



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:56 PM UTC

PDB ID : 2EYQ / pdb_00002eyq
Title : Crystal structure of Escherichia coli transcription-repair coupling factor
Authors : Deaconescu, A.M.; Darst, S.A.
Deposited on : 2005-11-09
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

<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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

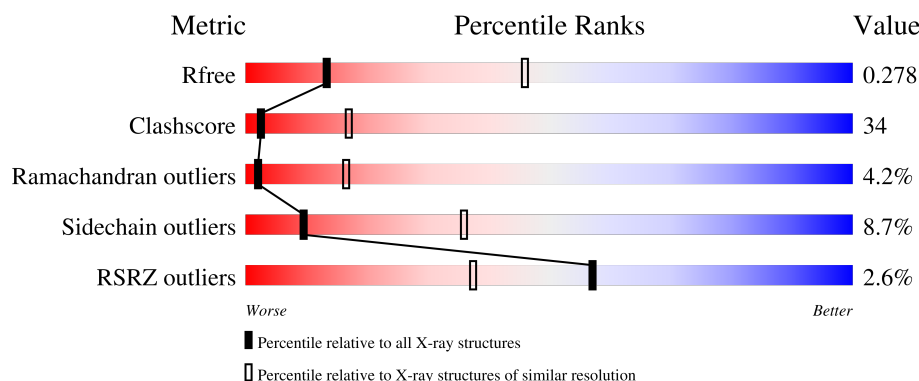
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

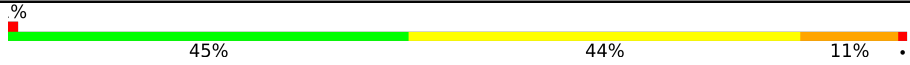
The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	1151	
1	B	1151	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EPE	A	1151	-	-	X	-
3	EPE	B	1150	-	-	X	-
3	EPE	B	1151	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18063 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 Transcription-repair coupling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1146	Total	C	N	O	S	0	0	0
			8980	5683	1605	1656	36			
1	B	1143	Total	C	N	O	S	0	0	0
			8873	5611	1584	1642	36			

There are 6 discrepancies between the modelled and reference sequences:

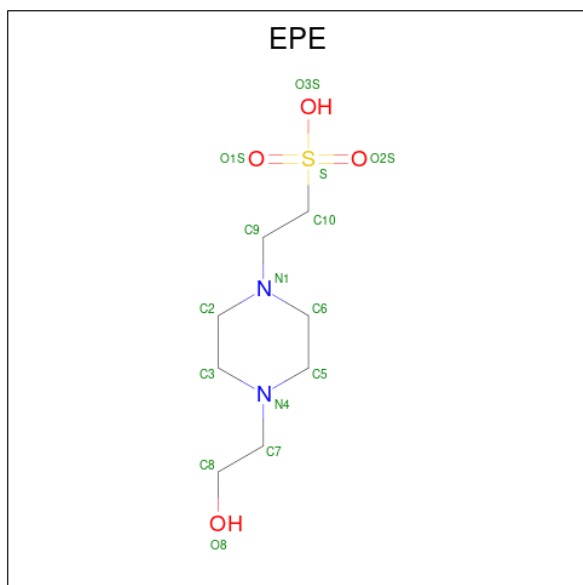
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P30958
A	-1	PRO	-	cloning artifact	UNP P30958
A	0	HIS	-	cloning artifact	UNP P30958
B	-2	GLY	-	cloning artifact	UNP P30958
B	-1	PRO	-	cloning artifact	UNP P30958
B	0	HIS	-	cloning artifact	UNP P30958

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 15 8 2 4 1	0	0
3	A	1	Total C N O S 15 8 2 4 1	0	0
3	B	1	Total C N O S 15 8 2 4 1	0	0
3	B	1	Total C N O S 15 8 2 4 1	0	0
3	B	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	68	Total O 68 68	0	0

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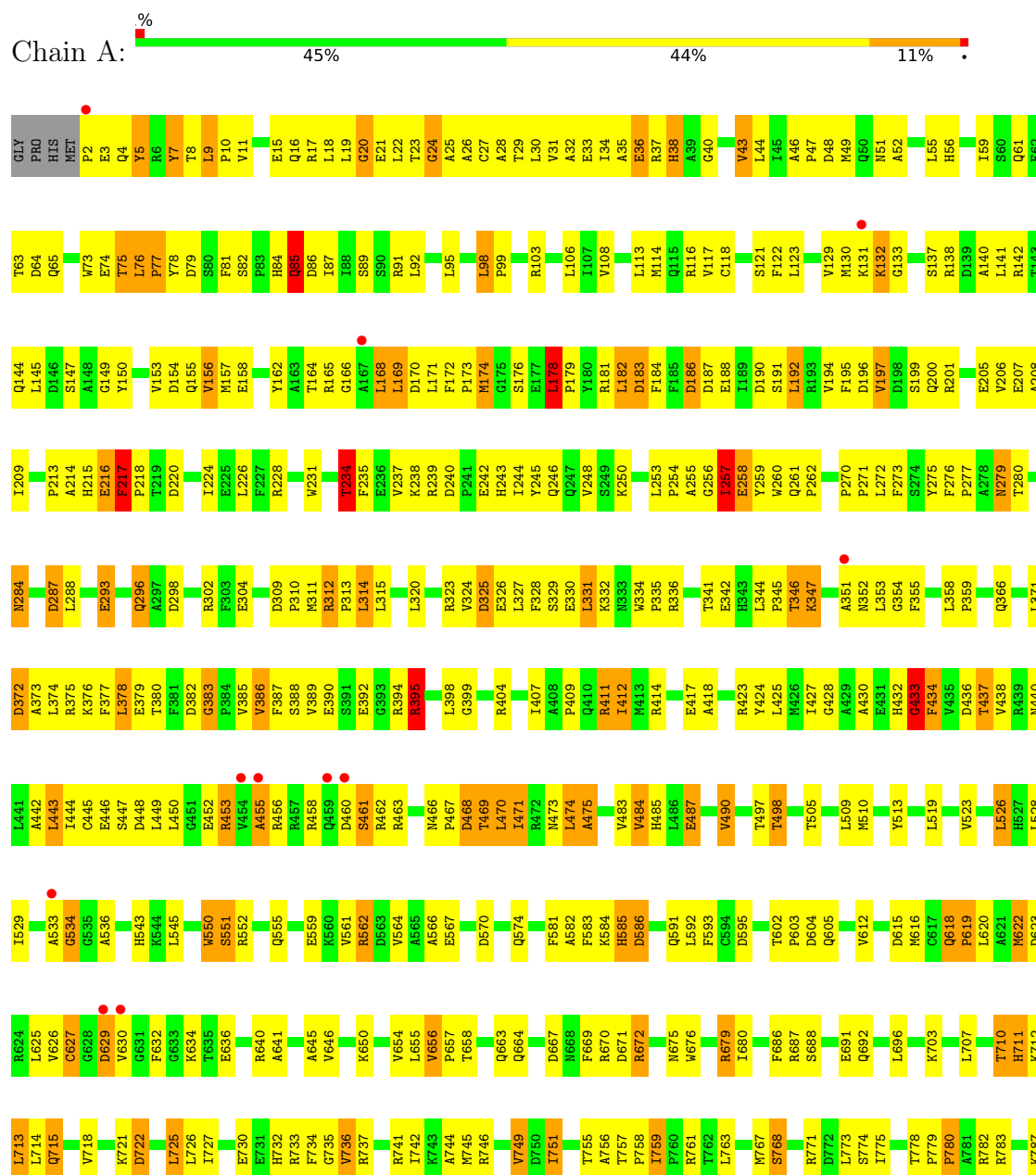
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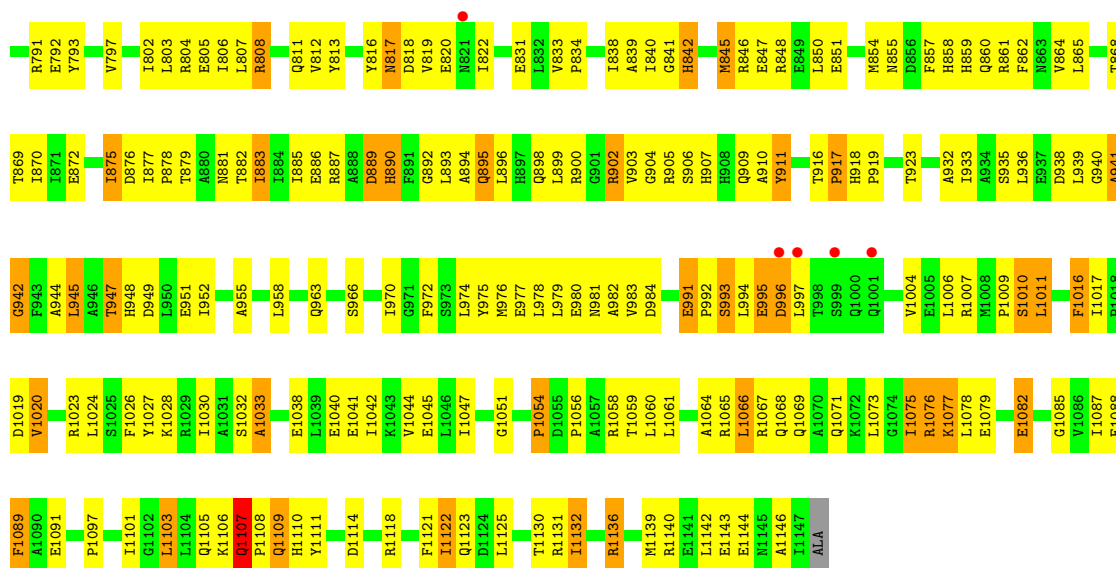
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	52	Total	O	0	0
			52	52		

3 Residue-property plots

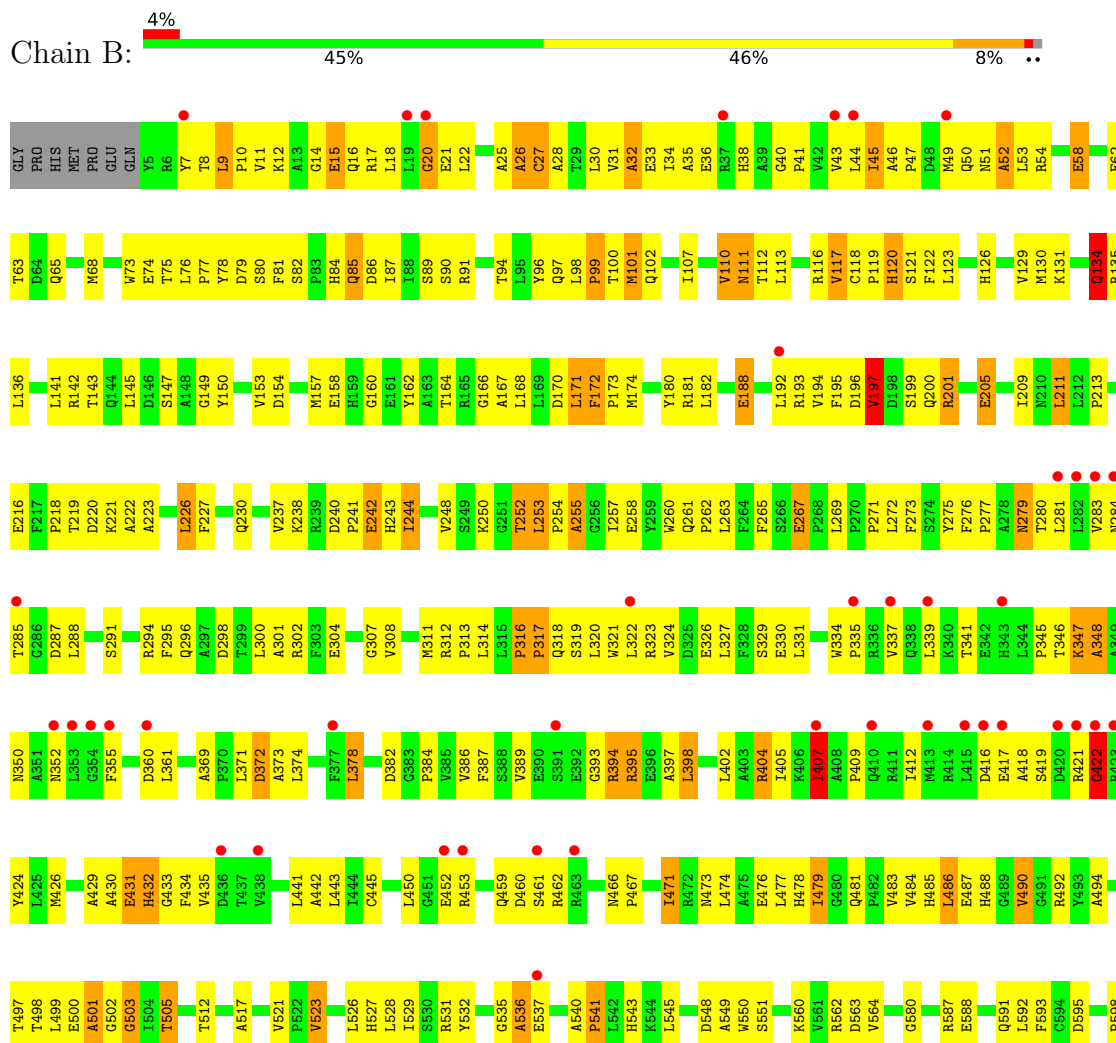
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Transcription-repair coupling factor





• Molecule 1: Transcription-repair coupling factor



L1073	L986	H907	G841	W599	B681
G1074	E991	H908	H842	T602	M682
I1075	P992	Q909	Q843	P603	S683
R1076	S993	A910	Q844	D604	S684
K1077	L994	Y911	M845	F605	R685
L1078	E995		B846		F686
	D996		E847		R687
G1085		L915	R848	I609	S688
		T916	E849		A689
F1089	Q1000	P917	L850	V612	K690
A1090	Q1001	H918		L613	E691
E1091		P919		S614	E692
K1092		K920	M854	D615	
		A921	M855	K616	
L1100	L1006	H922	D856	C617	
	R1007	T923	F857	Q618	
Q1095	M1008	T924	H858	P619	
N1096	P1009	D925	H859		
	S1010	Q927	Q860	M622	
L1104	L1011		R861	D623	
Q1105	I1012	L930	F862	M624	
K1106	P1013		M863	L625	
Q1107	F1016	I933	C867	V626	
P1108	V1020		T868	C627	
Q1109	M1021	L936	T869	G628	
H1110		E937	I870	D629	
	F1026		R871	V630	
L1113	Y1027	G940	E872	G631	
L1119	K1028	A941	T873	K634	
K1120	T1035	Q942	C874	T635	
F1121	E1036		I875		
I1122	M1037	L945	D876	A642	
	E1038		T879	F643	
L1125	L1039	H948	A880	V646	
	E1040	E951	N881		
R1128	K1043	T952	T882	K650	
K1129	V1044	R953	I883		
T1130	E1045		T884	V654	
I1131	L1046	G956	T885	L655	
E1132	I1047		E886	V656	
		Q963	R887	P657	
R1136	G1051	S964	A888	T658	
	L1052		D889	T659	
M1139	L1053	H967	H890	L660	
R1140	P1054	E968		L661	
E1141	D1055	T969	L893	A662	
L1142	P1056	I970	A894	Q663	
E1143	A1057		Q895	G664	
E1144	R1058	L974	L896	H665	
	L1059	Y975	R897	Y666	
I1147	L1060	M976	Q898	D667	
ALA		E977	L899	L751	
		L978	R900	A747	
	L1066	L979	G901	M748	
R1067	R1067	E980	E902	V749	
Q1068	Q1068	H981	V903	L752	
		V982	G904	T753	
	Q1071	V983	R905	F669	
	K1072		T986	L754	
			T837	A670	
			I838	D671	
			A839	R672	
			T840	T757	
				P758	
				I680	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.87Å 161.99Å 161.73Å 90.00° 105.09° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 98.2 (40.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.295 0.222 , 0.278	Depositor DCC
R_{free} test set	3095 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18063	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 ⓘ

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

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	0.63	0/9162	1.12	66/12429 (0.5%)
1	B	0.60	0/9051	1.06	55/12284 (0.4%)
All	All	0.62	0/18213	1.09	121/24713 (0.5%)

There are no bond length outliers.

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	A	838	ILE	N-CA-C	9.09	121.57	109.21
1	B	40	GLY	CA-C-N	9.06	129.42	119.90
1	B	40	GLY	C-N-CA	9.06	129.42	119.90
1	B	422	GLY	N-CA-C	8.96	134.41	113.18
1	A	455	ALA	N-CA-C	8.74	123.29	109.39
1	A	178	LEU	CA-C-N	8.72	128.66	120.03
1	A	178	LEU	C-N-CA	8.72	128.66	120.03
1	A	257	ILE	N-CA-C	8.58	119.37	110.36
1	A	991	GLU	CA-C-N	8.48	128.21	119.56
1	A	991	GLU	C-N-CA	8.48	128.21	119.56
1	B	832	LEU	N-CA-C	-8.27	103.71	113.88
1	B	120	HIS	N-CA-C	-8.20	103.28	113.28
1	A	1107	GLN	CA-C-N	7.79	127.34	119.24
1	A	1107	GLN	C-N-CA	7.79	127.34	119.24
1	B	991	GLU	CA-C-N	7.62	127.34	119.56
1	B	991	GLU	C-N-CA	7.62	127.34	119.56
1	A	877	ILE	CA-C-N	7.46	127.17	119.64
1	A	877	ILE	C-N-CA	7.46	127.17	119.64
1	B	260	TRP	N-CA-C	-7.41	102.83	113.21
1	A	390	GLU	N-CA-C	7.20	119.21	111.36
1	A	174	MET	N-CA-C	7.15	119.98	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	672	ARG	N-CA-C	7.08	119.08	111.36
1	A	217	PHE	CA-C-N	7.01	127.04	119.89
1	A	217	PHE	C-N-CA	7.01	127.04	119.89
1	A	383	GLY	CA-C-N	6.91	126.87	120.03
1	A	383	GLY	C-N-CA	6.91	126.87	120.03
1	A	1016	PHE	N-CA-C	-6.88	104.88	113.55
1	B	172	PHE	CA-C-N	6.87	127.25	119.83
1	B	172	PHE	C-N-CA	6.87	127.25	119.83
1	A	121	SER	N-CA-C	-6.83	103.76	111.14
1	A	7	TYR	N-CA-C	6.82	119.76	110.55
1	A	656	VAL	CA-C-N	6.80	126.04	118.97
1	A	656	VAL	C-N-CA	6.80	126.04	118.97
1	A	347	LYS	N-CA-C	-6.74	98.71	109.76
1	A	85	GLN	CG-CD-NE2	6.64	126.36	116.40
1	B	618	GLN	CA-C-N	6.60	127.12	119.47
1	B	618	GLN	C-N-CA	6.60	127.12	119.47
1	B	656	VAL	CA-C-N	6.60	126.54	119.28
1	B	656	VAL	C-N-CA	6.60	126.54	119.28
1	A	484	VAL	N-CA-C	6.59	117.33	108.11
1	A	392	GLU	N-CA-C	-6.54	105.27	113.18
1	B	421	ARG	N-CA-C	6.43	118.92	107.80
1	B	503	GLY	N-CA-C	-6.35	106.13	115.72
1	B	1119	LEU	N-CA-C	-6.30	99.94	109.95
1	A	284	ASN	N-CA-C	6.27	119.35	110.14
1	B	1016	PHE	N-CA-C	-6.24	105.57	113.43
1	B	433	GLY	N-CA-C	6.18	122.06	112.60
1	B	490	VAL	N-CA-C	6.12	117.22	107.98
1	A	64	ASP	N-CA-C	-6.10	105.41	112.92
1	A	475	ALA	N-CA-C	6.10	118.00	111.36
1	B	941	ALA	N-CA-C	6.09	117.61	110.97
1	A	176	SER	N-CA-C	6.09	119.53	110.52
1	B	838	ILE	N-CA-C	6.07	117.87	109.80
1	B	407	ILE	N-CA-C	6.06	117.32	108.53
1	A	458	ARG	N-CA-C	6.05	120.50	113.18
1	B	321	TRP	N-CA-C	5.98	119.46	109.95
1	A	433	GLY	N-CA-C	5.98	127.34	113.18
1	B	521	VAL	N-CA-C	5.97	115.09	108.05
1	B	833	VAL	CA-C-N	5.96	126.39	119.47
1	B	833	VAL	C-N-CA	5.96	126.39	119.47
1	A	20	GLY	N-CA-C	5.94	121.92	112.06
1	B	32	ALA	N-CA-C	-5.91	104.42	111.69
1	A	234	THR	N-CA-C	5.90	121.13	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	LEU	N-CA-C	5.88	119.25	110.14
1	B	369	ALA	CA-C-N	5.87	125.49	119.56
1	B	369	ALA	C-N-CA	5.87	125.49	119.56
1	A	414	ARG	N-CA-C	-5.86	99.84	109.40
1	B	167	ALA	N-CA-C	-5.85	106.19	113.15
1	A	775	ILE	N-CA-C	5.82	116.32	108.17
1	A	216	GLU	N-CA-C	-5.82	103.32	110.65
1	A	797	VAL	N-CA-C	-5.75	105.51	110.74
1	A	593	PHE	N-CA-C	-5.71	104.96	111.07
1	B	121	SER	N-CA-C	-5.71	106.35	113.15
1	A	886	GLU	N-CA-C	5.71	118.23	111.33
1	A	108	VAL	N-CA-C	5.67	114.36	107.61
1	A	144	GLN	N-CA-C	-5.66	105.02	111.07
1	B	323	ARG	N-CA-C	-5.65	101.33	110.32
1	A	336	ARG	N-CA-C	5.62	117.28	107.49
1	B	953	ARG	N-CA-C	-5.62	105.15	111.28
1	B	1058	ARG	N-CA-C	-5.61	104.18	111.02
1	A	711	HIS	N-CA-C	-5.60	105.71	112.54
1	A	528	LEU	N-CA-C	-5.58	105.68	112.88
1	A	395	ARG	N-CA-C	-5.58	105.20	111.28
1	A	1089	PHE	N-CA-C	5.57	117.72	110.53
1	B	11	VAL	N-CA-C	5.50	119.03	113.47
1	B	316	PRO	CA-C-N	5.47	126.68	119.84
1	B	316	PRO	C-N-CA	5.47	126.68	119.84
1	B	90	SER	N-CA-C	-5.44	106.81	113.50
1	B	462	ARG	N-CA-C	5.41	120.56	113.20
1	B	20	GLY	N-CA-C	5.40	120.33	110.71
1	A	1066	LEU	N-CA-C	-5.40	105.08	110.97
1	B	395	ARG	N-CA-C	-5.40	105.31	111.14
1	B	393	GLY	N-CA-C	-5.39	107.25	115.66
1	A	813	TYR	N-CA-C	-5.39	101.75	110.32
1	B	796	MET	N-CA-C	-5.39	105.51	112.68
1	B	126	HIS	N-CA-C	5.37	119.00	112.23
1	A	9	LEU	CA-C-N	5.34	125.26	119.76
1	A	9	LEU	C-N-CA	5.34	125.26	119.76
1	A	895	GLN	N-CA-C	5.29	116.86	111.14
1	B	211	LEU	N-CA-C	5.29	117.28	108.02
1	B	250	LYS	N-CA-C	-5.24	106.66	113.16
1	A	46	ALA	CA-C-N	5.24	125.04	119.28
1	A	46	ALA	C-N-CA	5.24	125.04	119.28
1	A	1136	ARG	N-CA-C	-5.22	105.51	111.14
1	A	996	ASP	N-CA-C	-5.20	106.63	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	TRP	CA-C-N	5.18	124.94	119.76
1	B	334	TRP	C-N-CA	5.18	124.94	119.76
1	A	817	ASN	N-CA-C	5.17	117.59	111.33
1	B	778	THR	N-CA-C	-5.16	102.96	110.08
1	A	490	VAL	N-CA-C	5.15	116.11	108.23
1	A	9	LEU	N-CA-C	5.14	116.13	109.65
1	A	947	THR	N-CA-C	-5.13	105.87	111.82
1	A	314	LEU	N-CA-C	5.12	118.42	110.17
1	B	977	GLU	N-CA-C	-5.12	105.78	111.36
1	A	618	GLN	CA-C-N	5.10	126.22	119.84
1	A	618	GLN	C-N-CA	5.10	126.22	119.84
1	B	253	LEU	CA-C-N	5.09	126.20	119.84
1	B	253	LEU	C-N-CA	5.09	126.20	119.84
1	B	874	GLY	N-CA-C	-5.02	108.44	114.66
1	A	40	GLY	N-CA-C	5.01	122.56	112.34

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	8980	0	8865	629	0
1	B	8873	0	8675	602	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	30	0	36	10	0
3	B	45	0	54	26	0
4	A	68	0	0	5	0
4	B	52	0	0	3	0
All	All	18063	0	17630	1227	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 34.

All (1227) 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:254:PRO:HD2	1:B:257:ILE:HD12	1.17	1.15
1:A:474:LEU:HD21	1:A:1028:LYS:HG3	1.31	1.07
1:B:117:VAL:HG12	1:B:118:CYS:H	1.16	1.05
1:A:116:ARG:HG3	1:A:320:LEU:O	1.57	1.04
1:B:386:VAL:HB	1:B:443:LEU:HD12	1.39	1.03
1:B:659:THR:HG22	1:B:684:SER:HB2	1.39	1.01
1:B:612:VAL:HA	1:B:622:MET:HE1	1.43	1.01
1:B:562:ARG:HG3	1:B:992:PRO:HG3	1.04	1.00
1:B:20:GLY:HA3	1:B:352:ASN:HA	1.42	0.99
1:A:991:GLU:CD	1:A:992:PRO:HD2	1.87	0.98
1:B:490:VAL:H	1:B:543:HIS:HD2	1.07	0.98
1:A:279:ASN:HD22	1:A:279:ASN:H	1.01	0.97
1:A:822:ILE:HD12	1:A:868:THR:CG2	1.97	0.95
1:A:473:ASN:C	1:A:474:LEU:HD23	1.92	0.95
1:B:791:ARG:HG3	1:B:791:ARG:HH11	1.31	0.95
1:A:991:GLU:CG	1:A:992:PRO:HD2	1.98	0.93
1:B:562:ARG:CG	1:B:992:PRO:HG3	1.95	0.93
1:B:18:LEU:HD12	1:B:350:ASN:HB3	1.49	0.93
1:B:710:THR:HG23	1:B:712:LYS:H	1.31	0.93
1:A:409:PRO:HB2	1:A:425:LEU:HD23	1.50	0.92
1:B:605:GLN:HE21	1:B:634:LYS:HD2	1.33	0.92
1:B:726:LEU:HD23	1:B:751:ILE:HD11	1.51	0.92
1:A:155:GLN:O	1:A:156:VAL:HG12	1.69	0.91
1:B:63:THR:HG22	1:B:65:GLN:H	1.31	0.91
1:B:1136:ARG:HG3	1:B:1136:ARG:HH11	1.35	0.91
1:B:384:PRO:HG2	1:B:441:LEU:HD13	1.53	0.91
1:A:178:LEU:HD23	1:A:178:LEU:H	1.36	0.90
1:B:182:LEU:CD2	1:B:192:LEU:HD13	2.02	0.90
1:A:612:VAL:HG13	1:A:622:MET:HE1	1.52	0.89
1:B:562:ARG:HG3	1:B:992:PRO:CG	1.98	0.87
1:A:170:ASP:OD1	1:A:181:ARG:HG3	1.75	0.87
1:A:412:ILE:HG22	1:A:417:GLU:HB2	1.57	0.87
1:A:562:ARG:HD2	1:A:992:PRO:HG3	1.53	0.86
1:A:344:LEU:HB2	1:A:352:ASN:ND2	1.91	0.86
1:B:615:ASP:HB2	1:B:622:MET:HE3	1.58	0.86
1:A:1091:GLU:CD	1:A:1091:GLU:H	1.83	0.85
1:B:481:GLN:HE22	1:B:531:ARG:HH12	1.25	0.84
1:B:389:VAL:CG1	1:B:394:ARG:HB3	2.06	0.84
1:B:940:GLY:N	3:B:1151:EPE:O1S	2.11	0.84
1:A:881:ASN:HA	1:A:903:VAL:HG13	1.58	0.84
1:A:887:ARG:HG2	1:A:890:HIS:CE1	2.12	0.84
1:B:922:MET:HE3	1:B:927:GLN:HG2	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:VAL:HG12	1:B:118:CYS:N	1.93	0.83
1:B:113:LEU:HD12	1:B:272:LEU:HD23	1.60	0.83
1:A:279:ASN:H	1:A:279:ASN:ND2	1.74	0.83
1:A:627:CYS:SG	1:A:773:LEU:HD11	2.18	0.82
1:A:279:ASN:HD22	1:A:279:ASN:N	1.69	0.82
1:B:182:LEU:HD21	1:B:192:LEU:HD13	1.61	0.82
1:A:276:PHE:HB3	1:A:280:THR:HG21	1.61	0.82
1:B:490:VAL:H	1:B:543:HIS:CD2	1.95	0.82
1:A:7:TYR:CE1	1:A:37:ARG:NH1	2.48	0.82
1:A:787:LYS:HG3	1:A:909:GLN:NE2	1.94	0.82
1:B:157:MET:HA	1:B:197:VAL:HG12	1.62	0.82
1:A:615:ASP:HB2	1:A:622:MET:HE3	1.62	0.81
1:B:31:VAL:HA	1:B:34:ILE:HG22	1.61	0.81
1:B:937:GLU:HG2	3:B:1151:EPE:H31	1.61	0.81
1:A:994:LEU:C	1:A:996:ASP:H	1.89	0.80
1:B:389:VAL:HG13	1:B:394:ARG:HB3	1.63	0.80
1:A:277:PRO:O	1:A:280:THR:HG22	1.81	0.80
1:B:78:TYR:CD2	1:B:314:LEU:HD13	2.16	0.79
1:B:994:LEU:C	1:B:996:ASP:H	1.91	0.79
1:A:63:THR:HG22	1:A:65:GLN:H	1.47	0.79
1:A:296:GLN:HE22	1:A:323:ARG:HA	1.46	0.79
1:B:1035:THR:HB	1:B:1038:GLU:HG3	1.64	0.79
1:B:936:LEU:HB3	3:B:1151:EPE:H101	1.63	0.78
1:B:62:PHE:HE2	1:B:426:MET:HE1	1.48	0.78
1:B:242:GLU:HG3	1:B:311:MET:HE3	1.66	0.78
1:A:497:THR:HG22	1:A:498:THR:N	1.98	0.78
1:A:273:PHE:CD1	1:A:330:GLU:HG2	2.20	0.77
1:B:982:ALA:O	1:B:986:LEU:HD13	1.82	0.77
1:B:302:ARG:HH11	1:B:302:ARG:HB3	1.48	0.77
1:A:903:VAL:HG12	1:A:910:ALA:HB1	1.66	0.77
1:B:602:THR:HB	1:B:605:GLN:HB2	1.65	0.77
1:A:21:GLU:HA	1:A:341:THR:O	1.84	0.76
1:B:170:ASP:OD1	1:B:181:ARG:HG3	1.86	0.76
1:B:903:VAL:CG1	1:B:910:ALA:HB1	2.15	0.76
1:B:1035:THR:HG22	1:B:1037:ASN:H	1.48	0.76
1:B:726:LEU:HD23	1:B:751:ILE:CD1	2.15	0.76
1:A:434:PHE:HD1	1:A:434:PHE:C	1.92	0.76
1:B:970:ILE:HB	1:B:974:LEU:HD23	1.67	0.76
1:B:98:LEU:HB3	1:B:99:PRO:HD3	1.67	0.76
1:A:411:ARG:HH21	1:A:427:ILE:HD11	1.51	0.76
1:B:659:THR:HG21	1:B:685:ARG:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:GLU:OE2	1:A:755:THR:HA	1.86	0.75
1:B:490:VAL:N	1:B:543:HIS:HD2	1.83	0.75
1:A:65:GLN:HE22	1:A:103:ARG:HG2	1.51	0.75
1:B:791:ARG:HH11	1:B:791:ARG:CG	2.00	0.75
1:A:254:PRO:HD2	1:A:257:ILE:HD12	1.67	0.75
1:B:298:ASP:O	1:B:302:ARG:HG3	1.87	0.74
1:A:373:ALA:HA	1:A:376:LYS:HE2	1.68	0.74
1:A:936:LEU:HD22	3:A:1151:EPE:H62	1.70	0.74
1:A:562:ARG:CD	1:A:992:PRO:HG3	2.18	0.74
1:A:992:PRO:C	1:A:994:LEU:H	1.96	0.74
1:B:942:GLY:N	3:B:1151:EPE:O2S	2.21	0.74
1:A:4:GLN:HB2	1:A:5:TYR:CE1	2.23	0.74
1:A:425:LEU:HD12	1:A:425:LEU:O	1.87	0.73
1:A:991:GLU:HG3	1:A:992:PRO:HD2	1.69	0.73
1:A:726:LEU:HD23	1:A:751:ILE:HD11	1.70	0.73
1:B:481:GLN:NE2	1:B:531:ARG:HH12	1.86	0.73
1:B:839:ALA:HB2	1:B:862:PHE:CD2	2.23	0.73
1:A:178:LEU:HD23	1:A:178:LEU:N	2.04	0.72
1:B:845:MET:HE2	1:B:875:ILE:CD1	2.19	0.72
1:A:848:ARG:NH2	1:B:685:ARG:O	2.23	0.72
1:B:992:PRO:C	1:B:994:LEU:H	1.98	0.72
1:B:96:TYR:O	1:B:99:PRO:HD2	1.90	0.72
1:B:117:VAL:CG1	1:B:118:CYS:H	1.99	0.72
1:A:156:VAL:HG11	1:A:170:ASP:HB3	1.72	0.72
1:A:899:LEU:O	1:A:902:ARG:HG3	1.89	0.72
1:B:956:GLY:HA2	1:B:967:MET:HE1	1.70	0.72
1:B:630:VAL:HG12	1:B:630:VAL:O	1.89	0.72
1:B:1136:ARG:HH11	1:B:1136:ARG:CG	2.02	0.71
1:A:378:LEU:HD12	1:A:407:ILE:CD1	2.21	0.71
1:A:474:LEU:HD23	1:A:474:LEU:N	2.04	0.71
1:A:181:ARG:HG3	1:A:181:ARG:HH11	1.55	0.71
1:B:91:ARG:HD3	1:B:216:GLU:OE1	1.91	0.71
1:B:685:ARG:HG3	3:B:1150:EPE:H61	1.71	0.71
1:A:707:LEU:HD21	1:A:713:LEU:HD21	1.73	0.71
1:B:994:LEU:O	1:B:996:ASP:N	2.23	0.71
1:B:31:VAL:HA	1:B:34:ILE:CG2	2.20	0.71
1:B:1125:LEU:HB3	1:B:1131:ARG:HB2	1.72	0.71
1:A:497:THR:CG2	1:A:498:THR:N	2.53	0.71
1:B:587:ARG:O	1:B:591:GLN:HG2	1.91	0.70
1:A:434:PHE:C	1:A:434:PHE:CD1	2.67	0.70
1:B:386:VAL:HB	1:B:443:LEU:CD1	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLY:C	1:A:26:ALA:H	1.99	0.70
1:A:616:MET:HE1	1:A:641:ALA:HB1	1.72	0.70
1:B:699:VAL:HG21	1:B:707:LEU:HD22	1.73	0.70
1:A:174:MET:HG3	1:A:214:ALA:HA	1.74	0.70
1:A:375:ARG:O	1:A:379:GLU:HG2	1.92	0.70
1:A:655:LEU:HD11	1:A:714:LEU:HD21	1.73	0.70
1:B:1140:ARG:O	1:B:1144:GLU:HG3	1.90	0.70
1:A:47:PRO:HG2	1:A:51:ASN:HD22	1.56	0.70
1:B:131:LYS:H	1:B:134:GLN:HG3	1.55	0.70
1:A:76:LEU:O	1:A:79:ASP:HB2	1.91	0.70
1:A:240:ASP:HB3	1:A:311:MET:HE1	1.73	0.70
1:A:940:GLY:N	3:A:1151:EPE:O1S	2.25	0.70
1:A:377:PHE:HD2	1:A:378:LEU:HD23	1.55	0.70
1:A:260:TRP:HH2	1:A:312:ARG:HG2	1.56	0.70
1:A:903:VAL:CG1	1:A:910:ALA:HB1	2.21	0.70
1:B:27:CYS:SG	1:B:339:LEU:HD13	2.31	0.70
1:B:76:LEU:O	1:B:79:ASP:HB2	1.92	0.70
1:A:20:GLY:N	1:A:344:LEU:HD11	2.07	0.70
1:A:117:VAL:HG12	1:A:118:CYS:O	1.92	0.69
1:A:20:GLY:HA3	1:A:344:LEU:HG	1.73	0.69
1:A:98:LEU:HB3	1:A:99:PRO:HD3	1.73	0.69
1:B:307:GLY:HA2	1:B:314:LEU:HG	1.75	0.69
1:B:671:ASP:CG	1:B:848:ARG:HH11	1.99	0.69
1:A:344:LEU:HB2	1:A:352:ASN:HD21	1.56	0.69
1:B:196:ASP:HB3	1:B:199:SER:HB3	1.74	0.69
1:A:178:LEU:N	1:A:178:LEU:CD2	2.56	0.69
1:A:936:LEU:HD13	3:A:1151:EPE:H102	1.74	0.69
1:A:1078:LEU:C	1:A:1078:LEU:HD23	2.18	0.69
1:B:903:VAL:HG12	1:B:910:ALA:HB1	1.74	0.69
1:A:36:GLU:OE2	1:A:63:THR:HG23	1.93	0.68
1:B:1106:LYS:C	1:B:1108:PRO:HD3	2.18	0.68
1:A:63:THR:HG21	1:A:65:GLN:HB2	1.76	0.68
1:A:1082:GLU:HA	1:A:1125:LEU:O	1.93	0.68
1:A:73:TRP:CH2	1:A:258:GLU:HB3	2.29	0.68
1:A:1038:GLU:O	1:A:1042:ILE:HG13	1.94	0.68
1:B:378:LEU:HD21	1:B:407:ILE:HD13	1.75	0.68
1:A:490:VAL:H	1:A:543:HIS:CD2	2.12	0.68
1:B:182:LEU:HD23	1:B:192:LEU:HD13	1.74	0.68
1:B:634:LYS:HE2	1:B:776:ILE:HG21	1.76	0.68
1:A:37:ARG:O	1:A:37:ARG:HG3	1.93	0.68
1:A:114:MET:HG2	1:A:327:LEU:HD22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ARG:HD2	1:B:319:SER:O	1.94	0.68
1:A:679:ARG:HD3	1:A:703:LYS:O	1.94	0.67
1:B:89:SER:HB2	1:B:174:MET:HE3	1.75	0.67
1:B:937:GLU:CG	3:B:1151:EPE:H31	2.23	0.67
1:B:612:VAL:CA	1:B:622:MET:HE1	2.21	0.67
1:B:905:ARG:HD3	1:B:908:HIS:CD2	2.29	0.67
1:B:1119:LEU:HD12	1:B:1120:LYS:H	1.57	0.67
1:A:1069:GLN:HB2	1:A:1139:MET:HE2	1.75	0.67
1:A:1073:LEU:HD11	1:A:1143:GLU:HB3	1.74	0.67
1:A:842:HIS:CE1	3:B:1150:EPE:H62	2.30	0.67
1:A:916:THR:HB	1:A:917:PRO:HD2	1.76	0.67
1:A:468:ASP:O	1:A:469:THR:C	2.38	0.67
1:A:842:HIS:NE2	3:B:1150:EPE:H62	2.09	0.67
1:A:1122:ILE:O	1:A:1123:GLN:HG2	1.95	0.67
1:B:7:TYR:HD2	1:B:8:THR:H	1.41	0.67
1:B:136:LEU:HD13	1:B:141:LEU:HB2	1.75	0.67
1:B:386:VAL:HG11	1:B:426:MET:HE3	1.76	0.67
1:B:688:SER:OG	1:B:691:GLU:HG3	1.95	0.67
1:B:134:GLN:O	1:B:188:GLU:HG2	1.95	0.67
1:B:153:VAL:HG12	1:B:154:ASP:H	1.59	0.67
1:B:153:VAL:HG12	1:B:154:ASP:N	2.08	0.67
1:A:872:GLU:O	1:A:875:ILE:HG13	1.95	0.67
1:B:936:LEU:HD22	3:B:1151:EPE:H62	1.76	0.67
1:B:1107:GLN:HA	1:B:1109:GLN:HE22	1.60	0.67
1:A:47:PRO:HG2	1:A:48:ASP:OD1	1.96	0.66
1:A:153:VAL:HG12	1:A:154:ASP:N	2.10	0.66
1:B:135:ARG:HG2	1:B:188:GLU:HG3	1.76	0.66
1:B:378:LEU:HD21	1:B:407:ILE:CD1	2.25	0.66
1:B:523:VAL:HA	1:B:526:LEU:HD23	1.77	0.66
1:A:490:VAL:H	1:A:543:HIS:HD2	1.41	0.66
1:A:585:HIS:O	1:A:586:ASP:HB3	1.94	0.66
1:B:171:LEU:HG	1:B:173:PRO:HD3	1.77	0.66
1:A:434:PHE:HD1	1:A:434:PHE:O	1.78	0.66
1:B:10:PRO:HB2	1:B:15:GLU:HB3	1.76	0.66
1:A:386:VAL:HA	1:A:424:TYR:O	1.96	0.66
1:B:930:LEU:O	1:B:933:ILE:HG22	1.96	0.66
1:B:46:ALA:O	1:B:110:VAL:HG23	1.96	0.65
1:B:629:ASP:OD1	1:B:634:LYS:CE	2.43	0.65
1:B:817:ASN:O	1:B:818:ASP:HB2	1.95	0.65
1:A:244:ILE:O	1:A:248:VAL:HG23	1.97	0.65
1:A:182:LEU:O	1:A:183:ASP:HB3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:ASP:OD1	1:B:634:LYS:HG2	1.96	0.65
1:A:460:ASP:O	1:A:462:ARG:N	2.29	0.65
1:A:411:ARG:NH2	1:A:427:ILE:HD11	2.11	0.65
1:B:117:VAL:HG21	1:B:272:LEU:HD13	1.79	0.65
1:A:10:PRO:HB3	1:A:15:GLU:O	1.96	0.65
1:A:122:PHE:CE1	1:A:218:PRO:HD3	2.31	0.65
1:A:1073:LEU:HD13	1:A:1142:LEU:HG	1.77	0.65
1:B:145:LEU:HD21	1:B:211:LEU:HD11	1.77	0.65
1:B:625:LEU:HD13	1:B:753:THR:HG22	1.79	0.65
1:A:467:PRO:O	1:A:471:ILE:HG13	1.97	0.65
1:A:763:LEU:HA	1:A:976:MET:HE1	1.77	0.65
1:A:199:SER:O	1:A:200:GLN:HB2	1.97	0.65
1:B:157:MET:HA	1:B:197:VAL:CG1	2.26	0.65
1:A:10:PRO:HG3	1:A:17:ARG:HB2	1.78	0.65
1:A:63:THR:CG2	1:A:65:GLN:HB2	2.26	0.65
1:A:1107:GLN:N	1:A:1108:PRO:HD3	2.10	0.65
1:B:147:SER:C	1:B:149:GLY:H	2.03	0.65
1:A:432:HIS:HA	1:A:445:CYS:HB2	1.77	0.64
1:B:605:GLN:HE21	1:B:634:LYS:CD	2.10	0.64
1:A:896:LEU:HA	1:A:899:LEU:HD12	1.79	0.64
1:B:302:ARG:HB3	1:B:302:ARG:NH1	2.12	0.64
1:B:794:ASP:C	1:B:796:MET:H	2.05	0.64
1:A:630:VAL:HG12	1:A:630:VAL:O	1.97	0.64
1:A:881:ASN:CA	1:A:903:VAL:HG13	2.27	0.64
1:B:38:HIS:CD2	1:B:281:LEU:HD23	2.33	0.64
1:A:181:ARG:NH2	1:A:200:GLN:O	2.30	0.64
1:A:456:ARG:HE	1:A:876:ASP:CG	2.05	0.64
1:A:1017:ILE:O	1:A:1023:ARG:HD3	1.98	0.64
1:B:794:ASP:HB3	1:B:797:VAL:HG23	1.78	0.64
1:B:180:TYR:HB3	1:B:192:LEU:HD11	1.78	0.64
1:B:725:LEU:HD12	1:B:726:LEU:H	1.63	0.64
1:B:991:GLU:CD	1:B:992:PRO:HD2	2.23	0.64
1:A:170:ASP:OD1	1:A:181:ARG:NH1	2.31	0.64
1:A:170:ASP:OD2	1:A:181:ARG:NH1	2.31	0.64
1:B:220:ASP:OD1	1:B:222:ALA:HB3	1.98	0.64
1:B:254:PRO:HD2	1:B:257:ILE:CD1	2.12	0.64
1:A:30:LEU:HD11	1:A:353:LEU:CD1	2.28	0.64
1:B:869:THR:H	1:B:872:GLU:HG2	1.61	0.64
1:B:211:LEU:HD23	1:B:211:LEU:O	1.98	0.63
1:B:466:ASN:OD1	1:B:467:PRO:HD2	1.98	0.63
1:A:432:HIS:HB2	1:A:448:ASP:OD1	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:ILE:O	1:A:1136:ARG:HG3	1.99	0.63
1:B:492:ARG:NH2	1:B:540:ALA:O	2.31	0.63
1:B:523:VAL:HA	1:B:526:LEU:CD2	2.27	0.63
1:A:240:ASP:CB	1:A:311:MET:HE1	2.28	0.63
1:B:685:ARG:HD2	3:B:1150:EPE:H61	1.80	0.63
1:B:936:LEU:HA	3:B:1151:EPE:H51	1.81	0.63
1:B:964:SER:HA	1:B:967:MET:HE3	1.80	0.63
1:A:1040:GLU:O	1:A:1044:VAL:HG23	1.99	0.63
1:B:484:VAL:HG22	1:B:490:VAL:HG22	1.80	0.63
1:A:78:TYR:CD2	1:A:314:LEU:HD13	2.34	0.63
1:A:936:LEU:HA	3:A:1151:EPE:H51	1.81	0.63
1:A:870:ILE:CD1	1:A:895:GLN:HB3	2.29	0.63
1:B:386:VAL:HA	1:B:424:TYR:CB	2.29	0.63
1:B:936:LEU:HB3	3:B:1151:EPE:C10	2.29	0.63
1:A:73:TRP:NE1	1:A:91:ARG:HH11	1.95	0.63
1:A:386:VAL:HG22	1:A:424:TYR:HB2	1.80	0.63
1:A:436:ASP:O	1:A:440:ASN:N	2.32	0.62
1:A:942:GLY:N	3:A:1151:EPE:O2S	2.32	0.62
1:B:802:ILE:O	1:B:806:ILE:HG13	1.99	0.62
1:A:10:PRO:CG	1:A:17:ARG:HB2	2.30	0.62
1:A:254:PRO:HD2	1:A:257:ILE:CD1	2.30	0.62
1:B:612:VAL:HA	1:B:622:MET:CE	2.23	0.62
1:B:1000:GLN:O	1:B:1071:GLN:NE2	2.32	0.62
1:B:945:LEU:O	1:B:948:HIS:HB3	1.99	0.62
1:A:155:GLN:O	1:A:156:VAL:CG1	2.46	0.62
1:A:156:VAL:HG13	1:A:156:VAL:O	2.00	0.62
1:A:885:ILE:HD13	1:A:899:LEU:HD13	1.81	0.62
1:A:570:ASP:O	1:A:574:GLN:HG3	1.99	0.62
1:B:692:GLN:HE22	1:B:712:LYS:HD3	1.64	0.62
1:A:30:LEU:O	1:A:34:ILE:HG13	2.00	0.62
1:A:117:VAL:HG12	1:A:118:CYS:N	2.15	0.62
1:B:494:ALA:HB2	1:B:512:THR:HG23	1.81	0.62
1:A:47:PRO:CG	1:A:51:ASN:HD22	2.12	0.62
1:A:116:ARG:HG3	1:A:320:LEU:C	2.25	0.62
1:A:298:ASP:O	1:A:302:ARG:HG3	1.99	0.62
1:A:870:ILE:HD11	1:A:895:GLN:HB3	1.82	0.61
1:B:430:ALA:HB1	1:B:445:CYS:SG	2.40	0.61
1:A:688:SER:OG	1:A:691:GLU:HG3	2.00	0.61
1:A:474:LEU:CD2	1:A:1028:LYS:HG3	2.20	0.61
1:A:629:ASP:O	1:A:634:LYS:HG3	2.01	0.61
1:B:906:SER:O	1:B:907:HIS:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:GLN:HG2	1:A:857:PHE:CD2	2.35	0.61
1:A:1016:PHE:CD2	1:A:1017:ILE:HG13	2.35	0.61
1:B:262:PRO:HG3	1:B:269:LEU:HD12	1.83	0.61
1:B:881:ASN:HA	1:B:903:VAL:HG13	1.82	0.61
1:B:1011:LEU:HD22	1:B:1056:PRO:HB3	1.82	0.61
1:A:117:VAL:CG1	1:A:118:CYS:N	2.63	0.61
1:A:358:LEU:HD21	1:A:444:ILE:HG12	1.83	0.61
1:B:710:THR:HG23	1:B:712:LYS:N	2.12	0.61
1:B:811:GLN:HG2	1:B:857:PHE:CD2	2.35	0.61
1:B:845:MET:HE2	1:B:875:ILE:HD13	1.83	0.61
1:A:131:LYS:O	1:A:133:GLY:N	2.33	0.61
1:A:214:ALA:O	1:A:215:HIS:CG	2.53	0.61
1:B:747:ALA:O	1:B:748:ASN:CB	2.48	0.61
1:B:874:GLY:HA2	1:B:902:ARG:NH1	2.16	0.61
1:B:1108:PRO:HD2	1:B:1109:GLN:HE21	1.65	0.61
1:A:763:LEU:O	1:A:767:MET:HG2	2.01	0.61
1:A:767:MET:HE2	1:A:958:LEU:HD21	1.83	0.60
1:A:629:ASP:OD1	1:A:634:LYS:HE3	1.99	0.60
1:A:802:ILE:HD12	1:A:833:VAL:HG21	1.83	0.60
1:A:822:ILE:HD12	1:A:868:THR:HG23	1.80	0.60
1:B:498:THR:O	1:B:499:LEU:HD23	2.01	0.60
1:A:78:TYR:HD2	1:A:314:LEU:HD22	1.67	0.60
1:B:168:LEU:CD2	1:B:181:ARG:HD3	2.31	0.60
1:B:386:VAL:HG11	1:B:426:MET:CE	2.30	0.60
1:A:9:LEU:HD11	1:A:37:ARG:HG3	1.82	0.60
1:B:845:MET:HE2	1:B:875:ILE:HD11	1.83	0.60
1:A:235:PHE:HZ	1:A:315:LEU:HD23	1.66	0.60
1:A:911:TYR:N	1:A:911:TYR:CD1	2.69	0.60
1:B:17:ARG:HB2	1:B:337:VAL:HG13	1.83	0.60
1:B:80:SER:O	1:B:255:ALA:HB1	2.02	0.60
1:B:412:ILE:HD13	1:B:418:ALA:HB2	1.83	0.60
1:A:24:GLY:O	1:A:26:ALA:N	2.35	0.60
1:A:497:THR:CG2	1:A:498:THR:H	2.14	0.60
1:A:562:ARG:CG	1:A:992:PRO:HG3	2.31	0.60
1:B:432:HIS:CD2	1:B:432:HIS:H	2.19	0.60
1:A:562:ARG:HG3	1:A:992:PRO:HG3	1.84	0.60
1:A:584:LYS:O	1:A:585:HIS:HB2	2.01	0.60
1:A:1009:PRO:HD2	4:A:1207:HOH:O	2.01	0.60
1:B:1129:LYS:O	1:B:1132:ILE:HG22	2.02	0.60
1:A:73:TRP:HE1	1:A:91:ARG:HH11	1.50	0.59
1:A:564:VAL:HG21	1:A:963:GLN:CD	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:VAL:HG12	1:B:238:LYS:N	2.16	0.59
1:B:659:THR:H	3:B:1150:EPE:H92	1.66	0.59
1:B:659:THR:CG2	1:B:684:SER:HB2	2.23	0.59
1:A:1078:LEU:HD23	1:A:1078:LEU:O	2.01	0.59
1:A:840:ILE:HG22	1:A:841:GLY:N	2.18	0.59
1:B:119:PRO:HD2	1:B:265:PHE:CE2	2.37	0.59
1:A:412:ILE:CG2	1:A:417:GLU:HB2	2.31	0.59
1:A:692:GLN:HE22	1:A:712:LYS:HE2	1.67	0.59
1:A:1103:LEU:HD21	1:A:1111:TYR:CE1	2.37	0.59
1:B:49:MET:O	1:B:52:ALA:HB3	2.02	0.59
1:A:966:SER:O	1:A:970:ILE:HG12	2.02	0.59
1:A:244:ILE:HD13	1:A:311:MET:O	2.01	0.59
1:B:291:SER:O	1:B:294:ARG:HB3	2.03	0.59
1:B:778:THR:HG22	1:B:779:PRO:HD2	1.83	0.59
1:A:434:PHE:CE1	1:A:443:LEU:HB2	2.38	0.58
1:A:1011:LEU:HD23	1:A:1056:PRO:HB3	1.85	0.58
1:B:642:ALA:O	1:B:646:VAL:HG23	2.02	0.58
1:A:224:ILE:O	1:A:228:ARG:HG3	2.03	0.58
1:B:63:THR:HG22	1:B:65:GLN:N	2.11	0.58
1:A:555:GLN:HE21	1:A:559:GLU:HG3	1.68	0.58
1:B:629:ASP:OD1	1:B:634:LYS:CD	2.51	0.58
1:B:1035:THR:HG22	1:B:1036:GLU:N	2.17	0.58
1:B:1109:GLN:H	1:B:1109:GLN:NE2	2.02	0.58
1:A:192:LEU:N	1:A:192:LEU:HD22	2.19	0.58
1:B:122:PHE:CE1	1:B:218:PRO:HD3	2.39	0.58
1:B:873:THR:O	1:B:902:ARG:HD2	2.02	0.58
1:A:73:TRP:NE1	1:A:91:ARG:NH1	2.52	0.58
1:B:994:LEU:C	1:B:996:ASP:N	2.60	0.58
1:A:444:ILE:CG2	1:A:449:LEU:HD13	2.33	0.58
1:A:1109:GLN:H	1:A:1109:GLN:NE2	2.01	0.58
1:A:52:ALA:HA	1:A:55:LEU:HD12	1.86	0.58
1:A:196:ASP:HB3	1:A:199:SER:HB3	1.85	0.58
1:A:323:ARG:HB2	1:A:326:GLU:HG3	1.85	0.58
1:A:261:GLN:HB3	1:A:262:PRO:HD3	1.85	0.57
1:B:1008:MET:HE3	1:B:1128:ARG:HG2	1.85	0.57
1:B:394:ARG:O	1:B:397:ALA:HB3	2.05	0.57
1:B:659:THR:HG21	1:B:685:ARG:H	1.69	0.57
1:A:82:SER:OG	1:A:255:ALA:O	2.17	0.57
1:A:899:LEU:O	1:A:902:ARG:CG	2.52	0.57
1:B:31:VAL:CA	1:B:34:ILE:HG22	2.35	0.57
1:B:435:VAL:HA	1:B:442:ALA:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:PRO:HB2	1:B:223:ALA:HB2	1.85	0.57
1:A:745:MET:HG2	1:A:745:MET:O	2.04	0.57
1:A:412:ILE:HG12	1:A:424:TYR:HB3	1.86	0.57
1:B:281:LEU:HD12	1:B:281:LEU:C	2.29	0.57
1:B:1078:LEU:HD12	1:B:1078:LEU:C	2.30	0.57
1:A:467:PRO:HG2	1:A:468:ASP:H	1.70	0.57
1:A:783:ARG:HD2	4:A:1186:HOH:O	2.03	0.57
1:B:145:LEU:CD2	1:B:211:LEU:HD11	2.35	0.57
1:A:129:VAL:HG12	1:A:130:MET:N	2.20	0.56
1:B:21:GLU:O	1:B:355:PHE:HB2	2.05	0.56
1:B:749:VAL:HG12	1:B:750:ASP:N	2.20	0.56
1:B:1091:GLU:CD	1:B:1092:LYS:H	2.13	0.56
1:B:73:TRP:CH2	1:B:258:GLU:HB3	2.40	0.56
1:B:147:SER:C	1:B:149:GLY:N	2.60	0.56
1:B:710:THR:CG2	1:B:712:LYS:H	2.12	0.56
1:B:68:MET:HE1	1:B:101:MET:HE2	1.85	0.56
1:B:869:THR:HG22	1:B:870:ILE:N	2.20	0.56
1:A:726:LEU:HD23	1:A:751:ILE:CD1	2.35	0.56
1:B:18:LEU:CD1	1:B:350:ASN:HB3	2.30	0.56
1:B:180:TYR:CE2	1:B:194:VAL:HG22	2.41	0.56
1:B:432:HIS:CD2	1:B:432:HIS:N	2.73	0.56
1:A:296:GLN:OE1	1:A:324:VAL:HG23	2.04	0.56
1:B:823:GLN:O	1:B:827:GLU:HG3	2.06	0.56
1:B:98:LEU:HD23	1:B:275:TYR:CB	2.36	0.56
1:B:441:LEU:HD12	1:B:442:ALA:H	1.70	0.56
1:A:78:TYR:CG	1:A:314:LEU:HD13	2.40	0.56
1:A:284:ASN:OD1	1:A:288:LEU:HD11	2.06	0.56
1:B:710:THR:HG23	1:B:711:HIS:N	2.21	0.56
1:A:612:VAL:CG1	1:A:622:MET:HE1	2.31	0.56
1:A:667:ASP:OD1	1:A:670:ARG:NH2	2.39	0.56
1:B:432:HIS:H	1:B:432:HIS:HD2	1.51	0.56
1:B:459:GLN:C	1:B:461:SER:H	2.14	0.56
1:B:564:VAL:HG21	1:B:963:GLN:CD	2.31	0.56
1:B:744:ALA:O	1:B:746:ARG:N	2.38	0.56
1:B:1119:LEU:HD12	1:B:1120:LYS:N	2.21	0.56
1:A:5:TYR:N	1:A:5:TYR:CD1	2.73	0.56
1:A:351:ALA:O	1:A:352:ASN:HB2	2.05	0.56
1:A:802:ILE:HG22	1:A:806:ILE:CD1	2.36	0.56
1:A:18:LEU:O	1:A:19:LEU:HD23	2.05	0.56
1:A:170:ASP:CG	1:A:181:ARG:NH1	2.63	0.56
1:A:216:GLU:O	1:A:217:PHE:HB3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:ASP:OD1	1:A:889:ASP:N	2.37	0.56
1:A:939:LEU:HA	3:A:1151:EPE:O1S	2.06	0.56
1:A:1010:SER:O	1:A:1011:LEU:HB3	2.06	0.56
1:B:100:THR:O	1:B:101:MET:C	2.48	0.56
1:B:725:LEU:HD12	1:B:726:LEU:N	2.20	0.56
1:B:786:VAL:HG22	1:B:910:ALA:HB3	1.88	0.56
1:B:992:PRO:O	1:B:994:LEU:N	2.39	0.56
1:A:171:LEU:HG	1:A:173:PRO:HD3	1.88	0.55
1:B:416:ASP:C	1:B:418:ALA:H	2.14	0.55
1:A:168:LEU:HD23	1:A:181:ARG:HD3	1.88	0.55
1:A:714:LEU:HB3	1:A:741:ARG:HG2	1.86	0.55
1:B:27:CYS:O	1:B:30:LEU:HB3	2.05	0.55
1:B:32:ALA:O	1:B:36:GLU:HG3	2.06	0.55
1:B:44:LEU:O	1:B:107:ILE:HA	2.05	0.55
1:B:244:ILE:O	1:B:248:VAL:HG23	2.06	0.55
1:B:261:GLN:N	1:B:262:PRO:CD	2.69	0.55
1:B:501:ALA:C	1:B:503:GLY:H	2.14	0.55
1:A:903:VAL:HG12	1:A:904:GLY:N	2.22	0.55
1:B:791:ARG:O	1:B:915:LEU:HA	2.06	0.55
1:A:153:VAL:HG12	1:A:154:ASP:H	1.70	0.55
1:A:181:ARG:HG3	1:A:181:ARG:NH1	2.22	0.55
1:A:893:LEU:O	1:A:894:ALA:C	2.49	0.55
1:A:895:GLN:O	1:A:896:LEU:C	2.49	0.55
1:B:316:PRO:C	1:B:318:GLN:H	2.15	0.55
1:B:1008:MET:HE3	1:B:1128:ARG:CG	2.37	0.55
1:A:629:ASP:OD1	1:A:629:ASP:N	2.40	0.55
1:B:625:LEU:HD13	1:B:753:THR:CG2	2.37	0.55
1:B:625:LEU:HB3	1:B:773:LEU:HD23	1.89	0.55
1:A:242:GLU:HB2	1:A:311:MET:HE3	1.87	0.55
1:A:382:ASP:CG	1:A:383:GLY:N	2.64	0.55
1:A:629:ASP:CG	1:A:634:LYS:HE3	2.31	0.55
1:A:840:ILE:CG2	1:A:841:GLY:N	2.69	0.55
1:B:7:TYR:HD2	1:B:8:THR:N	2.04	0.55
1:B:916:THR:OG1	1:B:917:PRO:HD2	2.07	0.55
1:A:460:ASP:O	1:A:461:SER:C	2.50	0.55
1:B:91:ARG:NH1	1:B:216:GLU:OE1	2.40	0.55
1:B:157:MET:O	1:B:197:VAL:HG11	2.06	0.55
1:B:346:THR:O	1:B:347:LYS:C	2.49	0.55
1:A:463:ARG:O	1:A:782:ARG:HA	2.07	0.54
1:A:10:PRO:HB2	1:A:335:PRO:HB2	1.89	0.54
1:A:473:ASN:O	1:A:474:LEU:C	2.49	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:HIS:O	1:A:586:ASP:CB	2.55	0.54
1:B:827:GLU:C	1:B:829:LEU:H	2.14	0.54
1:B:1107:GLN:HA	1:B:1109:GLN:NE2	2.22	0.54
1:A:260:TRP:C	1:A:262:PRO:HD2	2.32	0.54
1:A:994:LEU:O	1:A:996:ASP:N	2.41	0.54
1:B:170:ASP:OD2	1:B:181:ARG:NH1	2.40	0.54
1:A:382:ASP:CG	1:A:383:GLY:H	2.16	0.54
1:B:244:ILE:HD13	1:B:312:ARG:HG2	1.89	0.54
1:B:685:ARG:CG	3:B:1150:EPE:H61	2.36	0.54
1:A:164:THR:O	1:A:165:ARG:HG3	2.08	0.54
1:A:846:ARG:NH2	1:B:686:PHE:CE2	2.76	0.54
1:B:244:ILE:CD1	1:B:312:ARG:HG2	2.38	0.54
1:B:685:ARG:HG3	3:B:1150:EPE:H22	1.89	0.54
1:B:273:PHE:HA	1:B:276:PHE:CD1	2.43	0.54
1:B:483:VAL:HG12	1:B:484:VAL:N	2.23	0.54
1:B:22:LEU:O	1:B:341:THR:HG22	2.07	0.54
1:B:89:SER:HB2	1:B:174:MET:CE	2.37	0.54
1:B:887:ARG:HG2	1:B:887:ARG:HH11	1.71	0.54
1:A:182:LEU:O	1:A:183:ASP:CB	2.56	0.54
1:A:242:GLU:HB2	1:A:311:MET:CE	2.37	0.54
1:A:377:PHE:CD2	1:A:378:LEU:HD23	2.41	0.54
1:A:868:THR:N	1:A:872:GLU:OE1	2.25	0.54
1:A:896:LEU:O	1:A:899:LEU:N	2.41	0.54
1:A:1121:PHE:C	1:A:1122:ILE:HD13	2.33	0.54
1:B:976:MET:O	1:B:980:GLU:HG3	2.08	0.54
1:B:1132:ILE:HG23	1:B:1133:GLU:N	2.23	0.54
1:A:387:PHE:N	1:A:424:TYR:O	2.37	0.54
1:A:129:VAL:C	1:A:130:MET:HG3	2.34	0.53
1:A:372:ASP:O	1:A:376:LYS:HG2	2.08	0.53
1:B:629:ASP:OD1	1:B:634:LYS:HE2	2.08	0.53
1:A:707:LEU:CD2	1:A:713:LEU:HD21	2.37	0.53
1:A:1076:ARG:O	1:A:1077:LYS:HB2	2.08	0.53
1:B:174:MET:HG3	1:B:213:PRO:O	2.08	0.53
1:A:48:ASP:OD1	1:A:48:ASP:N	2.41	0.53
1:A:327:LEU:O	1:A:331:LEU:HB2	2.08	0.53
1:A:447:SER:OG	1:A:453:ARG:HG3	2.07	0.53
1:A:533:ALA:O	1:A:534:GLY:C	2.51	0.53
1:A:733:ARG:HB2	1:B:821:ASN:ND2	2.24	0.53
1:A:76:LEU:HD12	1:A:807:LEU:HD12	1.90	0.53
1:B:158:GLU:C	1:B:172:PHE:HD1	2.16	0.53
1:B:284:ASN:CB	1:B:288:LEU:HD11	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:GLU:OE2	1:B:505:THR:HG23	2.08	0.53
1:B:1089:PHE:CE2	1:B:1095:VAL:HG21	2.43	0.53
1:A:460:ASP:CB	1:A:782:ARG:HD3	2.37	0.53
1:A:758:PRO:O	1:A:759:ILE:HD12	2.09	0.53
1:A:841:GLY:O	1:A:842:HIS:O	2.26	0.53
1:B:615:ASP:CB	1:B:622:MET:HE3	2.34	0.53
1:A:27:CYS:O	1:A:28:ALA:C	2.52	0.53
1:A:671:ASP:OD1	1:B:688:SER:HB3	2.09	0.53
1:B:850:LEU:HB3	1:B:854:MET:HE3	1.89	0.53
1:B:888:ALA:O	1:B:889:ASP:C	2.50	0.53
1:A:842:HIS:O	1:A:845:MET:HG2	2.08	0.53
1:B:85:GLN:CD	1:B:158:GLU:HB3	2.34	0.53
1:A:18:LEU:C	1:A:19:LEU:HD23	2.34	0.53
1:A:271:PRO:O	1:A:272:LEU:C	2.49	0.53
1:A:378:LEU:HD12	1:A:407:ILE:HD13	1.91	0.53
1:A:1085:GLY:HA3	1:A:1121:PHE:CZ	2.44	0.53
1:B:486:LEU:O	1:B:550:TRP:NE1	2.41	0.53
1:A:994:LEU:C	1:A:996:ASP:N	2.61	0.52
1:A:1077:LYS:HG3	1:A:1078:LEU:N	2.23	0.52
1:A:385:VAL:O	1:A:442:ALA:O	2.27	0.52
1:B:91:ARG:O	1:B:94:THR:N	2.36	0.52
1:B:181:ARG:NH2	1:B:200:GLN:O	2.42	0.52
1:A:76:LEU:HD13	1:A:804:ARG:HA	1.90	0.52
1:A:715:GLN:OE1	1:A:737:ARG:NH2	2.43	0.52
1:B:34:ILE:HD13	1:B:283:VAL:HG21	1.90	0.52
1:B:450:LEU:HB3	1:B:598:PRO:HB2	1.90	0.52
1:A:77:PRO:O	1:A:302:ARG:NH1	2.41	0.52
1:B:1055:ASP:HB2	1:B:1056:PRO:HD3	1.91	0.52
1:A:859:HIS:CD2	1:A:861:ARG:NH2	2.77	0.52
1:A:875:ILE:HG22	1:A:876:ASP:N	2.24	0.52
1:B:830:ALA:HB2	1:B:838:ILE:HD12	1.92	0.52
1:A:26:ALA:O	1:A:29:THR:HG22	2.10	0.52
1:B:669:PHE:HB3	1:B:680:ILE:HD13	1.92	0.52
1:A:287:ASP:CG	1:A:287:ASP:O	2.52	0.52
1:A:456:ARG:NE	1:A:876:ASP:OD1	2.42	0.52
1:A:612:VAL:HA	1:A:622:MET:CE	2.39	0.52
1:B:1006:LEU:O	1:B:1131:ARG:NH1	2.43	0.52
1:A:206:VAL:HG12	1:A:207:GLU:N	2.24	0.52
1:A:385:VAL:HA	1:A:442:ALA:HB3	1.92	0.52
1:A:30:LEU:HD11	1:A:353:LEU:HD12	1.91	0.51
1:A:376:LYS:O	1:A:380:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:PRO:CD	1:B:257:ILE:HD12	2.12	0.51
1:B:898:GLN:HE21	1:B:902:ARG:NH2	2.07	0.51
1:A:792:GLU:O	1:A:793:TYR:C	2.53	0.51
1:A:974:LEU:O	1:A:977:GLU:HB3	2.10	0.51
1:B:50:GLN:HG2	1:B:860:GLN:NE2	2.26	0.51
1:B:62:PHE:CE2	1:B:426:MET:HE1	2.37	0.51
1:A:1077:LYS:HB3	1:A:1088:GLU:HB3	1.91	0.51
1:A:178:LEU:H	1:A:178:LEU:CD2	2.11	0.51
1:A:526:LEU:HD22	1:A:1027:TYR:HB3	1.93	0.51
1:A:992:PRO:O	1:A:994:LEU:N	2.43	0.51
1:A:1114:ASP:OD2	1:A:1118:ARG:HD3	2.10	0.51
1:B:656:VAL:HG21	1:B:662:ALA:HA	1.91	0.51
1:B:807:LEU:HD13	1:B:807:LEU:C	2.35	0.51
1:B:887:ARG:HG2	1:B:887:ARG:NH1	2.26	0.51
1:A:436:ASP:O	1:A:440:ASN:HA	2.10	0.51
1:A:822:ILE:HD12	1:A:868:THR:HG21	1.88	0.51
1:B:10:PRO:CB	1:B:15:GLU:HB3	2.40	0.51
1:B:43:VAL:HG12	1:B:43:VAL:O	2.10	0.51
1:B:794:ASP:OD2	1:B:796:MET:HB3	2.10	0.51
1:B:1121:PHE:C	1:B:1122:ILE:HD12	2.35	0.51
1:A:625:LEU:HD23	1:A:773:LEU:HD13	1.93	0.51
1:A:742:ILE:C	1:A:744:ALA:N	2.69	0.51
1:B:540:ALA:O	1:B:541:PRO:O	2.28	0.51
1:B:593:PHE:CD1	1:B:643:PHE:CD1	2.98	0.51
1:B:1136:ARG:CG	1:B:1136:ARG:NH1	2.65	0.51
1:A:37:ARG:O	1:A:38:HIS:HB2	2.11	0.51
1:A:261:GLN:N	1:A:262:PRO:CD	2.74	0.51
1:B:31:VAL:HG12	1:B:31:VAL:O	2.10	0.51
1:B:535:GLY:O	1:B:536:ALA:HB2	2.09	0.51
1:B:850:LEU:HD23	1:B:854:MET:HE1	1.91	0.51
1:B:1026:PHE:CD2	1:B:1046:LEU:HD21	2.46	0.51
1:A:324:VAL:O	1:A:328:PHE:HD1	1.94	0.51
1:B:25:ALA:HB3	1:B:434:PHE:CD2	2.45	0.51
1:B:501:ALA:HB2	4:B:1176:HOH:O	2.10	0.51
1:B:629:ASP:C	1:B:631:GLY:H	2.19	0.51
1:B:791:ARG:CG	1:B:791:ARG:NH1	2.67	0.51
1:B:835:GLU:OE1	1:B:835:GLU:N	2.36	0.51
1:A:279:ASN:ND2	1:A:279:ASN:N	2.42	0.51
1:A:686:PHE:O	1:A:687:ARG:HG2	2.11	0.51
1:B:74:GLU:HG2	1:B:808:ARG:HD3	1.92	0.51
1:A:509:LEU:HD23	1:A:529:ILE:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1122:ILE:C	1:A:1123:GLN:HG2	2.36	0.50
1:B:685:ARG:CD	3:B:1150:EPE:H61	2.40	0.50
1:B:713:LEU:CD2	1:B:718:VAL:HG21	2.41	0.50
1:B:873:THR:CG2	1:B:902:ARG:HG3	2.41	0.50
1:B:1011:LEU:HD23	1:B:1011:LEU:C	2.36	0.50
1:A:1091:GLU:OE1	1:A:1091:GLU:N	2.41	0.50
1:B:30:LEU:C	1:B:32:ALA:H	2.20	0.50
1:B:430:ALA:HB1	1:B:445:CYS:HB3	1.93	0.50
1:A:602:THR:HB	1:A:605:GLN:HB2	1.93	0.50
1:A:916:THR:HB	1:A:917:PRO:CD	2.42	0.50
1:A:1114:ASP:O	1:A:1118:ARG:HB2	2.11	0.50
1:B:17:ARG:O	1:B:18:LEU:HD23	2.10	0.50
1:B:47:PRO:HD3	1:B:285:THR:HB	1.93	0.50
1:B:936:LEU:HA	3:B:1151:EPE:C5	2.41	0.50
1:B:1096:ASN:OD1	1:B:1147:ILE:HD11	2.11	0.50
1:A:1032:SER:O	1:A:1033:ALA:C	2.54	0.50
1:B:63:THR:CG2	1:B:65:GLN:HB2	2.40	0.50
1:B:279:ASN:C	1:B:279:ASN:ND2	2.69	0.50
1:B:662:ALA:C	1:B:682:MET:CE	2.85	0.50
1:A:22:LEU:HD23	1:A:355:PHE:HD1	1.77	0.50
1:A:141:LEU:O	1:A:145:LEU:HG	2.10	0.50
1:A:622:MET:HG2	1:A:623:ASP:N	2.25	0.50
1:A:1082:GLU:OE1	1:A:1131:ARG:NH2	2.44	0.50
1:B:33:GLU:HG3	1:B:34:ILE:N	2.26	0.50
1:B:605:GLN:NE2	1:B:634:LYS:HD2	2.15	0.50
1:A:519:LEU:HB2	1:A:545:LEU:HD21	1.94	0.50
1:A:1140:ARG:O	1:A:1144:GLU:HG3	2.12	0.50
1:B:117:VAL:HG21	1:B:272:LEU:CD1	2.40	0.50
1:A:195:PHE:HB2	1:A:201:ARG:O	2.12	0.50
1:A:258:GLU:OE1	1:A:258:GLU:N	2.33	0.50
1:A:452:GLU:HG2	1:A:855:ASN:OD1	2.12	0.50
1:A:483:VAL:HG12	1:A:484:VAL:N	2.27	0.50
1:B:295:PHE:C	1:B:295:PHE:CD2	2.89	0.50
1:B:1107:GLN:N	1:B:1108:PRO:HD3	2.25	0.50
1:A:87:ILE:O	1:A:91:ARG:HG3	2.12	0.50
1:A:326:GLU:HA	1:A:329:SER:HB3	1.94	0.50
1:A:436:ASP:O	1:A:440:ASN:CA	2.60	0.50
1:B:711:HIS:C	1:B:713:LEU:H	2.19	0.50
1:B:629:ASP:OD1	1:B:634:LYS:CG	2.59	0.50
1:B:936:LEU:CD2	3:B:1151:EPE:H62	2.40	0.50
1:A:153:VAL:CG1	1:A:154:ASP:N	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LEU:N	1:A:474:LEU:CD2	2.73	0.49
1:A:645:ALA:O	1:A:650:LYS:HB2	2.10	0.49
1:A:859:HIS:C	1:A:861:ARG:H	2.18	0.49
1:A:78:TYR:CD2	1:A:314:LEU:HD22	2.46	0.49
1:A:732:HIS:CE1	1:A:733:ARG:HD3	2.47	0.49
1:A:802:ILE:HG22	1:A:806:ILE:HD11	1.94	0.49
1:A:949:ASP:O	1:A:952:ILE:HB	2.12	0.49
1:B:25:ALA:O	1:B:26:ALA:C	2.54	0.49
1:B:28:ALA:HB2	1:B:58:GLU:HG2	1.93	0.49
1:B:481:GLN:NE2	1:B:531:ARG:NH1	2.59	0.49
1:A:61:GLN:OE1	1:A:430:ALA:HB2	2.12	0.49
1:B:98:LEU:HD23	1:B:275:TYR:HB3	1.95	0.49
1:B:691:GLU:O	1:B:695:ILE:HG13	2.12	0.49
1:A:182:LEU:HD22	1:A:192:LEU:HD13	1.93	0.49
1:A:237:VAL:HG12	1:A:238:LYS:N	2.27	0.49
1:A:805:GLU:OE2	1:A:881:ASN:HB2	2.12	0.49
1:B:84:HIS:CD2	1:B:86:ASP:HB2	2.47	0.49
1:B:98:LEU:HD23	1:B:275:TYR:HB2	1.95	0.49
1:A:22:LEU:HD21	1:A:353:LEU:HD12	1.93	0.49
1:A:61:GLN:CD	1:A:428:GLY:HA3	2.38	0.49
1:A:309:ASP:OD1	1:A:310:PRO:HD2	2.11	0.49
1:A:749:VAL:HA	4:A:1199:HOH:O	2.12	0.49
1:A:1061:LEU:O	1:A:1064:ALA:HB3	2.12	0.49
1:B:10:PRO:HA	1:B:15:GLU:OE1	2.12	0.49
1:B:1076:ARG:HE	1:B:1090:ALA:CB	2.24	0.49
1:A:147:SER:C	1:A:149:GLY:N	2.69	0.49
1:B:227:PHE:HA	1:B:263:LEU:O	2.12	0.49
1:A:2:PRO:HG2	1:A:3:GLU:H	1.77	0.49
1:A:387:PHE:CD2	1:A:444:ILE:HB	2.48	0.49
1:A:805:GLU:HG2	1:A:882:THR:OG1	2.13	0.49
1:A:869:THR:HG22	1:A:870:ILE:N	2.26	0.49
1:B:300:LEU:O	1:B:304:GLU:HG2	2.13	0.49
1:B:993:SER:O	1:B:995:GLU:N	2.39	0.49
1:A:235:PHE:CD2	1:A:313:PRO:HB2	2.47	0.49
1:A:388:SER:HB3	1:A:445:CYS:SG	2.53	0.49
1:A:455:ALA:O	1:A:878:PRO:HG2	2.13	0.49
1:A:636:GLU:O	1:A:640:ARG:HG3	2.13	0.49
1:A:899:LEU:HA	1:A:902:ARG:HD2	1.94	0.49
1:A:1019:ASP:O	1:A:1020:VAL:C	2.54	0.49
1:B:12:LYS:C	1:B:335:PRO:HG3	2.38	0.49
1:B:477:LEU:O	1:B:1021:ASN:ND2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:923:THR:HG22	1:B:925:ASP:H	1.77	0.49
1:A:1103:LEU:HD22	1:A:1111:TYR:CD1	2.48	0.49
1:B:75:THR:HG22	1:B:76:LEU:H	1.78	0.49
1:A:287:ASP:O	1:A:287:ASP:OD1	2.31	0.49
1:A:418:ALA:HA	1:A:424:TYR:CE1	2.47	0.49
1:A:467:PRO:HG2	1:A:468:ASP:N	2.26	0.49
1:A:626:VAL:HA	1:A:774:SER:O	2.13	0.49
1:A:1016:PHE:CE1	1:A:1054:PRO:HD3	2.47	0.49
1:B:634:LYS:CE	1:B:776:ILE:HG21	2.41	0.49
1:A:533:ALA:CB	1:A:972:PHE:HB3	2.44	0.48
1:B:869:THR:HG22	1:B:870:ILE:H	1.77	0.48
1:A:394:ARG:HD3	1:A:446:GLU:OE1	2.13	0.48
1:A:811:GLN:HG2	1:A:857:PHE:HD2	1.78	0.48
1:A:869:THR:HB	1:A:872:GLU:HG3	1.94	0.48
1:B:77:PRO:HG2	1:B:302:ARG:HD3	1.95	0.48
1:B:657:PRO:C	1:B:658:THR:HG23	2.38	0.48
1:B:660:LEU:HD13	1:B:844:GLN:NE2	2.28	0.48
1:A:632:PHE:HB2	1:A:854:MET:HE1	1.95	0.48
1:A:756:ALA:O	1:A:757:THR:C	2.55	0.48
1:A:887:ARG:HG2	1:A:890:HIS:NE2	2.28	0.48
1:B:262:PRO:HG2	1:B:319:SER:HB3	1.95	0.48
1:B:794:ASP:C	1:B:796:MET:N	2.70	0.48
1:B:842:HIS:O	1:B:845:MET:HG2	2.12	0.48
1:A:32:ALA:O	1:A:36:GLU:HG2	2.13	0.48
1:A:201:ARG:CD	1:A:1045:GLU:HG3	2.44	0.48
1:A:239:ARG:O	1:A:240:ASP:C	2.55	0.48
1:B:612:VAL:HG13	1:B:622:MET:HE1	1.96	0.48
1:B:798:VAL:O	1:B:802:ILE:HG13	2.13	0.48
1:B:805:GLU:CG	1:B:882:THR:OG1	2.61	0.48
1:B:30:LEU:O	1:B:33:GLU:HG2	2.12	0.48
1:B:816:TYR:CZ	1:B:822:ILE:HG23	2.47	0.48
1:B:850:LEU:HB3	1:B:854:MET:CE	2.42	0.48
1:B:993:SER:C	1:B:995:GLU:H	2.20	0.48
1:A:179:PRO:HG2	1:A:195:PHE:O	2.14	0.48
1:A:498:THR:O	1:A:498:THR:HG22	2.13	0.48
1:A:581:PHE:CZ	1:A:650:LYS:HE3	2.49	0.48
1:A:11:VAL:HG12	1:A:11:VAL:O	2.14	0.48
1:A:425:LEU:HD12	1:A:425:LEU:C	2.38	0.48
1:A:859:HIS:O	1:A:861:ARG:N	2.46	0.48
1:A:992:PRO:C	1:A:994:LEU:N	2.65	0.48
1:B:82:SER:OG	1:B:258:GLU:OE1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ALA:HB1	1:B:545:LEU:HD12	1.96	0.48
1:B:867:CYS:HB3	1:B:872:GLU:HB2	1.94	0.48
1:B:30:LEU:C	1:B:32:ALA:N	2.72	0.48
1:B:97:GLN:O	1:B:97:GLN:HG2	2.13	0.48
1:B:180:TYR:HB3	1:B:192:LEU:CD1	2.41	0.48
1:B:1085:GLY:HA3	1:B:1121:PHE:CZ	2.48	0.48
1:A:859:HIS:C	1:A:861:ARG:N	2.70	0.48
1:A:1032:SER:C	1:A:1033:ALA:O	2.56	0.48
1:B:120:HIS:C	1:B:122:PHE:H	2.22	0.48
1:B:833:VAL:O	1:B:836:ALA:HB3	2.14	0.48
1:B:899:LEU:O	1:B:900:ARG:C	2.56	0.48
1:A:1091:GLU:CD	1:A:1091:GLU:N	2.62	0.48
1:B:316:PRO:O	1:B:318:GLN:N	2.45	0.48
1:B:1047:ILE:HA	1:B:1051:GLY:O	2.13	0.48
1:A:33:GLU:C	1:A:35:ALA:N	2.72	0.47
1:A:73:TRP:CZ3	1:A:258:GLU:HB3	2.48	0.47
1:A:592:LEU:HD23	1:A:595:ASP:OD2	2.14	0.47
1:B:168:LEU:HD21	1:B:181:ARG:HD3	1.96	0.47
1:B:523:VAL:O	1:B:526:LEU:HD23	2.14	0.47
1:B:827:GLU:C	1:B:829:LEU:N	2.70	0.47
1:A:654:VAL:HA	1:A:727:ILE:O	2.14	0.47
1:A:979:LEU:O	1:A:980:GLU:C	2.57	0.47
1:B:25:ALA:HB3	1:B:434:PHE:HD2	1.79	0.47
1:B:168:LEU:HD23	1:B:181:ARG:HD3	1.95	0.47
1:B:833:VAL:N	1:B:834:PRO:HD3	2.29	0.47
1:B:899:LEU:HA	1:B:902:ARG:HG2	1.96	0.47
1:B:986:LEU:N	1:B:986:LEU:HD12	2.29	0.47
1:B:1040:GLU:O	1:B:1043:LYS:HB3	2.14	0.47
1:A:153:VAL:CG1	1:A:154:ASP:H	2.27	0.47
1:A:995:GLU:C	1:A:997:LEU:N	2.71	0.47
1:B:683:ILE:HD12	1:B:692:GLN:HG2	1.96	0.47
1:A:328:PHE:O	1:A:332:LYS:HG3	2.14	0.47
1:A:940:GLY:H	3:A:1151:EPE:H92	1.79	0.47
1:A:1110:HIS:C	1:A:1111:TYR:CD1	2.92	0.47
1:B:537:GLU:O	1:B:537:GLU:HG2	2.14	0.47
1:B:588:GLU:O	1:B:592:LEU:HD23	2.15	0.47
1:B:659:THR:HA	1:B:662:ALA:HB3	1.97	0.47
1:A:91:ARG:O	1:A:92:LEU:C	2.55	0.47
1:A:618:GLN:C	1:A:620:LEU:H	2.22	0.47
1:A:696:LEU:HD22	1:A:718:VAL:HG13	1.97	0.47
1:A:906:SER:O	1:A:907:HIS:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:GLN:OE1	1:B:459:GLN:HA	2.15	0.47
1:B:903:VAL:HG12	1:B:904:GLY:N	2.29	0.47
1:B:1100:LEU:HD11	1:B:1119:LEU:HD22	1.97	0.47
1:A:43:VAL:O	1:A:43:VAL:HG12	2.13	0.47
1:A:95:LEU:HD13	1:A:117:VAL:HG13	1.96	0.47
1:A:206:VAL:CG1	1:A:207:GLU:N	2.77	0.47
1:A:550:TRP:O	1:A:552:ARG:N	2.47	0.47
1:B:74:GLU:HG2	1:B:808:ARG:CD	2.43	0.47
1:B:227:PHE:CE2	1:B:248:VAL:HG21	2.49	0.47
1:B:271:PRO:HB3	1:B:322:LEU:HD21	1.97	0.47
1:B:710:THR:CG2	1:B:712:LYS:HB2	2.43	0.47
1:B:881:ASN:CA	1:B:903:VAL:HG13	2.45	0.47
1:B:1045:GLU:O	1:B:1046:LEU:C	2.57	0.47
1:B:1075:ILE:HD12	1:B:1139:MET:HE1	1.97	0.47
1:A:33:GLU:C	1:A:35:ALA:H	2.22	0.47
1:A:386:VAL:HG13	1:A:412:ILE:HD11	1.97	0.47
1:A:471:ILE:HD13	1:A:948:HIS:CD2	2.49	0.47
1:A:636:GLU:CD	1:A:672:ARG:HH21	2.22	0.47
1:A:945:LEU:O	1:A:948:HIS:HB3	2.15	0.47
1:A:1132:ILE:O	1:A:1136:ARG:CG	2.61	0.47
1:B:129:VAL:HG12	1:B:130:MET:N	2.29	0.47
1:B:158:GLU:C	1:B:172:PHE:CD1	2.93	0.47
1:B:162:TYR:CD1	1:B:162:TYR:C	2.93	0.47
1:B:307:GLY:HA2	1:B:314:LEU:CG	2.44	0.47
1:B:347:LYS:HB2	1:B:350:ASN:HD22	1.79	0.47
1:B:372:ASP:O	1:B:373:ALA:C	2.57	0.47
1:B:564:VAL:CG2	1:B:963:GLN:NE2	2.78	0.47
1:B:662:ALA:O	1:B:682:MET:HE3	2.15	0.47
1:B:936:LEU:HD13	3:B:1151:EPE:O3S	2.15	0.47
1:B:1040:GLU:O	1:B:1044:VAL:HG23	2.14	0.47
1:A:377:PHE:HA	1:A:380:THR:CG2	2.44	0.47
1:A:432:HIS:HA	1:A:445:CYS:CB	2.44	0.47
1:B:237:VAL:CG1	1:B:238:LYS:N	2.78	0.47
1:B:312:ARG:O	1:B:314:LEU:HD23	2.15	0.47
1:B:478:HIS:O	1:B:481:GLN:HG3	2.15	0.47
1:B:655:LEU:HA	1:B:655:LEU:HD23	1.72	0.47
1:B:671:ASP:CG	1:B:848:ARG:NH1	2.71	0.47
1:B:711:HIS:C	1:B:713:LEU:N	2.73	0.47
1:B:760:PRO:HG3	1:B:951:GLU:HB3	1.97	0.47
1:B:991:GLU:CB	1:B:992:PRO:HD2	2.44	0.47
1:B:1066:LEU:O	1:B:1067:ARG:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LEU:HD13	1:A:169:LEU:C	2.40	0.47
1:A:1097:PRO:O	1:A:1101:ILE:HG22	2.14	0.47
1:B:526:LEU:HD13	1:B:529:ILE:HG13	1.97	0.47
1:A:783:ARG:HA	1:A:939:LEU:O	2.15	0.47
1:B:316:PRO:HA	1:B:317:PRO:HD3	1.77	0.47
1:B:326:GLU:O	1:B:329:SER:HB3	2.15	0.47
1:B:805:GLU:HG3	1:B:882:THR:HB	1.96	0.47
1:A:92:LEU:HD22	1:A:123:LEU:HD21	1.97	0.46
1:A:616:MET:HE1	1:A:641:ALA:CB	2.41	0.46
1:A:817:ASN:O	1:A:818:ASP:HB2	2.15	0.46
1:B:41:PRO:HD2	1:B:279:ASN:O	2.15	0.46
1:B:279:ASN:O	1:B:280:THR:HB	2.15	0.46
1:B:560:LYS:HB3	1:B:963:GLN:HE22	1.80	0.46
1:A:206:VAL:HG12	1:A:208:ALA:H	1.79	0.46
1:A:484:VAL:O	1:A:529:ILE:HA	2.15	0.46
1:B:243:HIS:O	1:B:244:ILE:C	2.58	0.46
1:B:911:TYR:N	1:B:911:TYR:CD1	2.83	0.46
1:A:162:TYR:HA	1:A:170:ASP:O	2.16	0.46
1:A:201:ARG:HD3	1:A:1045:GLU:HG3	1.97	0.46
1:A:371:LEU:HD11	1:A:404:ARG:HE	1.79	0.46
1:A:805:GLU:CG	1:A:882:THR:OG1	2.63	0.46
1:A:933:ILE:C	1:A:935:SER:N	2.73	0.46
1:A:1082:GLU:H	1:A:1082:GLU:HG2	1.46	0.46
1:B:262:PRO:HG3	1:B:269:LEU:CD1	2.46	0.46
1:B:799:ARG:O	1:B:803:LEU:HB2	2.15	0.46
1:B:1008:MET:CE	1:B:1128:ARG:HG2	2.45	0.46
1:A:132:LYS:O	1:A:132:LYS:HG3	2.15	0.46
1:A:412:ILE:HG22	1:A:417:GLU:OE1	2.16	0.46
1:B:625:LEU:HB3	1:B:773:LEU:CD2	2.45	0.46
1:B:690:LYS:O	1:B:691:GLU:C	2.56	0.46
1:A:182:LEU:HD22	1:A:192:LEU:CD1	2.46	0.46
1:A:377:PHE:HA	1:A:380:THR:HG22	1.97	0.46
1:A:566:ALA:O	1:A:567:GLU:C	2.58	0.46
1:B:98:LEU:HB3	1:B:99:PRO:CD	2.42	0.46
1:B:153:VAL:CG1	1:B:154:ASP:N	2.77	0.46
1:B:605:GLN:O	1:B:609:ILE:HG13	2.15	0.46
1:B:711:HIS:HA	1:B:714:LEU:HD12	1.98	0.46
1:A:686:PHE:C	1:A:687:ARG:HG2	2.40	0.46
1:B:120:HIS:HD1	1:B:275:TYR:HE2	1.62	0.46
1:B:683:ILE:HD11	1:B:695:ILE:HB	1.98	0.46
1:A:150:TYR:CE1	1:A:214:ALA:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLY:H	1:A:312:ARG:HH22	1.63	0.46
1:A:485:HIS:CE1	1:A:487:GLU:HB2	2.51	0.46
1:A:831:GLU:O	1:A:834:PRO:HD3	2.15	0.46
1:A:1006:LEU:HD12	1:A:1132:ILE:HD11	1.97	0.46
1:A:277:PRO:O	1:A:280:THR:CG2	2.57	0.46
1:A:839:ALA:HB2	1:A:862:PHE:CD2	2.51	0.46
1:A:1109:GLN:H	1:A:1109:GLN:HE21	1.62	0.46
1:B:1125:LEU:HB3	1:B:1131:ARG:CB	2.44	0.46
1:A:433:GLY:HA3	1:A:443:LEU:O	2.15	0.46
1:B:226:LEU:HD22	1:B:230:GLN:NE2	2.31	0.46
1:B:361:LEU:HD22	1:B:374:LEU:HD12	1.98	0.46
1:B:827:GLU:O	1:B:829:LEU:N	2.49	0.46
1:A:602:THR:HG22	1:A:604:ASP:H	1.81	0.45
1:B:7:TYR:OH	1:B:17:ARG:CZ	2.64	0.45
1:B:76:LEU:O	1:B:77:PRO:C	2.56	0.45
1:B:712:LYS:CD	3:B:1150:EPE:H72	2.46	0.45
1:B:805:GLU:HG2	1:B:882:THR:OG1	2.16	0.45
1:A:359:PRO:HG2	1:A:377:PHE:CE1	2.52	0.45
1:A:533:ALA:O	1:A:534:GLY:O	2.33	0.45
1:A:692:GLN:NE2	1:A:712:LYS:HE2	2.31	0.45
1:A:983:VAL:O	1:A:984:ASP:C	2.59	0.45
1:A:1103:LEU:HD21	1:A:1111:TYR:CZ	2.51	0.45
1:B:598:PRO:HD2	1:B:599:PHE:CE1	2.51	0.45
1:B:659:THR:HG23	3:B:1150:EPE:H21	1.97	0.45
1:B:778:THR:CG2	1:B:779:PRO:HD2	2.46	0.45
1:B:992:PRO:C	1:B:994:LEU:N	2.64	0.45
1:A:328:PHE:HA	1:A:331:LEU:HB2	1.98	0.45
1:A:903:VAL:CG1	1:A:904:GLY:N	2.79	0.45
1:B:312:ARG:O	1:B:313:PRO:C	2.59	0.45
1:A:244:ILE:CD1	1:A:312:ARG:HG3	2.47	0.45
1:A:1066:LEU:O	1:A:1067:ARG:C	2.59	0.45
1:B:327:LEU:O	1:B:331:LEU:HB2	2.16	0.45
1:B:1108:PRO:CD	1:B:1109:GLN:HE21	2.27	0.45
1:A:19:LEU:HD22	1:A:351:ALA:HB3	1.99	0.45
1:A:37:ARG:O	1:A:37:ARG:CG	2.64	0.45
1:A:201:ARG:NH1	1:A:201:ARG:HB3	2.31	0.45
1:A:377:PHE:C	1:A:380:THR:HG22	2.41	0.45
1:A:446:GLU:HG2	1:A:450:LEU:HD12	1.98	0.45
1:A:892:GLY:O	1:A:893:LEU:C	2.60	0.45
1:B:384:PRO:O	1:B:441:LEU:HD12	2.17	0.45
1:A:9:LEU:HA	1:A:10:PRO:HD3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:O	1:A:260:TRP:HB2	2.16	0.45
1:A:1054:PRO:O	1:A:1058:ARG:HG3	2.17	0.45
1:A:1068:GLN:O	1:A:1069:GLN:C	2.59	0.45
1:B:416:ASP:C	1:B:418:ALA:N	2.74	0.45
1:B:873:THR:HG22	1:B:902:ARG:HG3	1.99	0.45
1:B:110:VAL:O	1:B:112:THR:N	2.49	0.45
1:B:384:PRO:HA	1:B:422:GLY:N	2.31	0.45
1:B:532:TYR:OH	1:B:968:GLU:O	2.33	0.45
1:B:800:GLU:O	1:B:804:ARG:N	2.45	0.45
1:A:23:THR:O	1:A:24:GLY:O	2.35	0.45
1:A:271:PRO:O	1:A:273:PHE:N	2.50	0.45
1:A:592:LEU:O	1:A:595:ASP:HB2	2.17	0.45
1:A:993:SER:C	1:A:995:GLU:H	2.25	0.45
1:A:1078:LEU:HG	1:A:1087:ILE:HD13	1.97	0.45
1:B:14:GLY:O	1:B:16:GLN:HG2	2.17	0.45
1:B:254:PRO:O	1:B:257:ILE:HB	2.16	0.45
1:A:952:ILE:O	1:A:955:ALA:HB3	2.16	0.45
1:A:1103:LEU:CD2	1:A:1111:TYR:CE1	3.00	0.45
1:B:193:ARG:NH1	1:B:205:GLU:HG2	2.32	0.45
1:B:654:VAL:HA	1:B:727:ILE:O	2.17	0.45
1:B:720:PHE:CD1	1:B:723:LEU:HD22	2.52	0.45
1:B:744:ALA:C	1:B:746:ARG:N	2.75	0.45
1:B:909:GLN:HG3	1:B:910:ALA:N	2.32	0.45
1:A:404:ARG:NH1	1:A:591:GLN:HG2	2.32	0.45
1:B:170:ASP:OD1	1:B:181:ARG:NH1	2.50	0.45
1:B:452:GLU:OE2	1:B:859:HIS:CE1	2.70	0.45
1:B:760:PRO:HA	1:B:951:GLU:OE1	2.16	0.45
1:B:1104:LEU:HD13	1:B:1113:LEU:HD11	1.99	0.45
1:A:244:ILE:HD11	1:A:312:ARG:HG3	2.00	0.44
1:A:455:ALA:HB2	1:A:858:HIS:ND1	2.32	0.44
1:A:710:THR:HG22	1:A:711:HIS:ND1	2.31	0.44
1:B:113:LEU:CD1	1:B:272:LEU:HD23	2.40	0.44
1:B:666:TYR:HA	1:B:708:ILE:CD1	2.47	0.44
1:B:1013:PRO:HG2	1:B:1054:PRO:HB2	1.98	0.44
1:B:1035:THR:CB	1:B:1038:GLU:HG3	2.41	0.44
1:A:1006:LEU:CD1	1:A:1132:ILE:HD13	2.48	0.44
1:A:1107:GLN:N	1:A:1108:PRO:CD	2.80	0.44
1:B:150:TYR:CD2	1:B:160:GLY:HA2	2.51	0.44
1:B:295:PHE:C	1:B:295:PHE:HD2	2.25	0.44
1:B:710:THR:HG21	3:B:1150:EPE:H32	1.98	0.44
1:B:817:ASN:C	1:B:819:VAL:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1075:ILE:HD12	1:B:1139:MET:CE	2.46	0.44
1:A:325:ASP:OD1	1:A:325:ASP:N	2.50	0.44
1:B:153:VAL:CG1	1:B:154:ASP:H	2.28	0.44
1:B:412:ILE:HD12	1:B:424:TYR:CB	2.48	0.44
1:B:713:LEU:HD23	1:B:718:VAL:HG21	1.99	0.44
1:A:84:HIS:CD2	1:A:86:ASP:H	2.36	0.44
1:A:164:THR:C	1:A:165:ARG:HG3	2.42	0.44
1:A:280:THR:HG23	1:A:334:TRP:CD1	2.51	0.44
1:A:550:TRP:O	1:A:551:SER:C	2.60	0.44
1:B:710:THR:HG21	3:B:1150:EPE:C3	2.48	0.44
1:A:497:THR:OG1	1:A:510:MET:HE2	2.18	0.44
1:A:771:ARG:HG3	1:A:771:ARG:HH11	1.83	0.44
1:A:812:VAL:HB	1:A:864:VAL:HG22	1.98	0.44
1:B:498:THR:C	1:B:499:LEU:HD23	2.42	0.44
1:A:626:VAL:HG22	1:A:774:SER:HB2	1.99	0.44
1:A:778:THR:O	1:A:779:PRO:C	2.61	0.44
1:A:1065:ARG:O	1:A:1069:GLN:HG3	2.17	0.44
1:B:116:ARG:HD3	1:B:269:LEU:O	2.18	0.44
1:B:329:SER:C	1:B:331:LEU:H	2.24	0.44
1:B:430:ALA:O	1:B:431:GLU:C	2.61	0.44
1:B:473:ASN:O	1:B:474:LEU:C	2.59	0.44
1:B:1011:LEU:C	1:B:1011:LEU:CD2	2.90	0.44
1:A:51:ASN:C	1:A:55:LEU:HD12	2.43	0.44
1:A:84:HIS:HD2	1:A:86:ASP:N	2.15	0.44
1:A:387:PHE:HD2	1:A:444:ILE:HB	1.81	0.44
1:A:460:ASP:C	1:A:462:ARG:N	2.73	0.44
1:A:948:HIS:O	1:A:949:ASP:C	2.58	0.44
1:A:1006:LEU:CD1	1:A:1132:ILE:CD1	2.95	0.44
1:B:119:PRO:HG2	1:B:265:PHE:CD2	2.52	0.44
1:B:564:VAL:HG21	1:B:963:GLN:NE2	2.33	0.44
1:B:746:ARG:HG3	1:B:751:ILE:HG13	1.98	0.44
1:A:257:ILE:CG2	1:A:258:GLU:N	2.79	0.44
1:A:812:VAL:HG22	1:A:882:THR:HB	1.99	0.44
1:A:981:ASN:O	1:A:982:ALA:C	2.58	0.44
1:B:8:THR:O	1:B:9:LEU:CB	2.65	0.44
1:B:660:LEU:HD23	1:B:660:LEU:HA	1.68	0.44
1:B:855:ASN:O	1:B:856:ASP:C	2.61	0.44
1:A:34:ILE:HG22	1:A:34:ILE:O	2.18	0.44
1:A:138:ARG:NH1	1:A:166:GLY:O	2.49	0.44
1:A:470:LEU:HD23	1:A:475:ALA:HB3	2.00	0.44
1:A:552:ARG:O	1:A:555:GLN:N	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:PHE:CE1	1:A:851:GLU:HB3	2.53	0.44
1:A:995:GLU:C	1:A:997:LEU:H	2.24	0.44
1:A:1032:SER:O	1:A:1033:ALA:O	2.35	0.44
1:B:395:ARG:C	1:B:397:ALA:N	2.74	0.44
1:B:488:HIS:O	1:B:550:TRP:CG	2.71	0.44
1:B:975:TYR:C	1:B:975:TYR:CD2	2.96	0.44
1:A:1077:LYS:HE3	1:A:1079:GLU:HG2	2.01	0.43
1:B:346:THR:O	1:B:346:THR:HG22	2.18	0.43
1:B:1027:TYR:O	1:B:1028:LYS:C	2.60	0.43
1:A:33:GLU:HA	1:A:36:GLU:HG3	1.99	0.43
1:A:43:VAL:HG22	1:A:106:LEU:HD23	1.99	0.43
1:A:654:VAL:HG13	1:A:727:ILE:HB	1.99	0.43
1:A:742:ILE:C	1:A:744:ALA:H	2.25	0.43
1:A:1103:LEU:CD2	1:A:1111:TYR:CD1	3.01	0.43
1:B:25:ALA:HB2	1:B:432:HIS:O	2.18	0.43
1:B:62:PHE:HE2	1:B:426:MET:CE	2.23	0.43
1:B:77:PRO:C	1:B:78:TYR:CD1	2.96	0.43
1:B:402:LEU:C	1:B:404:ARG:H	2.26	0.43
1:B:592:LEU:O	1:B:595:ASP:HB2	2.17	0.43
1:B:936:LEU:HD22	3:B:1151:EPE:H102	1.99	0.43
1:A:31:VAL:HG11	1:A:44:LEU:HD22	2.01	0.43
1:A:98:LEU:HD12	1:A:98:LEU:O	2.18	0.43
1:A:138:ARG:HG3	1:A:184:PHE:CE1	2.53	0.43
1:A:257:ILE:O	1:A:259:TYR:N	2.51	0.43
1:A:791:ARG:HD2	4:A:1156:HOH:O	2.18	0.43
1:B:267:GLU:O	1:B:267:GLU:HG3	2.18	0.43
1:B:899:LEU:O	1:B:902:ARG:HG2	2.17	0.43
1:A:56:HIS:C	1:A:56:HIS:CD2	2.96	0.43
1:A:117:VAL:CG1	1:A:118:CYS:H	2.31	0.43
1:A:583:PHE:O	1:A:584:LYS:HB2	2.18	0.43
1:A:883:ILE:HG22	1:A:903:VAL:HG21	2.00	0.43
1:A:883:ILE:CD1	1:A:885:ILE:HD11	2.48	0.43
1:A:938:ASP:O	3:A:1151:EPE:H101	2.18	0.43
1:B:84:HIS:O	1:B:87:ILE:HB	2.18	0.43
1:B:295:PHE:HD2	1:B:295:PHE:O	2.01	0.43
1:B:453:ARG:CZ	1:B:453:ARG:CB	2.96	0.43
1:B:816:TYR:CZ	1:B:818:ASP:HA	2.53	0.43
1:A:169:LEU:HD13	1:A:170:ASP:N	2.34	0.43
1:A:618:GLN:HA	1:A:619:PRO:HD3	1.83	0.43
1:A:627:CYS:HA	1:A:755:THR:O	2.19	0.43
1:A:713:LEU:HA	1:A:713:LEU:HD23	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:LEU:O	1:A:981:ASN:HB3	2.19	0.43
1:A:1007:ARG:O	1:A:1007:ARG:HG2	2.17	0.43
1:B:166:GLY:C	1:B:168:LEU:H	2.26	0.43
1:B:483:VAL:CG1	1:B:484:VAL:N	2.81	0.43
1:A:3:GLU:O	1:A:4:GLN:C	2.61	0.43
1:A:21:GLU:O	1:A:21:GLU:HG3	2.18	0.43
1:A:216:GLU:O	1:A:217:PHE:CB	2.67	0.43
1:A:583:PHE:CE2	1:A:645:ALA:HA	2.54	0.43
1:A:932:ALA:O	1:A:935:SER:HB3	2.19	0.43
1:B:38:HIS:HD2	1:B:281:LEU:HD23	1.79	0.43
1:B:122:PHE:HB2	1:B:265:PHE:HE2	1.83	0.43
1:B:272:LEU:O	1:B:272:LEU:HD12	2.18	0.43
1:A:75:THR:HG21	1:A:81:PHE:O	2.18	0.43
1:A:767:MET:O	1:A:768:SER:C	2.62	0.43
1:A:991:GLU:CD	1:A:992:PRO:CD	2.76	0.43
1:B:110:VAL:O	1:B:111:ASN:C	2.61	0.43
1:B:347:LYS:O	1:B:348:ALA:C	2.61	0.43
1:B:634:LYS:HD2	1:B:634:LYS:HA	1.82	0.43
1:B:667:ASP:OD2	1:B:846:ARG:NE	2.51	0.43
1:A:186:ASP:C	1:A:188:GLU:H	2.27	0.43
1:A:231:TRP:CZ2	1:A:243:HIS:HE1	2.37	0.43
1:A:840:ILE:HG21	1:A:842:HIS:CE1	2.53	0.43
1:A:1004:VAL:O	1:A:1004:VAL:HG12	2.18	0.43
1:B:683:ILE:HD13	1:B:683:ILE:HA	1.94	0.43
1:B:1053:LEU:HA	1:B:1054:PRO:HD3	1.86	0.43
1:A:312:ARG:O	1:A:313:PRO:C	2.60	0.43
1:A:602:THR:HG22	1:A:603:PRO:N	2.33	0.43
1:A:905:ARG:HD3	3:A:1152:EPE:O3S	2.19	0.43
1:B:89:SER:CB	1:B:174:MET:HE3	2.46	0.43
1:B:117:VAL:O	1:B:269:LEU:HD22	2.18	0.43
1:B:312:ARG:N	1:B:313:PRO:HD3	2.34	0.43
1:B:662:ALA:C	1:B:682:MET:HE1	2.43	0.43
1:B:873:THR:O	1:B:873:THR:HG22	2.18	0.43
1:B:1001:GLN:HA	4:B:1195:HOH:O	2.18	0.43
1:B:1057:ALA:O	1:B:1058:ARG:C	2.59	0.43
1:A:95:LEU:HD13	1:A:117:VAL:CG1	2.49	0.43
1:A:842:HIS:NE2	3:B:1150:EPE:C6	2.81	0.43
1:A:1023:ARG:O	1:A:1024:LEU:C	2.61	0.43
1:A:1105:GLN:O	1:A:1108:PRO:HD3	2.19	0.43
1:B:20:GLY:HA3	1:B:352:ASN:CA	2.30	0.43
1:B:51:ASN:O	1:B:54:ARG:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:GLN:NE2	1:B:158:GLU:HB3	2.34	0.43
1:B:220:ASP:O	1:B:221:LYS:C	2.61	0.43
1:B:759:ILE:HG23	1:B:763:LEU:HD23	2.00	0.43
1:A:4:GLN:C	1:A:5:TYR:CG	2.97	0.42
1:A:8:THR:O	1:A:17:ARG:HG2	2.19	0.42
1:A:76:LEU:CD1	1:A:807:LEU:HD12	2.48	0.42
1:A:257:ILE:HG22	1:A:258:GLU:N	2.34	0.42
1:A:354:GLY:HA3	1:A:437:THR:HB	2.01	0.42
1:B:501:ALA:C	1:B:503:GLY:N	2.77	0.42
1:B:630:VAL:O	1:B:630:VAL:CG1	2.61	0.42
1:B:692:GLN:HE22	1:B:712:LYS:CD	2.32	0.42
1:B:758:PRO:HG2	1:B:951:GLU:HG2	2.01	0.42
1:A:656:VAL:C	1:A:734:PHE:CZ	2.97	0.42
1:A:979:LEU:C	1:A:981:ASN:N	2.77	0.42
1:A:1011:LEU:CD2	1:A:1056:PRO:HB3	2.49	0.42
1:A:1068:GLN:O	1:A:1071:GLN:N	2.52	0.42
1:B:33:GLU:C	1:B:35:ALA:N	2.76	0.42
1:B:296:GLN:OE1	1:B:324:VAL:HG23	2.19	0.42
1:B:550:TRP:O	1:B:551:SER:C	2.62	0.42
1:B:580:GLY:N	1:B:619:PRO:O	2.52	0.42
1:B:665:HIS:O	1:B:666:TYR:C	2.62	0.42
1:B:692:GLN:NE2	1:B:712:LYS:HD3	2.31	0.42
1:B:832:LEU:C	1:B:834:PRO:HD3	2.44	0.42
1:B:663:GLN:N	1:B:682:MET:HE1	2.34	0.42
1:A:113:LEU:HD12	1:A:272:LEU:HD23	2.01	0.42
1:A:885:ILE:CD1	1:A:899:LEU:HD13	2.48	0.42
1:B:77:PRO:C	1:B:78:TYR:HD1	2.26	0.42
1:B:650:LYS:HB3	1:B:724:GLY:HA3	2.01	0.42
1:B:1010:SER:OG	1:B:1060:LEU:HA	2.19	0.42
1:B:1073:LEU:HD13	1:B:1142:LEU:CD2	2.49	0.42
1:B:1110:HIS:O	1:B:1121:PHE:HA	2.19	0.42
1:A:675:ASN:C	1:A:676:TRP:CD1	2.97	0.42
1:B:1100:LEU:CD1	1:B:1119:LEU:HD22	2.49	0.42
1:A:23:THR:HG22	1:A:24:GLY:N	2.35	0.42
1:A:186:ASP:O	1:A:188:GLU:N	2.53	0.42
1:A:246:GLN:HE21	1:A:250:LYS:HE3	1.85	0.42
1:A:467:PRO:CG	1:A:468:ASP:H	2.33	0.42
1:A:534:GLY:C	1:A:536:ALA:H	2.27	0.42
1:A:895:GLN:O	1:A:898:GLN:HB3	2.19	0.42
1:B:301:ALA:O	1:B:304:GLU:HB2	2.19	0.42
1:B:398:LEU:O	1:B:402:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:681:GLU:HG3	1:B:682:MET:N	2.35	0.42
1:B:793:TYR:CE1	1:B:798:VAL:HG21	2.54	0.42
1:B:1035:THR:CG2	1:B:1036:GLU:N	2.83	0.42
1:A:61:GLN:NE2	1:A:428:GLY:HA3	2.35	0.42
1:A:742:ILE:O	1:A:744:ALA:N	2.53	0.42
1:B:81:PHE:CD2	1:B:911:TYR:HE2	2.38	0.42
1:B:371:LEU:HD11	1:B:404:ARG:HE	1.84	0.42
1:B:732:HIS:CE1	1:B:733:ARG:HG3	2.54	0.42
1:B:744:ALA:O	1:B:745:MET:C	2.62	0.42
1:B:1076:ARG:HE	1:B:1090:ALA:HB1	1.85	0.42
1:B:1132:ILE:CG2	1:B:1133:GLU:N	2.82	0.42
1:A:293:GLU:HG3	1:A:324:VAL:HG21	2.02	0.42
1:B:201:ARG:HD3	1:B:1045:GLU:HG3	2.02	0.42
1:B:846:ARG:O	1:B:849:GLU:HB2	2.20	0.42
1:B:903:VAL:CG1	1:B:904:GLY:N	2.83	0.42
1:B:1020:VAL:HB	4:B:1187:HOH:O	2.19	0.42
1:B:1109:GLN:HE21	1:B:1109:GLN:H	1.67	0.42
1:A:19:LEU:C	1:A:344:LEU:HD11	2.43	0.42
1:A:707:LEU:HD23	1:A:713:LEU:HD11	2.02	0.42
1:B:147:SER:O	1:B:149:GLY:N	2.53	0.42
1:B:402:LEU:C	1:B:404:ARG:N	2.78	0.42
1:B:887:ARG:C	1:B:889:ASP:N	2.77	0.42
1:A:17:ARG:HA	1:A:17:ARG:HD2	1.85	0.42
1:A:1041:GLU:HA	1:A:1041:GLU:OE1	2.20	0.42
1:B:478:HIS:O	1:B:479:ILE:C	2.62	0.42
1:A:395:ARG:NH1	1:A:425:LEU:HD21	2.35	0.41
1:A:669:PHE:HB3	1:A:680:ILE:HD13	2.01	0.41
1:A:1059:THR:O	1:A:1060:LEU:C	2.63	0.41
1:A:76:LEU:O	1:A:79:ASP:N	2.54	0.41
1:A:150:TYR:CD1	1:A:214:ALA:HB2	2.55	0.41
1:A:228:ARG:NH1	1:A:245:TYR:OH	2.53	0.41
1:A:273:PHE:CD2	1:A:276:PHE:HE2	2.37	0.41
1:A:618:GLN:O	1:A:620:LEU:N	2.52	0.41
1:A:721:LYS:O	1:A:722:ASP:HB2	2.21	0.41
1:A:870:ILE:HD13	1:A:895:GLN:HB3	2.02	0.41
1:A:941:ALA:O	1:A:944:ALA:N	2.53	0.41
1:A:257:ILE:O	1:A:258:GLU:C	2.63	0.41
1:A:270:PRO:HA	1:A:271:PRO:HD3	1.88	0.41
1:A:280:THR:HG23	1:A:334:TRP:NE1	2.36	0.41
1:A:385:VAL:O	1:A:386:VAL:O	2.37	0.41
1:B:135:ARG:HG2	1:B:188:GLU:CG	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:837:ARG:NH1	1:B:837:ARG:HG3	2.35	0.41
1:B:895:GLN:O	1:B:896:LEU:C	2.62	0.41
1:A:389:VAL:HG11	1:A:395:ARG:N	2.35	0.41
1:A:612:VAL:HA	1:A:622:MET:HE1	2.01	0.41
1:A:725:LEU:CD2	1:A:726:LEU:N	2.83	0.41
1:A:761:ARG:HG3	1:A:761:ARG:HH11	1.85	0.41
1:A:1026:PHE:O	1:A:1030:ILE:HG13	2.21	0.41
1:B:430:ALA:HB1	1:B:445:CYS:CB	2.50	0.41
1:B:430:ALA:O	1:B:431:GLU:O	2.38	0.41
1:B:527:HIS:CE1	1:B:528:LEU:HD21	2.55	0.41
1:B:840:ILE:HG22	1:B:841:GLY:N	2.36	0.41
1:A:147:SER:C	1:A:149:GLY:H	2.27	0.41
1:A:377:PHE:CD2	1:A:377:PHE:C	2.98	0.41
1:A:875:ILE:CG2	1:A:876:ASP:N	2.84	0.41
1:B:52:ALA:O	1:B:53:LEU:C	2.63	0.41
1:B:131:LYS:N	1:B:134:GLN:HG3	2.27	0.41
1:B:918:HIS:HB3	1:B:920:LYS:HG2	2.02	0.41
1:A:85:GLN:H	1:A:85:GLN:HG3	1.43	0.41
1:A:137:SER:O	1:A:140:ALA:HB3	2.21	0.41
1:A:663:GLN:O	1:A:664:GLN:C	2.64	0.41
1:A:805:GLU:HG3	1:A:882:THR:HB	2.02	0.41
1:A:975:TYR:CD2	1:A:975:TYR:C	2.99	0.41
1:B:45:ILE:HD12	1:B:113:LEU:HD22	2.02	0.41
1:B:170:ASP:CG	1:B:181:ARG:NH1	2.79	0.41
1:A:55:LEU:O	1:A:59:ILE:HG13	2.20	0.41
1:A:581:PHE:CD2	1:A:582:ALA:O	2.74	0.41
1:A:735:GLY:O	1:A:736:VAL:C	2.64	0.41
1:A:763:LEU:HA	1:A:976:MET:CE	2.49	0.41
1:A:1069:GLN:HB2	1:A:1139:MET:CE	2.48	0.41
1:B:244:ILE:CD1	1:B:244:ILE:H	2.33	0.41
1:B:347:LYS:O	1:B:350:ASN:N	2.54	0.41
1:B:548:ASP:O	1:B:549:ALA:C	2.63	0.41
1:B:627:CYS:HA	1:B:755:THR:O	2.20	0.41
1:A:74:GLU:HG2	1:A:808:ARG:HB2	2.03	0.41
1:A:911:TYR:N	1:A:911:TYR:HD1	2.17	0.41
1:A:1047:ILE:O	1:A:1051:GLY:HA2	2.20	0.41
1:B:26:ALA:O	1:B:27:CYS:C	2.63	0.41
1:B:49:MET:O	1:B:52:ALA:CB	2.67	0.41
1:B:614:SER:O	1:B:617:CYS:HB2	2.20	0.41
1:B:656:VAL:HG22	1:B:709:GLY:O	2.19	0.41
1:B:686:PHE:C	1:B:687:ARG:HG2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1037:ASN:C	1:B:1039:LEU:N	2.76	0.41
1:A:9:LEU:CD1	1:A:37:ARG:O	2.69	0.41
1:A:21:GLU:HG3	1:A:353:LEU:O	2.21	0.41
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.82	0.41
1:A:656:VAL:HA	1:A:657:PRO:HD3	1.83	0.41
1:A:710:THR:HB	1:A:712:LYS:H	1.86	0.41
1:A:726:LEU:HB3	1:A:751:ILE:HG12	2.02	0.41
1:A:1106:LYS:C	1:A:1108:PRO:HD3	2.46	0.41
1:B:73:TRP:HB3	1:B:75:THR:OG1	2.21	0.41
1:B:77:PRO:HG2	1:B:302:ARG:CD	2.51	0.41
1:B:96:TYR:HA	1:B:123:LEU:HD21	2.02	0.41
1:B:196:ASP:O	1:B:200:GLN:N	2.36	0.41
1:B:430:ALA:CB	1:B:445:CYS:HB3	2.51	0.41
1:B:659:THR:HG23	3:B:1150:EPE:C2	2.51	0.41
1:B:710:THR:O	1:B:713:LEU:HB2	2.21	0.41
1:B:791:ARG:HG3	1:B:791:ARG:NH1	2.12	0.41
1:B:874:GLY:O	1:B:876:ASP:N	2.54	0.41
1:B:883:ILE:HG12	1:B:885:ILE:HD12	2.02	0.41
1:B:1039:LEU:HD23	1:B:1039:LEU:HA	1.82	0.41
1:B:1091:GLU:CD	1:B:1091:GLU:N	2.78	0.41
1:A:456:ARG:HG2	1:A:876:ASP:OD2	2.21	0.41
1:A:1078:LEU:O	1:A:1078:LEU:CD2	2.68	0.41
1:A:1142:LEU:C	1:A:1142:LEU:HD12	2.46	0.41
1:B:195:PHE:CD1	1:B:195:PHE:C	2.98	0.41
1:B:485:HIS:HD2	1:B:486:LEU:N	2.19	0.41
1:B:499:LEU:O	1:B:505:THR:HA	2.20	0.41
1:B:811:GLN:HG3	1:B:863:ASN:HA	2.03	0.41
1:B:979:LEU:O	1:B:983:VAL:HG23	2.20	0.41
1:A:178:LEU:HB2	1:A:179:PRO:HD2	2.02	0.40
1:A:273:PHE:C	1:A:275:TYR:N	2.76	0.40
1:A:779:PRO:HA	1:A:780:PRO:HD3	1.83	0.40
1:A:1040:GLU:O	1:A:1041:GLU:C	2.64	0.40
1:A:1075:ILE:HA	1:A:1089:PHE:HA	2.02	0.40
1:A:1078:LEU:C	1:A:1078:LEU:CD2	2.89	0.40
1:B:276:PHE:HA	1:B:277:PRO:HD3	1.93	0.40
1:B:471:ILE:H	1:B:471:ILE:HG13	1.58	0.40
1:B:613:LEU:HA	1:B:613:LEU:HD23	1.77	0.40
1:B:873:THR:HG22	1:B:902:ARG:CG	2.51	0.40
1:B:1047:ILE:HG12	1:B:1053:LEU:HD13	2.03	0.40
1:A:76:LEU:O	1:A:77:PRO:C	2.65	0.40
1:A:157:MET:O	1:A:197:VAL:HG11	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLU:C	1:A:172:PHE:HD1	2.28	0.40
1:A:191:SER:C	1:A:192:LEU:HD22	2.47	0.40
1:A:345:PRO:O	1:A:347:LYS:N	2.54	0.40
1:A:377:PHE:CA	1:A:380:THR:HG22	2.51	0.40
1:A:513:TYR:CD1	1:A:545:LEU:HD13	2.56	0.40
1:A:592:LEU:HA	1:A:595:ASP:OD2	2.20	0.40
1:A:936:LEU:HD13	3:A:1151:EPE:C10	2.48	0.40
1:A:1142:LEU:HD12	1:A:1142:LEU:O	2.21	0.40
1:B:45:ILE:HD12	1:B:113:LEU:CD2	2.50	0.40
1:B:257:ILE:O	1:B:257:ILE:HG12	2.22	0.40
1:B:416:ASP:O	1:B:418:ALA:N	2.54	0.40
1:B:563:ASP:O	1:B:564:VAL:C	2.65	0.40
1:B:735:GLY:O	1:B:739:LYS:HE3	2.22	0.40
1:B:991:GLU:CG	1:B:992:PRO:HD2	2.51	0.40
1:A:16:GLN:O	1:A:17:ARG:CD	2.69	0.40
1:A:117:VAL:HG21	1:A:272:LEU:HD13	2.04	0.40
1:A:129:VAL:CG1	1:A:130:MET:N	2.84	0.40
1:A:209:ILE:O	1:A:209:ILE:HG23	2.22	0.40
1:A:466:ASN:HB2	1:A:469:THR:CB	2.51	0.40
1:A:505:THR:HB	4:A:1208:HOH:O	2.20	0.40
1:A:763:LEU:O	1:A:763:LEU:HG	2.20	0.40
1:A:1047:ILE:O	1:A:1051:GLY:N	2.52	0.40
1:B:75:THR:HG22	1:B:79:ASP:CB	2.52	0.40
1:B:502:GLY:HA3	1:B:1007:ARG:HH12	1.86	0.40
1:B:602:THR:HG23	1:B:603:PRO:HD2	2.03	0.40
1:B:906:SER:O	1:B:907:HIS:CB	2.69	0.40
1:A:48:ASP:OD1	1:A:51:ASN:ND2	2.54	0.40
1:A:231:TRP:O	1:A:234:THR:N	2.44	0.40
1:A:526:LEU:CD2	1:A:1027:TYR:HB3	2.51	0.40
1:A:562:ARG:HG3	1:A:992:PRO:CG	2.50	0.40
1:B:387:PHE:HB2	1:B:424:TYR:O	2.21	0.40
1:A:156:VAL:CG1	1:A:156:VAL:O	2.69	0.40
1:A:385:VAL:HG23	1:A:423:ARG:NH1	2.36	0.40
1:A:398:LEU:O	1:A:399:GLY:C	2.63	0.40
1:A:933:ILE:C	1:A:935:SER:H	2.29	0.40
1:A:947:THR:O	1:A:951:GLU:HG3	2.21	0.40
1:B:252:THR:O	1:B:253:LEU:HD23	2.22	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	1144/1151 (99%)	941 (82%)	153 (13%)	50 (4%)	2	15
1	B	1141/1151 (99%)	942 (83%)	153 (13%)	46 (4%)	2	17
All	All	2285/2302 (99%)	1883 (82%)	306 (13%)	96 (4%)	2	16

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	A	25	ALA
1	A	38	HIS
1	A	132	LYS
1	A	187	ASP
1	A	346	THR
1	A	386	VAL
1	A	461	SER
1	A	469	THR
1	A	585	HIS
1	A	736	VAL
1	A	842	HIS
1	A	1146	ALA
1	B	244	ILE
1	B	255	ALA
1	B	419	SER
1	B	422	GLY
1	B	431	GLU
1	B	541	PRO
1	B	745	MET
1	B	819	VAL
1	B	993	SER
1	B	995	GLU
1	A	217	PHE
1	A	433	GLY

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Mol	Chain	Res	Type
1	A	438	VAL
1	A	534	GLY
1	A	551	SER
1	A	586	ASP
1	A	820	GLU
1	A	942	GLY
1	A	993	SER
1	A	995	GLU
1	A	1075	ILE
1	B	52	ALA
1	B	241	PRO
1	B	317	PRO
1	B	360	ASP
1	B	372	ASP
1	B	429	ALA
1	B	875	ILE
1	B	994	LEU
1	A	183	ASP
1	A	220	ASP
1	A	470	LEU
1	A	550	TRP
1	A	619	PRO
1	A	722	ASP
1	A	1033	ALA
1	A	1077	LYS
1	B	101	MET
1	B	111	ASN
1	B	347	LYS
1	B	348	ALA
1	B	409	PRO
1	B	417	GLU
1	B	501	ALA
1	B	630	VAL
1	B	715	GLN
1	B	746	ARG
1	B	828	ARG
1	A	182	LEU
1	A	186	ASP
1	A	190	ASP
1	A	258	GLU
1	A	437	THR
1	A	468	ASP

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Mol	Chain	Res	Type
1	A	941	ALA
1	B	9	LEU
1	B	345	PRO
1	B	382	ASP
1	B	479	ILE
1	B	536	ALA
1	B	748	ASN
1	A	213	PRO
1	A	768	SER
1	A	780	PRO
1	A	860	GLN
1	A	919	PRO
1	A	1054	PRO
1	B	26	ALA
1	B	744	ALA
1	B	917	PRO
1	A	156	VAL
1	A	819	VAL
1	B	134	GLN
1	B	242	GLU
1	B	308	VAL
1	B	460	ASP
1	B	623	ASP
1	B	117	VAL
1	A	875	ILE
1	A	917	PRO
1	B	110	VAL
1	B	197	VAL
1	A	1020	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	930/975 (95%)	840 (90%)	90 (10%)	8	32
1	B	904/975 (93%)	834 (92%)	70 (8%)	12	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1834/1950 (94%)	1674 (91%)	160 (9%)	9 36

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	36	GLU
1	A	43	VAL
1	A	49	MET
1	A	75	THR
1	A	76	LEU
1	A	77	PRO
1	A	85	GLN
1	A	89	SER
1	A	98	LEU
1	A	142	ARG
1	A	169	LEU
1	A	178	LEU
1	A	192	LEU
1	A	194	VAL
1	A	197	VAL
1	A	205	GLU
1	A	226	LEU
1	A	234	THR
1	A	257	ILE
1	A	279	ASN
1	A	287	ASP
1	A	293	GLU
1	A	296	GLN
1	A	304	GLU
1	A	312	ARG
1	A	325	ASP
1	A	331	LEU
1	A	342	GLU
1	A	346	THR
1	A	366	GLN
1	A	372	ASP
1	A	374	LEU
1	A	378	LEU
1	A	395	ARG
1	A	411	ARG
1	A	412	ILE

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Mol	Chain	Res	Type
1	A	434	PHE
1	A	443	LEU
1	A	453	ARG
1	A	471	ILE
1	A	474	LEU
1	A	487	GLU
1	A	498	THR
1	A	523	VAL
1	A	526	LEU
1	A	561	VAL
1	A	562	ARG
1	A	622	MET
1	A	627	CYS
1	A	629	ASP
1	A	646	VAL
1	A	658	THR
1	A	672	ARG
1	A	679	ARG
1	A	710	THR
1	A	713	LEU
1	A	715	GLN
1	A	725	LEU
1	A	746	ARG
1	A	749	VAL
1	A	751	ILE
1	A	759	ILE
1	A	803	LEU
1	A	808	ARG
1	A	816	TYR
1	A	845	MET
1	A	847	GLU
1	A	850	LEU
1	A	865	LEU
1	A	879	THR
1	A	883	ILE
1	A	889	ASP
1	A	890	HIS
1	A	900	ARG
1	A	902	ARG
1	A	911	TYR
1	A	918	HIS
1	A	923	THR

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Mol	Chain	Res	Type
1	A	945	LEU
1	A	1010	SER
1	A	1011	LEU
1	A	1076	ARG
1	A	1082	GLU
1	A	1103	LEU
1	A	1107	GLN
1	A	1109	GLN
1	A	1122	ILE
1	A	1130	THR
1	A	1132	ILE
1	B	15	GLU
1	B	27	CYS
1	B	45	ILE
1	B	58	GLU
1	B	85	GLN
1	B	99	PRO
1	B	102	GLN
1	B	134	GLN
1	B	142	ARG
1	B	143	THR
1	B	164	THR
1	B	171	LEU
1	B	188	GLU
1	B	197	VAL
1	B	201	ARG
1	B	205	GLU
1	B	209	ILE
1	B	219	THR
1	B	226	LEU
1	B	240	ASP
1	B	252	THR
1	B	267	GLU
1	B	279	ASN
1	B	287	ASP
1	B	320	LEU
1	B	330	GLU
1	B	378	LEU
1	B	394	ARG
1	B	398	LEU
1	B	404	ARG
1	B	405	ILE

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Mol	Chain	Res	Type
1	B	407	ILE
1	B	432	HIS
1	B	471	ILE
1	B	476	GLU
1	B	486	LEU
1	B	487	GLU
1	B	497	THR
1	B	505	THR
1	B	523	VAL
1	B	635	THR
1	B	660	LEU
1	B	672	ARG
1	B	682	MET
1	B	713	LEU
1	B	716	SER
1	B	717	ASP
1	B	757	THR
1	B	783	ARG
1	B	791	ARG
1	B	803	LEU
1	B	816	TYR
1	B	822	ILE
1	B	845	MET
1	B	879	THR
1	B	890	HIS
1	B	893	LEU
1	B	906	SER
1	B	916	THR
1	B	945	LEU
1	B	991	GLU
1	B	1011	LEU
1	B	1053	LEU
1	B	1058	ARG
1	B	1068	GLN
1	B	1078	LEU
1	B	1091	GLU
1	B	1109	GLN
1	B	1119	LEU
1	B	1136	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	51	ASN
1	A	56	HIS
1	A	65	GLN
1	A	84	HIS
1	A	115	GLN
1	A	246	GLN
1	A	279	ASN
1	A	338	GLN
1	A	343	HIS
1	A	527	HIS
1	A	543	HIS
1	A	555	GLN
1	A	668	ASN
1	A	738	HIS
1	A	811	GLN
1	A	859	HIS
1	A	890	HIS
1	A	1071	GLN
1	A	1094	HIS
1	A	1107	GLN
1	A	1109	GLN
1	B	69	ASN
1	B	84	HIS
1	B	134	GLN
1	B	200	GLN
1	B	210	ASN
1	B	215	HIS
1	B	243	HIS
1	B	279	ASN
1	B	350	ASN
1	B	352	ASN
1	B	432	HIS
1	B	485	HIS
1	B	527	HIS
1	B	543	HIS
1	B	585	HIS
1	B	692	GLN
1	B	732	HIS
1	B	764	ASN
1	B	821	ASN
1	B	842	HIS
1	B	844	GLN

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Mol	Chain	Res	Type
1	B	855	ASN
1	B	890	HIS
1	B	898	GLN
1	B	948	HIS
1	B	963	GLN
1	B	1109	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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EPE	B	1152	-	15,15,15	1.07	0	19,20,20	1.26	2 (10%)
3	EPE	B	1150	-	15,15,15	0.96	0	19,20,20	1.43	2 (10%)
3	EPE	A	1152	-	15,15,15	1.06	0	19,20,20	1.39	3 (15%)
2	SO4	A	1149	-	4,4,4	0.36	0	6,6,6	0.27	0
3	EPE	A	1151	-	15,15,15	1.15	0	19,20,20	1.41	2 (10%)
2	SO4	B	1149	-	4,4,4	0.38	0	6,6,6	0.22	0
2	SO4	A	1150	-	4,4,4	0.34	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EPE	B	1151	-	15,15,15	1.39	1 (6%)	19,20,20	1.42	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	B	1152	-	-	0/9/19/19	0/1/1/1
3	EPE	B	1150	-	-	1/9/19/19	0/1/1/1
3	EPE	A	1152	-	-	1/9/19/19	0/1/1/1
3	EPE	A	1151	-	-	1/9/19/19	0/1/1/1
3	EPE	B	1151	-	-	1/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1151	EPE	C10-S	2.83	1.81	1.77

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1152	EPE	O1S-S-C10	4.29	113.21	106.73
3	A	1151	EPE	O1S-S-C10	4.24	113.13	106.73
3	B	1151	EPE	O1S-S-C10	3.92	112.65	106.73
3	B	1150	EPE	O1S-S-C10	3.88	112.59	106.73
3	B	1152	EPE	O1S-S-C10	3.64	112.23	106.73
3	B	1151	EPE	O3S-S-O1S	-3.56	102.50	111.40
3	A	1151	EPE	O3S-S-O1S	-2.93	104.06	111.40
3	B	1150	EPE	O3S-S-O2S	-2.62	104.84	111.40
3	A	1152	EPE	O3S-S-O2S	-2.25	105.76	111.40
3	B	1152	EPE	O3S-S-O1S	-2.18	105.93	111.40
3	A	1152	EPE	O3S-S-O1S	-2.07	106.22	111.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1151	EPE	N4-C7-C8-O8
3	A	1151	EPE	N4-C7-C8-O8
3	A	1152	EPE	N4-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
3	B	1150	EPE	N4-C7-C8-O8

There are no ring outliers.

4 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1150	EPE	14	0
3	A	1152	EPE	1	0
3	A	1151	EPE	9	0
3	B	1151	EPE	12	0

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

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	1146/1151 (99%)	-0.16	16 (1%) 73 54	4, 44, 83, 109	0
1	B	1143/1151 (99%)	0.08	44 (3%) 44 27	4, 53, 105, 123	0
All	All	2289/2302 (99%)	-0.04	60 (2%) 57 37	4, 48, 100, 123	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	282	LEU	4.4
1	B	630	VAL	3.5
1	B	353	LEU	3.4
1	B	283	VAL	3.3
1	B	284	ASN	3.3
1	B	19	LEU	3.2
1	B	44	LEU	3.2
1	A	1001	GLN	3.0
1	B	453	ARG	3.0
1	B	360	ASP	2.9
1	B	49	MET	2.9
1	B	421	ARG	2.9
1	B	355	PHE	2.8
1	A	630	VAL	2.8
1	B	20	GLY	2.8
1	A	996	ASP	2.8
1	A	459	GLN	2.8
1	B	377	PHE	2.7
1	B	410	GLN	2.6
1	B	192	LEU	2.6
1	B	438	VAL	2.6
1	A	460	ASP	2.6
1	B	422	GLY	2.6
1	B	339	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	352	ASN	2.5
1	A	454	VAL	2.5
1	B	322	LEU	2.4
1	B	407	ILE	2.4
1	B	43	VAL	2.4
1	B	337	VAL	2.4
1	A	533	ALA	2.3
1	B	281	LEU	2.3
1	A	131	LYS	2.3
1	B	391	SER	2.3
1	B	415	LEU	2.3
1	B	452	GLU	2.3
1	B	417	GLU	2.2
1	B	420	ASP	2.2
1	B	335	PRO	2.2
1	A	455	ALA	2.2
1	A	167	ALA	2.2
1	A	351	ALA	2.2
1	B	37	ARG	2.2
1	B	343	HIS	2.2
1	A	2	PRO	2.1
1	B	436	ASP	2.1
1	B	423	ARG	2.1
1	A	997	LEU	2.1
1	A	999	SER	2.1
1	A	821	ASN	2.1
1	B	463	ARG	2.1
1	B	461	SER	2.0
1	B	413	MET	2.0
1	B	416	ASP	2.0
1	B	354	GLY	2.0
1	B	7	TYR	2.0
1	B	285	THR	2.0
1	A	629	ASP	2.0
1	B	992	PRO	2.0
1	B	537	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	1149	5/5	0.54	0.13	120,120,120,121	0
3	EPE	B	1152	15/15	0.62	0.21	95,95,98,98	0
3	EPE	B	1151	15/15	0.66	0.22	105,108,109,109	0
2	SO4	A	1150	5/5	0.67	0.13	104,104,105,105	0
3	EPE	A	1152	15/15	0.72	0.19	88,89,91,92	0
3	EPE	B	1150	15/15	0.81	0.21	81,89,91,92	0
3	EPE	A	1151	15/15	0.84	0.15	104,105,105,106	0
2	SO4	A	1149	5/5	0.88	0.10	89,89,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.