEU:HG	1.84	0.77
1:B:278:LEU:HG	1:B:287:LEU:HD22	1.67	0.76
1:A:601:LYS:HD3	1:A:604:ARG:HE	1.50	0.75
1:B:499:VAL:HG21	1:B:540:VAL:CG1	2.15	0.75
1:A:298:THR:HB	1:A:406:ILE:HD13	1.69	0.75
1:B:234:ARG:NH2	1:B:235:ARG:HE	1.85	0.75
1:B:772:PRO:HD3	1:B:813:ALA:O	1.85	0.75
1:A:231:SER:O	1:A:233:GLN:HG2	1.87	0.75
1:A:841:ASP:HB3	1:A:844:VAL:HG23	1.67	0.75
1:B:152:GLY:O	1:B:153:ILE:HD12	1.87	0.74
1:B:608:ARG:HH11	1:B:613:ASN:ND2	1.86	0.74
1:A:201:LEU:HD12	1:A:202:GLY:H	1.52	0.74
1:A:304:THR:CG2	1:A:306:LEU:HG	2.19	0.72
1:A:772:PRO:HD3	1:A:813:ALA:O	1.88	0.72
1:B:941:MET:HA	1:B:941:MET:HE3	1.70	0.72
1:B:254:ARG:HH11	1:B:258:GLN:HE21	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:HH21	1:A:130:LEU:H	1.36	0.72
1:A:49:MET:HG3	1:A:68:VAL:HG13	1.71	0.71
1:A:640:GLU:O	1:A:644:ILE:HG13	1.91	0.71
1:A:632:ALA:H	1:A:647:THR:CG2	2.03	0.71
1:B:35:ASP:HB2	1:B:54:SER:OG	1.90	0.71
1:B:234:ARG:HH22	1:B:235:ARG:HE	1.35	0.71
1:A:350:GLN:HG3	1:A:406:ILE:HG12	1.72	0.70
1:A:608:ARG:HH11	1:A:613:ASN:HD22	1.38	0.70
1:B:753:ARG:NH1	1:B:753:ARG:HG2	2.07	0.70
1:B:609:THR:OG1	1:B:612:GLU:HG3	1.92	0.69
1:A:409:VAL:HG23	1:B:23:GLU:OE1	1.91	0.69
1:A:672:VAL:HG11	1:A:696:VAL:HG13	1.73	0.69
1:B:254:ARG:HH11	1:B:258:GLN:NE2	1.90	0.69
1:B:814:ARG:H	1:B:818:HIS:CD2	2.09	0.69
1:A:503:ALA:HB1	1:A:509:TYR:OH	1.92	0.69
1:A:119:ARG:NH2	1:A:130:LEU:H	1.90	0.69
1:A:119:ARG:HH21	1:A:130:LEU:HB2	1.57	0.69
1:A:304:THR:HG22	1:A:306:LEU:HG	1.75	0.69
1:A:642:ASP:HB2	1:A:646:ASN:HD22	1.56	0.69
1:A:753:ARG:HH11	1:A:753:ARG:HG2	1.59	0.68
1:B:992:ALA:HB3	1:B:993:PRO:HD3	1.75	0.68
1:B:632:ALA:HB2	1:B:647:THR:HG21	1.75	0.68
1:A:448:ARG:HD2	1:A:458:PHE:HE2	1.58	0.68
1:A:632:ALA:HB2	1:A:647:THR:HG21	1.74	0.68
1:A:232:MET:HE2	1:A:240:ILE:HD12	1.76	0.68
1:A:859:VAL:CG1	1:A:901:SER:HA	2.23	0.68
1:B:15:LEU:O	1:B:19:ARG:HG3	1.93	0.68
1:B:205:ARG:NH2	1:B:246:GLN:O	2.26	0.68
1:B:632:ALA:N	1:B:647:THR:HG21	2.08	0.68
1:A:326:LEU:HD12	1:A:326:LEU:H	1.59	0.68
1:B:642:ASP:HB2	1:B:646:ASN:ND2	2.09	0.68
1:A:743:ARG:HG3	1:A:743:ARG:HH11	1.58	0.67
1:B:64:ALA:O	1:B:68:VAL:HG23	1.94	0.67
1:B:632:ALA:CB	1:B:647:THR:HG21	2.25	0.67
1:B:1033:LEU:HA	1:B:1036:ARG:HD2	1.77	0.67
1:B:683:GLY:O	1:B:713:GLY:HA3	1.95	0.66
1:B:1:MET:N	1:B:24:LEU:HB3	2.10	0.66
1:A:1017:TYR:CE2	1:A:1037:LEU:HG	2.30	0.66
1:A:541:THR:O	1:A:544:GLN:HG2	1.94	0.66
1:B:607:ARG:NH1	1:B:607:ARG:HB3	2.11	0.66
1:A:539:LEU:N	1:A:539:LEU:HD23	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:VAL:CG2	1:A:519:GLU:HG3	2.27	0.65
1:B:517:VAL:HG22	1:B:526:VAL:HG22	1.79	0.64
1:A:607:ARG:NH2	1:A:712:GLU:OE2	2.30	0.64
1:A:850:PRO:HG2	1:A:975:ARG:HH22	1.62	0.64
1:A:104:PRO:HG3	1:A:291:PRO:HB2	1.77	0.64
1:A:776:ILE:O	1:A:798:GLY:HA3	1.98	0.64
1:B:315:ILE:HG13	1:B:324:LEU:HD21	1.80	0.64
1:A:351:LEU:HD13	1:A:425:LEU:HD11	1.79	0.64
1:A:79:PRO:HB2	1:A:85:SER:HA	1.81	0.63
1:A:540:VAL:HA	1:A:544:GLN:OE1	1.98	0.63
1:A:951:ALA:HB1	1:A:955:PHE:CE2	2.33	0.63
1:B:743:ARG:HG3	1:B:743:ARG:HH11	1.63	0.63
1:A:448:ARG:HH11	1:A:448:ARG:HG3	1.64	0.63
1:A:464:PRO:HG2	1:A:465:GLU:OE2	1.98	0.63
1:A:609:THR:HG23	1:A:612:GLU:OE1	1.98	0.63
1:B:51:LEU:HD21	1:B:65:LEU:HD23	1.80	0.63
1:A:114:ASN:HB3	1:A:117:ALA:HB3	1.81	0.63
1:A:415:ARG:HD2	1:A:419:ARG:HH12	1.64	0.63
1:A:1032:ASN:HB3	1:A:1036:ARG:NH1	2.13	0.62
1:B:272:LEU:HG	1:B:312:GLN:HG3	1.79	0.62
1:A:604:ARG:HH11	1:A:604:ARG:HG3	1.64	0.62
1:A:632:ALA:CB	1:A:647:THR:HG21	2.28	0.62
1:B:59:TYR:HB2	1:B:83:PHE:CE1	2.35	0.62
1:B:839:ALA:HB2	1:B:1066:ARG:NH1	2.15	0.61
1:B:607:ARG:NH2	1:B:712:GLU:OE2	2.33	0.61
1:B:934:LEU:HB3	1:B:974:LEU:HD11	1.82	0.61
1:A:1053:THR:OG1	1:A:1055:GLU:HG3	2.00	0.61
1:A:672:VAL:CG1	1:A:696:VAL:HG13	2.31	0.61
1:B:650:ASP:OD2	1:B:688:ARG:HB2	2.00	0.61
1:B:635:ARG:HG2	1:B:635:ARG:HH11	1.65	0.60
1:B:951:ALA:HB1	1:B:955:PHE:CE2	2.36	0.60
1:A:304:THR:HG22	1:A:306:LEU:H	1.67	0.60
1:B:753:ARG:HD3	1:B:794:PRO:HB3	1.84	0.60
1:A:373:ALA:HB3	1:A:431:GLU:HB2	1.84	0.60
1:B:1:MET:H3	1:B:24:LEU:HB3	1.64	0.60
1:B:618:VAL:HG13	1:B:657:ALA:HB1	1.83	0.60
1:A:1032:ASN:O	1:A:1036:ARG:HD3	2.01	0.60
1:B:119:ARG:O	1:B:123:ILE:HG13	2.02	0.60
1:B:205:ARG:HD2	1:B:453:TRP:CE3	2.37	0.59
1:B:258:GLN:HG2	1:B:337:VAL:HG11	1.83	0.59
1:A:703:LYS:HB2	1:A:705:LEU:HG	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:GLN:HG3	1:B:406:ILE:HG13	1.83	0.59
1:B:86:GLU:OE2	1:B:292:ARG:HD3	2.03	0.59
1:B:885:THR:HG23	1:B:916:LYS:HE2	1.84	0.59
1:A:618:VAL:HG13	1:A:657:ALA:HB1	1.84	0.59
1:B:743:ARG:HG3	1:B:743:ARG:NH1	2.16	0.58
1:A:216:ALA:HB3	1:A:221:HIS:CE1	2.39	0.58
1:A:213:ALA:HB3	1:A:269:LEU:HD23	1.85	0.58
1:B:1029:GLU:HB3	1:B:1032:ASN:ND2	2.17	0.58
1:A:119:ARG:NH2	1:A:130:LEU:HB2	2.19	0.58
1:A:131:ALA:HB3	1:A:199:ALA:N	2.19	0.58
1:A:119:ARG:HH21	1:A:130:LEU:N	2.02	0.58
1:A:647:THR:O	1:A:647:THR:HG22	2.04	0.58
1:B:114:ASN:HB3	1:B:117:ALA:HB3	1.85	0.58
1:A:688:ARG:HH11	1:A:688:ARG:HG3	1.69	0.58
1:B:156:LYS:HE2	1:B:166:MET:HE3	1.85	0.58
1:B:595:ARG:O	1:B:599:VAL:HG23	2.03	0.58
1:A:991:ARG:HH11	1:A:991:ARG:HG3	1.68	0.58
1:B:288:GLU:HG2	1:B:289:VAL:N	2.18	0.58
1:B:373:ALA:HB3	1:B:431:GLU:CB	2.33	0.58
1:A:717:ARG:HB2	1:A:720:ASP:OD2	2.04	0.57
1:B:216:ALA:HB3	1:B:221:HIS:CE1	2.39	0.57
1:B:712:GLU:HG3	1:B:751:SER:O	2.04	0.57
1:B:5:LEU:HB2	1:B:26:MET:CE	2.34	0.57
1:B:703:LYS:HB2	1:B:705:LEU:HG	1.86	0.57
1:B:230:CYS:SG	1:B:241:GLU:HG3	2.45	0.57
1:B:505:GLU:HG2	1:B:538:VAL:HG23	1.86	0.57
1:B:784:ILE:HD11	1:B:797:ILE:HD12	1.86	0.57
1:B:904:HIS:CD2	1:B:905:LEU:HG	2.40	0.57
1:A:586:ARG:HH21	1:A:644:ILE:HD13	1.69	0.57
1:B:415:ARG:NH1	1:B:419:ARG:HH22	2.02	0.57
1:A:511:ALA:HB2	1:A:531:ASP:HA	1.86	0.57
1:A:64:ALA:O	1:A:68:VAL:HG23	2.05	0.57
1:B:139:VAL:HG12	1:B:143:GLU:OE2	2.05	0.56
1:B:638:ARG:HD3	1:B:642:ASP:OD2	2.05	0.56
1:A:1013:VAL:HG21	1:A:1038:VAL:HG22	1.86	0.56
1:A:595:ARG:O	1:A:599:VAL:HG23	2.05	0.56
1:A:530:PRO:O	1:A:531:ASP:HB3	2.05	0.56
1:A:656:LEU:HD21	1:A:699:LEU:HD13	1.88	0.56
1:B:274:THR:HG21	1:B:294:GLN:OE1	2.06	0.56
1:B:632:ALA:H	1:B:647:THR:CG2	2.15	0.56
1:B:643:LEU:O	1:B:647:THR:HB	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:GLU:HB3	1:A:1032:ASN:HD22	1.70	0.56
1:A:448:ARG:NH1	1:A:448:ARG:HG3	2.20	0.56
1:A:1010:GLU:O	1:A:1014:ARG:HG3	2.05	0.56
1:B:871:SER:HB2	1:B:889:ARG:HB2	1.87	0.56
1:B:32:TYR:CE1	1:B:50:PRO:HB3	2.41	0.56
1:A:502:VAL:HG12	1:A:503:ALA:N	2.21	0.56
1:A:354:ASN:N	1:A:436:ASN:OD1	2.36	0.56
1:B:153:ILE:CG2	1:B:154:MET:N	2.69	0.55
1:B:234:ARG:O	1:B:237:GLN:HG2	2.06	0.55
1:A:447:GLN:HA	1:A:450:GLU:OE2	2.07	0.55
1:B:905:LEU:HB2	1:B:908:ALA:HB3	1.88	0.55
1:A:874:GLU:HA	1:A:886:ALA:HB2	1.88	0.55
1:A:1030:ARG:HG3	1:A:1031:GLN:N	2.21	0.55
1:B:688:ARG:HG3	1:B:688:ARG:HH11	1.72	0.55
1:B:986:ALA:HB1	1:B:993:PRO:CG	2.36	0.55
1:A:81:TYR:CZ	1:A:295:VAL:HG22	2.42	0.55
1:B:415:ARG:HG2	1:B:419:ARG:HH12	1.71	0.55
1:B:635:ARG:HG2	1:B:635:ARG:NH1	2.21	0.55
1:B:640:GLU:O	1:B:644:ILE:HG13	2.06	0.55
1:B:848:VAL:HG11	1:B:862:ALA:HA	1.87	0.55
1:B:986:ALA:HB1	1:B:993:PRO:HG2	1.88	0.55
1:A:20:THR:O	1:A:24:LEU:HG	2.07	0.55
1:A:635:ARG:HE	1:A:640:GLU:HB2	1.72	0.55
1:B:843:ARG:HG2	1:B:846:ARG:NH1	2.21	0.55
1:A:499:VAL:HG23	1:A:544:GLN:O	2.07	0.55
1:A:728:GLY:O	1:A:731:VAL:HG23	2.07	0.55
1:B:40:PRO:HG2	1:B:387:TYR:O	2.06	0.55
1:A:324:LEU:HB2	1:A:326:LEU:HD11	1.89	0.55
1:A:502:VAL:HG21	1:A:540:VAL:HG12	1.89	0.55
1:B:499:VAL:HA	1:B:518:LEU:HD23	1.89	0.55
1:B:1029:GLU:HB3	1:B:1032:ASN:HD21	1.72	0.54
1:B:248:LEU:HD22	1:B:252:LEU:HD23	1.89	0.54
1:A:1000:PRO:HD3	1:A:1060:ILE:O	2.07	0.54
1:A:511:ALA:CB	1:A:531:ASP:HA	2.38	0.54
1:B:536:VAL:HG12	1:B:537:ARG:HD3	1.89	0.54
1:A:743:ARG:HG3	1:A:743:ARG:NH1	2.23	0.54
1:B:241:GLU:HG2	1:B:296:GLU:CB	2.37	0.54
1:B:647:THR:HG22	1:B:647:THR:O	2.07	0.54
1:A:1032:ASN:HB3	1:A:1036:ARG:HH11	1.72	0.54
1:B:969:LEU:HD23	1:B:969:LEU:C	2.27	0.54
1:B:216:ALA:HB3	1:B:221:HIS:ND1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:THR:HG22	1:A:1053:THR:HG23	1.89	0.54
1:A:437:ILE:O	1:A:441:ARG:HB2	2.07	0.54
1:A:652:LEU:HD12	1:A:675:SER:O	2.07	0.54
1:A:711:ALA:O	1:A:712:GLU:HB2	2.07	0.54
1:B:1069:ILE:O	1:B:1072:LEU:HB2	2.08	0.54
1:A:992:ALA:HB3	1:A:993:PRO:HD3	1.90	0.54
1:B:487:GLY:O	1:B:556:THR:HG23	2.09	0.53
1:B:210:GLN:HE21	1:B:228:ARG:HH12	1.56	0.53
1:B:631:ILE:O	1:B:688:ARG:HG3	2.09	0.53
1:A:608:ARG:HD2	1:A:613:ASN:ND2	2.23	0.53
1:A:647:THR:HG22	1:A:650:ASP:HA	1.89	0.53
1:A:507:ALA:HB3	1:A:509:TYR:HE1	1.73	0.53
1:A:936:ASP:HA	1:A:976:LYS:O	2.09	0.53
1:B:257:HIS:O	1:B:261:VAL:HG22	2.09	0.53
1:A:507:ALA:HB3	1:A:509:TYR:CE1	2.43	0.53
1:A:980:LEU:HD23	1:A:983:MET:HE1	1.91	0.52
1:A:49:MET:SD	1:B:494:GLN:OE1	2.67	0.52
1:B:684:THR:OG1	1:B:717:ARG:HD3	2.09	0.52
1:A:536:VAL:HG12	1:A:537:ARG:HG3	1.91	0.52
1:A:738:ALA:O	1:A:741:ARG:HB2	2.10	0.52
1:B:153:ILE:HG23	1:B:154:MET:N	2.24	0.52
1:A:553:LEU:HD12	1:A:553:LEU:C	2.30	0.52
1:A:116:THR:HG22	1:A:120:ARG:NH2	2.25	0.52
1:A:504:PRO:HD2	1:A:509:TYR:HH	1.72	0.52
1:B:119:ARG:NH2	1:B:130:LEU:O	2.41	0.52
1:B:234:ARG:HH22	1:B:235:ARG:NE	2.03	0.52
1:B:843:ARG:NE	1:B:846:ARG:HH12	2.06	0.52
1:A:711:ALA:O	1:A:712:GLU:CB	2.57	0.52
1:A:489:ASP:OD2	1:A:557:ARG:NH1	2.43	0.52
1:A:505:GLU:HG2	1:A:538:VAL:HB	1.92	0.52
1:B:407:VAL:HB	1:B:420:LYS:HG2	1.92	0.52
1:A:797:ILE:C	1:A:799:PRO:HD3	2.30	0.52
1:B:850:PRO:HG3	1:B:855:ARG:O	2.10	0.52
1:B:167:ARG:O	1:B:169:VAL:HG23	2.10	0.51
1:B:1038:VAL:HG12	1:B:1039:ALA:N	2.25	0.51
1:A:249:SER:C	1:A:251:GLU:H	2.12	0.51
1:B:12:GLU:HG3	1:B:13:ILE:N	2.25	0.51
1:A:300:THR:O	1:A:304:THR:HB	2.10	0.51
1:B:204:ALA:O	1:B:455:ASN:HB2	2.09	0.51
1:A:632:ALA:CA	1:A:647:THR:HG21	2.40	0.51
1:A:874:GLU:HA	1:A:886:ALA:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:PRO:O	1:B:736:MET:HG3	2.10	0.51
1:B:975:ARG:O	1:B:1002:GLY:HA2	2.09	0.51
1:A:810:GLY:HA2	1:A:876:ARG:HG2	1.93	0.51
1:A:932:ILE:HD11	1:A:1069:ILE:HG21	1.91	0.51
1:A:326:LEU:HD12	1:A:326:LEU:N	2.25	0.51
1:A:443:LEU:O	1:A:443:LEU:HD23	2.10	0.51
1:A:503:ALA:HB1	1:A:504:PRO:HD2	1.93	0.51
1:B:753:ARG:NH1	1:B:753:ARG:CG	2.74	0.51
1:A:201:LEU:HD12	1:A:202:GLY:N	2.22	0.51
1:A:884:VAL:O	1:A:898:ILE:HA	2.11	0.51
1:B:105:ASP:OD1	1:B:106:GLY:N	2.44	0.51
1:B:791:VAL:O	1:B:791:VAL:HG13	2.10	0.51
1:A:858:ASP:OD2	1:A:860:HIS:HB2	2.11	0.51
1:B:234:ARG:O	1:B:235:ARG:C	2.49	0.51
1:A:210:GLN:HE21	1:A:228:ARG:NH1	1.88	0.50
1:A:418:MET:HE1	1:A:450:GLU:HA	1.93	0.50
1:B:498:THR:OG1	1:B:545:VAL:HG22	2.11	0.50
1:B:607:ARG:NH1	1:B:816:GLU:OE2	2.43	0.50
1:A:540:VAL:HG22	1:A:544:GLN:OE1	2.12	0.50
1:A:867:VAL:HG11	1:A:888:VAL:HG21	1.93	0.50
1:A:995:PHE:CD1	1:A:995:PHE:O	2.64	0.50
1:B:914:ALA:HA	1:B:958:MET:HE1	1.93	0.50
1:B:971:MET:CE	1:B:986:ALA:HB2	2.42	0.50
1:A:269:LEU:HG	1:A:270:ARG:N	2.26	0.50
1:B:671:ALA:HB2	1:B:706:PRO:HG2	1.93	0.50
1:A:380:PRO:HB3	1:B:383:ARG:CZ	2.41	0.50
1:A:298:THR:CB	1:A:406:ILE:HD13	2.39	0.50
1:B:495:LEU:O	1:B:495:LEU:HD23	2.11	0.50
1:B:841:ASP:O	1:B:844:VAL:HB	2.11	0.50
1:B:111:LEU:HD21	1:B:267:VAL:HG12	1.94	0.50
1:A:501:GLU:OE2	1:A:514:GLN:NE2	2.44	0.50
1:A:652:LEU:CD2	1:A:693:THR:HG23	2.41	0.50
1:B:1026:ASP:HB2	1:B:1030:ARG:HB3	1.94	0.50
1:B:810:GLY:HA2	1:B:876:ARG:HG2	1.94	0.50
1:A:614:ILE:HD11	1:A:675:SER:HB3	1.94	0.49
1:A:1057:ASP:O	1:A:1058:ASP:HB2	2.12	0.49
1:A:799:PRO:C	1:A:801:ALA:H	2.14	0.49
1:B:154:MET:HB2	1:B:200:LEU:HD13	1.94	0.49
1:B:541:THR:OG1	1:B:542:PRO:HD2	2.12	0.49
1:B:60:LEU:CD2	1:B:83:PHE:HD1	2.25	0.49
1:A:52:PRO:HG2	1:A:53:GLY:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:LYS:HG2	1:A:978:TYR:HE2	1.77	0.49
1:B:10:ARG:HG2	1:B:59:TYR:CZ	2.47	0.49
1:B:415:ARG:HH11	1:B:419:ARG:HH12	1.60	0.49
1:A:784:ILE:HD11	1:A:797:ILE:HD12	1.92	0.49
1:A:956:GLY:O	1:A:960:VAL:HG23	2.13	0.49
1:B:116:THR:O	1:B:119:ARG:HG2	2.13	0.49
1:B:12:GLU:HG3	1:B:13:ILE:H	1.78	0.49
1:B:871:SER:CB	1:B:889:ARG:HB2	2.42	0.49
1:B:941:MET:HA	1:B:941:MET:CE	2.41	0.49
1:B:825:GLN:HG2	1:B:873:LEU:HD22	1.94	0.49
1:A:661:ALA:O	1:A:664:PHE:O	2.29	0.49
1:A:971:MET:HE1	1:A:986:ALA:HB2	1.95	0.49
1:B:104:PRO:HG3	1:B:291:PRO:HB2	1.94	0.49
1:A:681:LEU:O	1:A:684:THR:HG23	2.13	0.49
1:A:750:VAL:O	1:A:770:ALA:HA	2.13	0.49
1:B:299:VAL:CG1	1:B:350:GLN:HB2	2.43	0.49
1:B:296:GLU:OE1	1:B:352:ARG:NH2	2.46	0.49
1:A:10:ARG:HG2	1:A:59:TYR:CE2	2.48	0.48
1:A:799:PRO:C	1:A:801:ALA:N	2.65	0.48
1:B:279:VAL:HG12	1:B:280:SER:N	2.28	0.48
1:B:602:ARG:HD3	1:B:679:THR:CG2	2.43	0.48
1:A:234:ARG:HH12	1:A:235:ARG:HE	1.59	0.48
1:A:632:ALA:HB3	1:A:643:LEU:HD22	1.95	0.48
1:A:980:LEU:HD23	1:A:983:MET:CE	2.43	0.48
1:B:533:LEU:HD12	1:B:533:LEU:O	2.14	0.48
1:B:547:GLY:H	1:B:550:ASP:CG	2.17	0.48
1:B:791:VAL:O	1:B:791:VAL:CG1	2.61	0.48
1:B:884:VAL:O	1:B:898:ILE:HA	2.13	0.48
1:B:210:GLN:NE2	1:B:228:ARG:HH12	2.10	0.48
1:B:355:ALA:HB1	1:B:433:VAL:HG11	1.95	0.48
1:B:448:ARG:O	1:B:451:THR:HG23	2.12	0.48
1:B:897:LEU:C	1:B:897:LEU:HD23	2.34	0.48
1:A:519:GLU:HG2	1:A:524:GLN:HG2	1.95	0.48
1:A:669:ALA:HA	1:A:831:GLN:NE2	2.29	0.48
1:B:426:SER:HB3	1:B:441:ARG:CZ	2.41	0.48
1:A:607:ARG:NH1	1:A:816:GLU:OE2	2.47	0.48
1:A:6:LEU:HD22	1:A:69:ALA:HB2	1.96	0.47
1:B:843:ARG:HA	1:B:846:ARG:HD2	1.96	0.47
1:A:1004:ILE:HG22	1:A:1005:GLY:N	2.29	0.47
1:A:643:LEU:O	1:A:647:THR:HB	2.15	0.47
1:B:792:TYR:CD1	1:B:792:TYR:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:ARG:HH11	1:B:607:ARG:HB3	1.78	0.47
1:B:975:ARG:HG3	1:B:975:ARG:HH11	1.78	0.47
1:A:249:SER:C	1:A:251:GLU:N	2.67	0.47
1:A:608:ARG:HD2	1:A:613:ASN:HD21	1.79	0.47
1:B:820:VAL:HG12	1:B:824:LYS:HE3	1.97	0.47
1:B:879:TYR:O	1:B:880:GLY:C	2.53	0.47
1:A:652:LEU:HD21	1:A:693:THR:HG23	1.96	0.47
1:A:814:ARG:H	1:A:818:HIS:HD2	1.63	0.47
1:B:511:ALA:HA	1:B:531:ASP:HA	1.97	0.47
1:B:607:ARG:NH1	1:B:816:GLU:CD	2.68	0.47
1:B:941:MET:HE2	1:B:942:VAL:H	1.80	0.47
1:A:383:ARG:CZ	1:B:380:PRO:HB3	2.45	0.47
1:A:446:GLU:OE1	1:A:466:LEU:HD21	2.15	0.47
1:B:81:TYR:CZ	1:B:295:VAL:HG22	2.50	0.47
1:B:498:THR:HG23	1:B:543:GLY:O	2.15	0.47
1:B:608:ARG:HD2	1:B:613:ASN:HD21	1.80	0.47
1:B:868:ASP:OD2	1:B:891:GLU:N	2.45	0.47
1:A:119:ARG:HH21	1:A:130:LEU:CB	2.25	0.47
1:A:287:LEU:O	1:A:288:GLU:HB2	2.15	0.47
1:B:388:GLY:HA2	1:B:392:LEU:HD22	1.97	0.47
1:B:579:ASP:OD1	1:B:580:LEU:N	2.47	0.47
1:A:698:ASP:O	1:A:702:ARG:HG2	2.15	0.46
1:A:975:ARG:O	1:A:1002:GLY:HA2	2.15	0.46
1:A:4:SER:HB3	1:A:75:THR:H	1.79	0.46
1:A:895:TYR:CD2	1:A:930:PRO:HG2	2.50	0.46
1:B:818:HIS:O	1:B:822:LEU:HG	2.14	0.46
1:A:40:PRO:HG2	1:A:387:TYR:O	2.15	0.46
1:A:921:LEU:HD22	1:A:965:LEU:HD11	1.97	0.46
1:B:205:ARG:NH1	1:B:229:ASP:OD2	2.49	0.46
1:B:675:SER:HB2	1:B:710:PHE:HB2	1.97	0.46
1:A:753:ARG:HH11	1:A:753:ARG:CG	2.24	0.46
1:A:814:ARG:H	1:A:818:HIS:CD2	2.34	0.46
1:A:227:ASP:H	1:A:344:GLN:HE22	1.63	0.46
1:B:441:ARG:HG2	1:B:441:ARG:NH1	2.31	0.46
1:B:49:MET:HG3	1:B:68:VAL:HG13	1.98	0.46
1:B:76:LEU:HD23	1:B:100:THR:HB	1.98	0.46
1:B:196:PHE:O	1:B:197:ALA:HB2	2.15	0.46
1:B:254:ARG:NH1	1:B:258:GLN:HE21	2.11	0.46
1:B:346:GLY:HA2	1:B:411:GLY:O	2.16	0.46
1:A:697:PHE:HB2	1:A:736:MET:HE2	1.97	0.45
1:B:634:GLN:O	1:B:634:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:ILE:CD1	1:B:797:ILE:HD12	2.45	0.45
1:A:741:ARG:HD2	1:A:741:ARG:C	2.36	0.45
1:B:254:ARG:O	1:B:258:GLN:HG3	2.17	0.45
1:B:288:GLU:HG2	1:B:289:VAL:H	1.81	0.45
1:A:863:ILE:O	1:A:867:VAL:HG22	2.17	0.45
1:B:31:VAL:HA	1:B:49:MET:O	2.16	0.45
1:B:803:GLN:HA	1:B:806:ASN:OD1	2.16	0.45
1:A:358:PHE:CE2	1:A:467:ALA:HA	2.50	0.45
1:A:608:ARG:HH11	1:A:613:ASN:ND2	2.11	0.45
1:B:803:GLN:OE1	1:B:803:GLN:HA	2.16	0.45
1:A:943:GLY:O	1:A:947:GLU:HG2	2.16	0.45
1:A:1029:GLU:OE2	1:A:1031:GLN:HB2	2.16	0.45
1:A:498:THR:O	1:A:518:LEU:HA	2.17	0.45
1:B:13:ILE:O	1:B:16:ARG:HB3	2.17	0.45
1:B:254:ARG:NH2	1:B:340:GLU:OE2	2.49	0.45
1:A:1010:GLU:CD	1:A:1010:GLU:H	2.19	0.45
1:A:395:SER:OG	1:A:397:GLN:HG3	2.16	0.45
1:A:504:PRO:O	1:A:506:GLY:N	2.50	0.45
1:A:586:ARG:HH11	1:A:586:ARG:HG2	1.82	0.45
1:A:647:THR:N	1:A:648:PRO:CD	2.80	0.45
1:A:811:LEU:HD21	1:A:875:LEU:HD23	1.99	0.45
1:B:1010:GLU:HB2	1:B:1014:ARG:NH1	2.31	0.45
1:B:122:ALA:HA	1:B:263:LEU:HD13	1.99	0.45
1:B:795:GLU:OE1	1:B:795:GLU:N	2.49	0.45
1:B:820:VAL:CG1	1:B:824:LYS:HE3	2.47	0.45
1:A:119:ARG:O	1:A:122:ALA:HB3	2.17	0.45
1:A:798:GLY:N	1:A:799:PRO:HD3	2.33	0.45
1:A:638:ARG:HD3	1:A:642:ASP:OD2	2.16	0.44
1:B:426:SER:CB	1:B:441:ARG:NH2	2.75	0.44
1:B:133:THR:CG2	1:B:137:SER:OG	2.64	0.44
1:A:840:PRO:HD3	1:A:868:ASP:HA	1.99	0.44
1:A:49:MET:CE	1:B:494:GLN:HB3	2.47	0.44
1:B:237:GLN:HE21	1:B:237:GLN:HA	1.83	0.44
1:B:10:ARG:NE	1:B:36:ASP:OD2	2.42	0.44
1:A:597:ASP:OD1	1:A:597:ASP:N	2.47	0.44
1:A:67:ALA:O	1:A:71:ASN:ND2	2.51	0.44
1:B:142:ILE:O	1:B:145:PHE:HB3	2.17	0.44
1:B:459:VAL:HG12	1:B:459:VAL:O	2.18	0.44
1:B:647:THR:N	1:B:648:PRO:CD	2.80	0.44
1:A:999:TRP:CD2	1:A:1062:PRO:HB3	2.53	0.44
1:A:229:ASP:HB3	1:A:242:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:NE	1:A:36:ASP:OD2	2.49	0.44
1:B:1000:PRO:HD3	1:B:1060:ILE:O	2.17	0.44
1:B:168:LYS:HE2	1:B:200:LEU:HD11	2.00	0.44
1:B:60:LEU:HD21	1:B:83:PHE:HD1	1.83	0.44
1:A:785:GLU:HA	1:A:790:GLY:O	2.18	0.44
1:B:848:VAL:HG11	1:B:862:ALA:CA	2.48	0.44
1:A:204:ALA:HA	1:A:279:VAL:O	2.18	0.43
1:A:681:LEU:H	1:A:681:LEU:HD23	1.83	0.43
1:B:703:LYS:HD3	1:B:705:LEU:HD11	2.00	0.43
1:B:755:PHE:HA	1:B:777:GLY:O	2.18	0.43
1:A:299:VAL:HG13	1:A:350:GLN:HB2	1.99	0.43
1:A:617:LEU:HA	1:A:824:LYS:HE3	1.98	0.43
1:B:502:VAL:HG12	1:B:503:ALA:N	2.33	0.43
1:A:632:ALA:HB2	1:A:647:THR:CG2	2.44	0.43
1:B:241:GLU:HG2	1:B:296:GLU:HB3	1.99	0.43
1:A:3:ALA:HB1	1:A:76:LEU:HD11	2.00	0.43
1:A:4:SER:HB3	1:A:74:ALA:HA	2.01	0.43
1:B:276:GLU:O	1:B:287:LEU:HB3	2.19	0.43
1:B:618:VAL:CG1	1:B:657:ALA:HB1	2.49	0.43
1:A:242:ILE:HD13	1:A:414:TRP:CH2	2.54	0.43
1:A:346:GLY:HA2	1:A:411:GLY:O	2.19	0.43
1:B:229:ASP:HB3	1:B:242:ILE:HB	2.01	0.43
1:B:272:LEU:CG	1:B:312:GLN:HG3	2.47	0.43
1:B:441:ARG:HG2	1:B:441:ARG:HH11	1.83	0.43
1:B:447:GLN:O	1:B:448:ARG:C	2.56	0.43
1:A:1033:LEU:HD12	1:A:1033:LEU:O	2.19	0.43
1:A:105:ASP:OD1	1:A:106:GLY:N	2.49	0.43
1:A:791:VAL:HG13	1:A:791:VAL:O	2.18	0.43
1:B:261:VAL:HG23	1:B:262:ARG:N	2.32	0.43
1:B:92:LYS:HG2	1:B:107:ARG:HH12	1.84	0.43
1:A:732:PRO:O	1:A:736:MET:HG3	2.18	0.43
1:B:261:VAL:HG23	1:B:262:ARG:H	1.83	0.43
1:B:648:PRO:O	1:B:649:ALA:HB3	2.19	0.43
1:B:921:LEU:HD22	1:B:965:LEU:HD11	2.00	0.43
1:A:1009:LEU:CD1	1:A:1042:TYR:HA	2.49	0.43
1:A:13:ILE:HB	1:A:81:TYR:CE2	2.54	0.43
1:A:784:ILE:CD1	1:A:797:ILE:CD1	2.96	0.43
1:B:652:LEU:O	1:B:692:LYS:NZ	2.37	0.43
1:B:797:ILE:C	1:B:799:PRO:HD3	2.39	0.43
1:B:850:PRO:CG	1:B:975:ARG:HH22	2.22	0.43
1:B:991:ARG:HD3	1:B:991:ARG:HA	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ARG:HG2	1:A:586:ARG:NH1	2.34	0.43
1:B:127:VAL:HA	1:B:128:PRO:HD2	1.81	0.43
1:B:415:ARG:NH1	1:B:419:ARG:NH2	2.66	0.43
1:B:33:ALA:HB1	1:B:54:SER:HA	1.99	0.43
1:B:690:HIS:CE1	1:B:731:VAL:HG11	2.54	0.43
1:B:437:ILE:O	1:B:441:ARG:HB2	2.19	0.42
1:B:682:ALA:O	1:B:713:GLY:HA2	2.19	0.42
1:B:925:GLU:HB2	1:B:965:LEU:HD23	2.01	0.42
1:A:973:ILE:HG21	1:A:1004:ILE:HD11	2.02	0.42
1:B:999:TRP:CD2	1:B:1062:PRO:HB3	2.54	0.42
1:B:511:ALA:CB	1:B:531:ASP:HA	2.49	0.42
1:B:746:LEU:O	1:B:765:CYS:HB3	2.19	0.42
1:A:208:GLU:HG2	1:A:276:GLU:HG2	2.02	0.42
1:A:753:ARG:NH1	1:A:753:ARG:CG	2.81	0.42
1:A:753:ARG:HD3	1:A:794:PRO:HB3	2.01	0.42
1:A:1033:LEU:O	1:A:1037:LEU:HB2	2.20	0.42
1:A:587:HIS:CE1	1:A:629:LEU:HD11	2.55	0.42
1:A:879:TYR:O	1:A:880:GLY:C	2.57	0.42
1:A:989:SER:C	1:A:991:ARG:H	2.22	0.42
1:A:827:LEU:O	1:A:831:GLN:HG3	2.20	0.42
1:B:248:LEU:HB2	1:B:253:ARG:HH12	1.84	0.42
1:A:978:TYR:OH	1:A:1003:GLU:HG3	2.20	0.42
1:A:361:ASP:C	1:A:363:SER:N	2.70	0.42
1:B:827:LEU:O	1:B:831:GLN:HG3	2.19	0.42
1:A:254:ARG:O	1:A:258:GLN:HG3	2.20	0.42
1:A:632:ALA:HA	1:A:650:ASP:OD1	2.20	0.42
1:A:997:VAL:CG2	1:A:1060:ILE:HG23	2.50	0.42
1:B:154:MET:CE	1:B:168:LYS:HB2	2.50	0.42
1:A:351:LEU:HD13	1:A:425:LEU:CD1	2.46	0.42
1:A:638:ARG:NH2	1:A:681:LEU:HD21	2.35	0.42
1:A:47:GLU:HG2	1:B:495:LEU:HB3	2.01	0.42
1:A:340:GLU:O	1:A:341:PRO:C	2.57	0.41
1:B:156:LYS:HE2	1:B:166:MET:CE	2.47	0.41
1:B:837:TRP:HZ3	1:B:839:ALA:HB2	1.85	0.41
1:A:241:GLU:HG2	1:A:296:GLU:HB3	2.02	0.41
1:A:23:GLU:OE1	1:B:409:VAL:HG22	2.20	0.41
1:B:686:GLY:H	1:B:689:ASN:ND2	2.18	0.41
1:A:521:MET:HA	1:A:521:MET:CE	2.50	0.41
1:A:980:LEU:HA	1:A:983:MET:HE3	2.03	0.41
1:B:468:ALA:C	1:B:470:ALA:H	2.23	0.41
1:A:119:ARG:O	1:A:123:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:HB3	1:A:287:LEU:HD23	2.02	0.41
1:A:298:THR:OG1	1:A:350:GLN:NE2	2.53	0.41
1:A:862:ALA:O	1:A:866:ILE:HG13	2.21	0.41
1:A:811:LEU:CD1	1:A:873:LEU:HD11	2.50	0.41
1:A:911:ALA:HB1	1:A:954:ARG:CZ	2.50	0.41
1:B:703:LYS:O	1:B:704:ARG:C	2.59	0.41
1:B:918:GLY:O	1:B:961:LEU:HD13	2.20	0.41
1:A:1013:VAL:HG13	1:A:1017:TYR:HD2	1.86	0.41
1:A:210:GLN:HG3	1:A:225:VAL:CG2	2.50	0.41
1:A:250:GLU:O	1:A:250:GLU:HG2	2.20	0.41
1:B:256:LEU:HD22	1:B:277:PHE:CD2	2.56	0.41
1:B:31:VAL:HB	1:B:51:LEU:HG	2.01	0.41
1:B:608:ARG:CD	1:B:613:ASN:ND2	2.83	0.41
1:B:753:ARG:HD3	1:B:794:PRO:CB	2.50	0.41
1:B:828:SER:HG	1:B:889:ARG:HH12	1.66	0.41
1:A:199:ALA:O	1:A:200:LEU:CG	2.60	0.41
1:A:4:SER:CB	1:A:74:ALA:HA	2.51	0.41
1:B:1017:TYR:CG	1:B:1037:LEU:HD23	2.56	0.41
1:A:642:ASP:O	1:A:646:ASN:N	2.54	0.41
1:A:799:PRO:O	1:A:801:ALA:N	2.54	0.41
1:A:4:SER:OG	1:A:74:ALA:HA	2.21	0.41
1:A:502:VAL:CG1	1:A:503:ALA:N	2.84	0.41
1:B:516:VAL:HG12	1:B:517:VAL:N	2.36	0.41
1:B:642:ASP:HB2	1:B:646:ASN:HD22	1.85	0.41
1:B:975:ARG:NH1	1:B:975:ARG:HG3	2.36	0.41
1:A:258:GLN:HG2	1:A:337:VAL:HG11	2.03	0.41
1:A:868:ASP:OD2	1:A:891:GLU:N	2.54	0.41
1:B:530:PRO:HD2	1:B:533:LEU:CD2	2.50	0.41
1:B:154:MET:HB2	1:B:200:LEU:CD1	2.51	0.40
1:B:270:ARG:NH1	1:B:270:ARG:HB3	2.36	0.40
1:A:201:LEU:HD23	1:A:278:LEU:HB3	2.02	0.40
1:A:448:ARG:HD2	1:A:458:PHE:CE2	2.48	0.40
1:A:509:TYR:HB3	1:A:513:ALA:HB3	2.03	0.40
1:A:638:ARG:HD2	1:A:643:LEU:CD2	2.51	0.40
1:A:681:LEU:N	1:A:681:LEU:HD23	2.35	0.40
1:A:79:PRO:CB	1:A:85:SER:HA	2.49	0.40
1:B:640:GLU:HG2	1:B:644:ILE:HD11	2.03	0.40
1:B:1057:ASP:O	1:B:1058:ASP:HB2	2.21	0.40
1:B:943:GLY:O	1:B:947:GLU:HG2	2.21	0.40
1:A:703:LYS:HD3	1:A:705:LEU:HD11	2.04	0.40
1:B:133:THR:O	1:B:196:PHE:CE1	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:VAL:HG11	1:B:540:VAL:CG1	2.52	0.40
1:B:499:VAL:CG2	1:B:540:VAL:HG11	2.37	0.40
1:B:635:ARG:HE	1:B:640:GLU:H	1.69	0.40
1:B:743:ARG:HG2	1:B:743:ARG:H	1.63	0.40
1:A:1029:GLU:HB3	1:A:1032:ASN:ND2	2.37	0.40
1:A:1051:ALA:HB2	1:A:1059:VAL:HG23	2.02	0.40
1:A:604:ARG:HH11	1:A:604:ARG:CG	2.32	0.40
1:A:975:ARG:HH11	1:A:975:ARG:HG3	1.86	0.40
1:B:258:GLN:O	1:B:262:ARG:HB2	2.22	0.40
1:B:623:PHE:CE2	1:B:625:GLU:HB2	2.57	0.40
1:B:731:VAL:HG12	1:B:733:THR:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	958/1093 (88%)	870 (91%)	64 (7%)	24 (2%)	6	29
1	B	984/1093 (90%)	893 (91%)	73 (7%)	18 (2%)	9	38
All	All	1942/2186 (89%)	1763 (91%)	137 (7%)	42 (2%)	7	32

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	LEU
1	A	520	ALA
1	A	712	GLU
1	B	360	ALA
1	B	520	ALA
1	B	712	GLU
1	A	53	GLY

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Mol	Chain	Res	Type
1	A	202	GLY
1	A	232	MET
1	A	505	GLU
1	A	579	ASP
1	A	979	GLY
1	A	1046	LYS
1	B	202	GLY
1	B	232	MET
1	B	853	ARG
1	A	61	ASN
1	A	335	THR
1	A	521	MET
1	A	575	LEU
1	A	869	VAL
1	A	1031	GLN
1	B	197	ALA
1	B	342	ALA
1	B	1031	GLN
1	A	413	SER
1	A	620	PRO
1	A	741	ARG
1	B	235	ARG
1	B	399	ASP
1	B	718	PRO
1	A	102	VAL
1	A	531	ASP
1	B	135	GLY
1	B	1027	PRO
1	B	469	ALA
1	B	620	PRO
1	A	1027	PRO
1	B	53	GLY
1	B	536	VAL
1	A	1045	GLY
1	A	536	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	718/796 (90%)	673 (94%)	45 (6%)	20	53
1	B	738/796 (93%)	697 (94%)	41 (6%)	23	59
All	All	1456/1592 (92%)	1370 (94%)	86 (6%)	21	56

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	36	ASP
1	A	54	SER
1	A	56	PRO
1	A	70	GLU
1	A	76	LEU
1	A	107	ARG
1	A	220	THR
1	A	232	MET
1	A	250	GLU
1	A	266	ARG
1	A	269	LEU
1	A	294	GLN
1	A	326	LEU
1	A	365	LEU
1	A	387	TYR
1	A	415	ARG
1	A	428	PHE
1	A	442	ARG
1	A	491	LEU
1	A	531	ASP
1	A	539	LEU
1	A	540	VAL
1	A	597	ASP
1	A	635	ARG
1	A	662	ASP
1	A	693	THR
1	A	718	PRO
1	A	741	ARG
1	A	764	VAL
1	A	771	THR
1	A	794	PRO
1	A	902	THR
1	A	903	HIS

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Mol	Chain	Res	Type
1	A	926	SER
1	A	948	THR
1	A	991	ARG
1	A	997	VAL
1	A	1001	THR
1	A	1030	ARG
1	A	1031	GLN
1	A	1037	LEU
1	A	1049	ARG
1	A	1052	THR
1	A	1071	ARG
1	B	1	MET
1	B	10	ARG
1	B	12	GLU
1	B	20	THR
1	B	36	ASP
1	B	56	PRO
1	B	107	ARG
1	B	115	LYS
1	B	140	GLU
1	B	205	ARG
1	B	237	GLN
1	B	241	GLU
1	B	283	ARG
1	B	292	ARG
1	B	293	ILE
1	B	319	GLU
1	B	326	LEU
1	B	363	SER
1	B	385	ASP
1	B	393	VAL
1	B	397	GLN
1	B	428	PHE
1	B	442	ARG
1	B	448	ARG
1	B	495	LEU
1	B	537	ARG
1	B	539	LEU
1	B	597	ASP
1	B	693	THR
1	B	718	PRO
1	B	743	ARG

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Mol	Chain	Res	Type
1	B	764	VAL
1	B	792	TYR
1	B	805	ARG
1	B	828	SER
1	B	868	ASP
1	B	948	THR
1	B	997	VAL
1	B	1001	THR
1	B	1052	THR
1	B	1070	THR

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	71	ASN
1	A	210	GLN
1	A	219	GLN
1	A	237	GLN
1	A	344	GLN
1	A	350	GLN
1	A	397	GLN
1	A	613	ASN
1	A	646	ASN
1	A	818	HIS
1	A	831	GLN
1	A	851	GLN
1	A	1032	ASN
1	B	43	HIS
1	B	206	HIS
1	B	210	GLN
1	B	219	GLN
1	B	233	GLN
1	B	237	GLN
1	B	258	GLN
1	B	290	ASN
1	B	344	GLN
1	B	350	GLN
1	B	397	GLN
1	B	613	ASN
1	B	646	ASN
1	B	818	HIS
1	B	904	HIS

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Mol	Chain	Res	Type
1	B	1032	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	972/1093 (88%)	-0.40	5 (0%) 90 74	35, 63, 96, 139	0
1	B	1000/1093 (91%)	-0.38	8 (0%) 86 64	34, 61, 101, 138	0
All	All	1972/2186 (90%)	-0.39	13 (0%) 87 67	34, 62, 99, 139	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1025	THR	4.0
1	B	520	ALA	3.4
1	A	1026	ASP	3.2
1	B	1026	ASP	2.8
1	B	195	LEU	2.7
1	B	136	PRO	2.4
1	A	1044	HIS	2.4
1	B	521	MET	2.3
1	B	1032	ASN	2.3
1	A	361	ASP	2.2
1	B	170	HIS	2.2
1	A	362	PHE	2.0
1	B	137	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.