



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:15 AM GMT

PDB ID : 3HO8
Title : Crystal Structure of S. aureus Pyruvate Carboxylase in complex with Coenzyme A
Authors : Tong, L.; Yu, L.P.C.
Deposited on : 2009-06-01
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

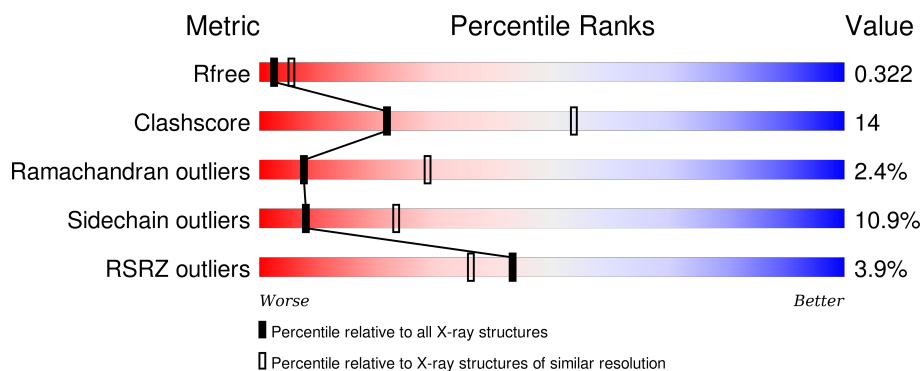
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	1150	<div> <div>4%</div> <div>57% 26% • 14%</div> </div>
1	B	1150	<div> <div>%</div> <div>52% 29% 5% 14%</div> </div>
1	C	1150	<div> <div>2%</div> <div>56% 26% • 13%</div> </div>
1	D	1150	<div> <div>6%</div> <div>54% 23% • 19%</div> </div>

2 Entry composition [i](#)

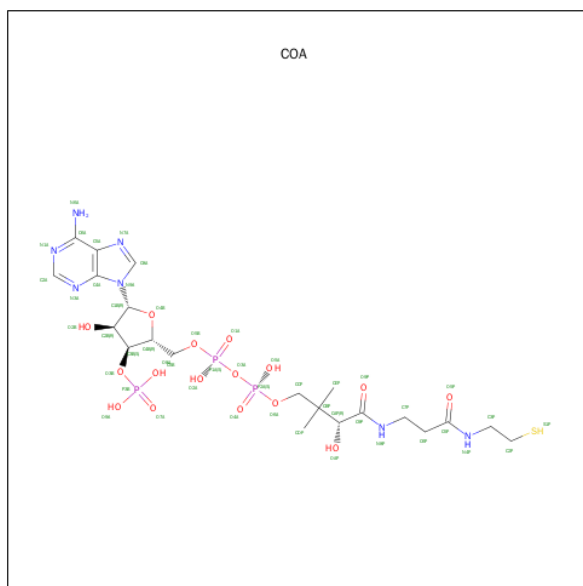
There are 4 unique types of molecules in this entry. The entry contains 31229 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7880	5000	1329	1525	26			
1	D	934	Total	C	N	O	S	0	0	0
			7396	4696	1250	1426	24			
1	C	995	Total	C	N	O	S	0	0	0
			7889	5005	1330	1528	26			
1	B	989	Total	C	N	O	S	0	0	0
			7838	4975	1321	1516	26			

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		
2	D	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		

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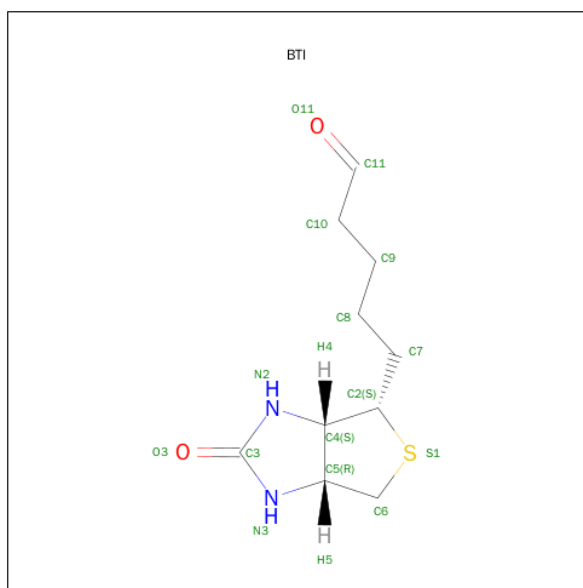
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: C₁₀H₁₆N₂O₂S).

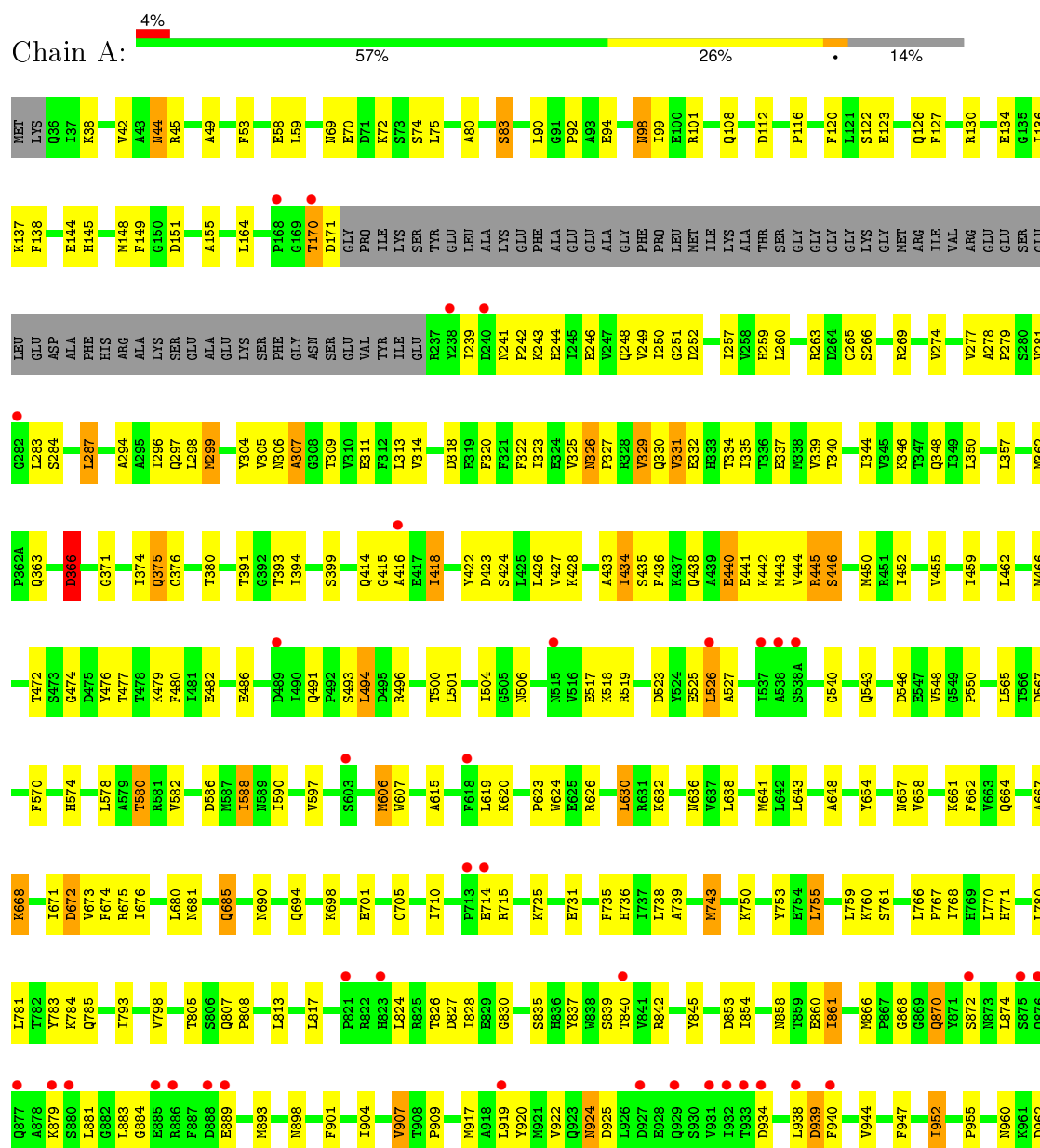


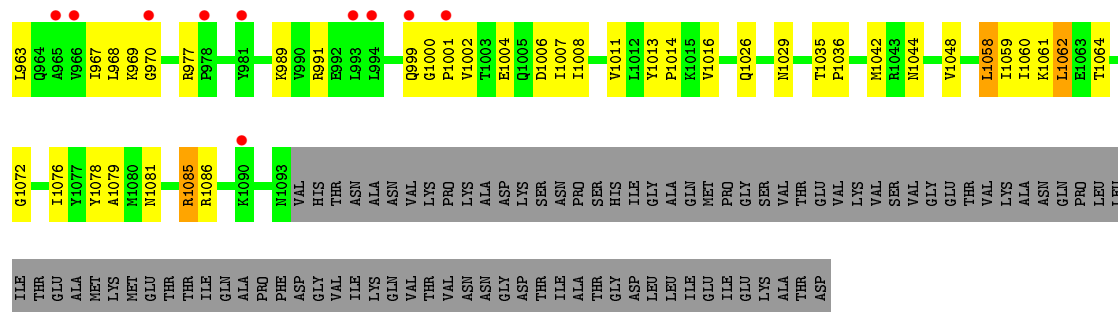
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
4	B	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

3 Residue-property plots

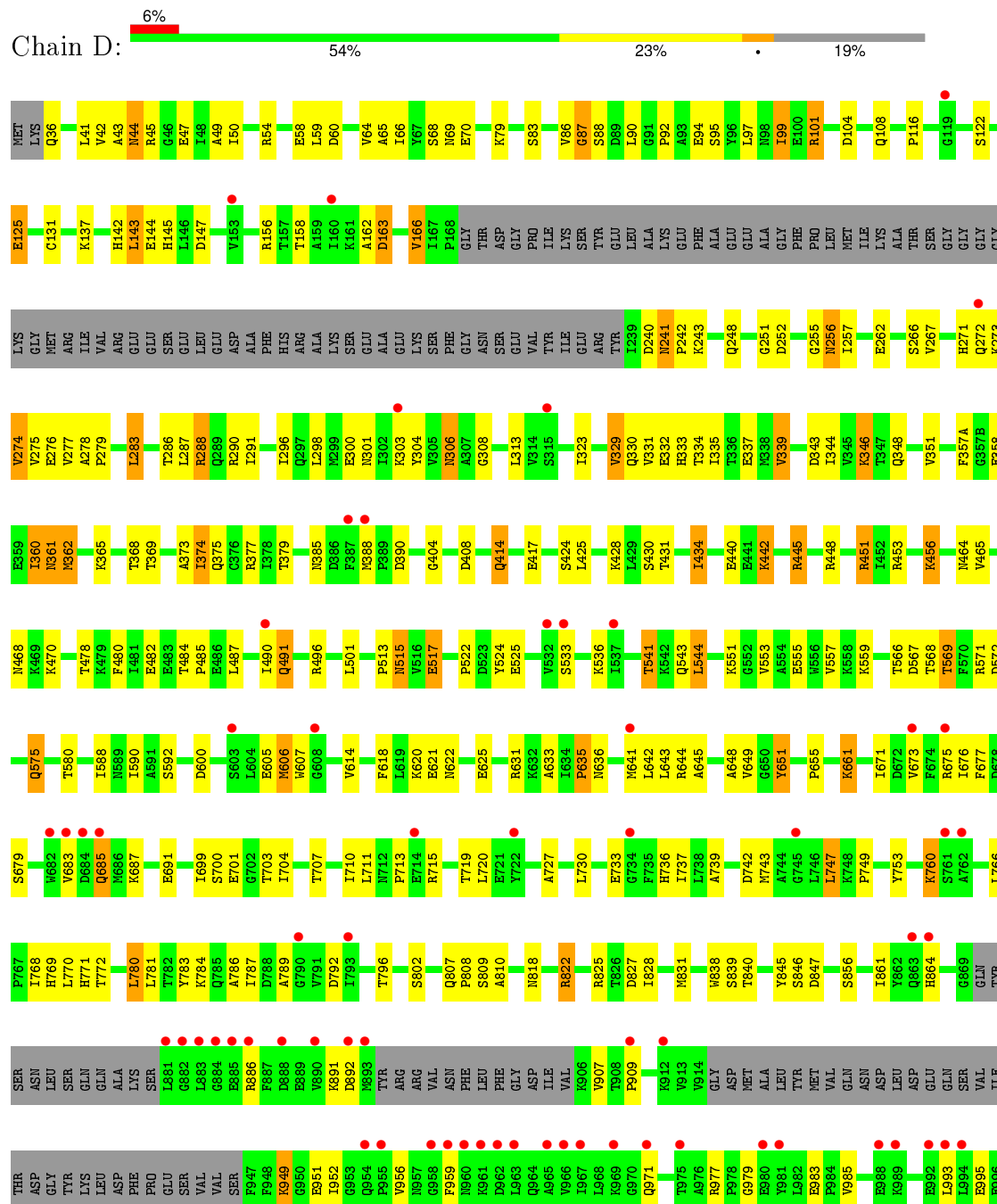
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

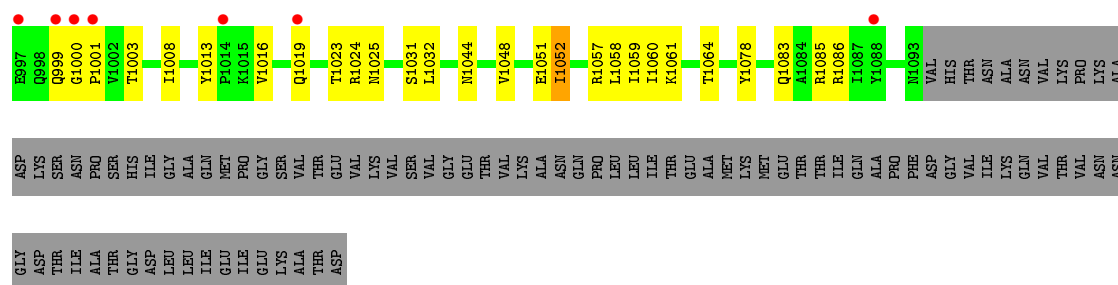
• Molecule 1: Pyruvate carboxylase



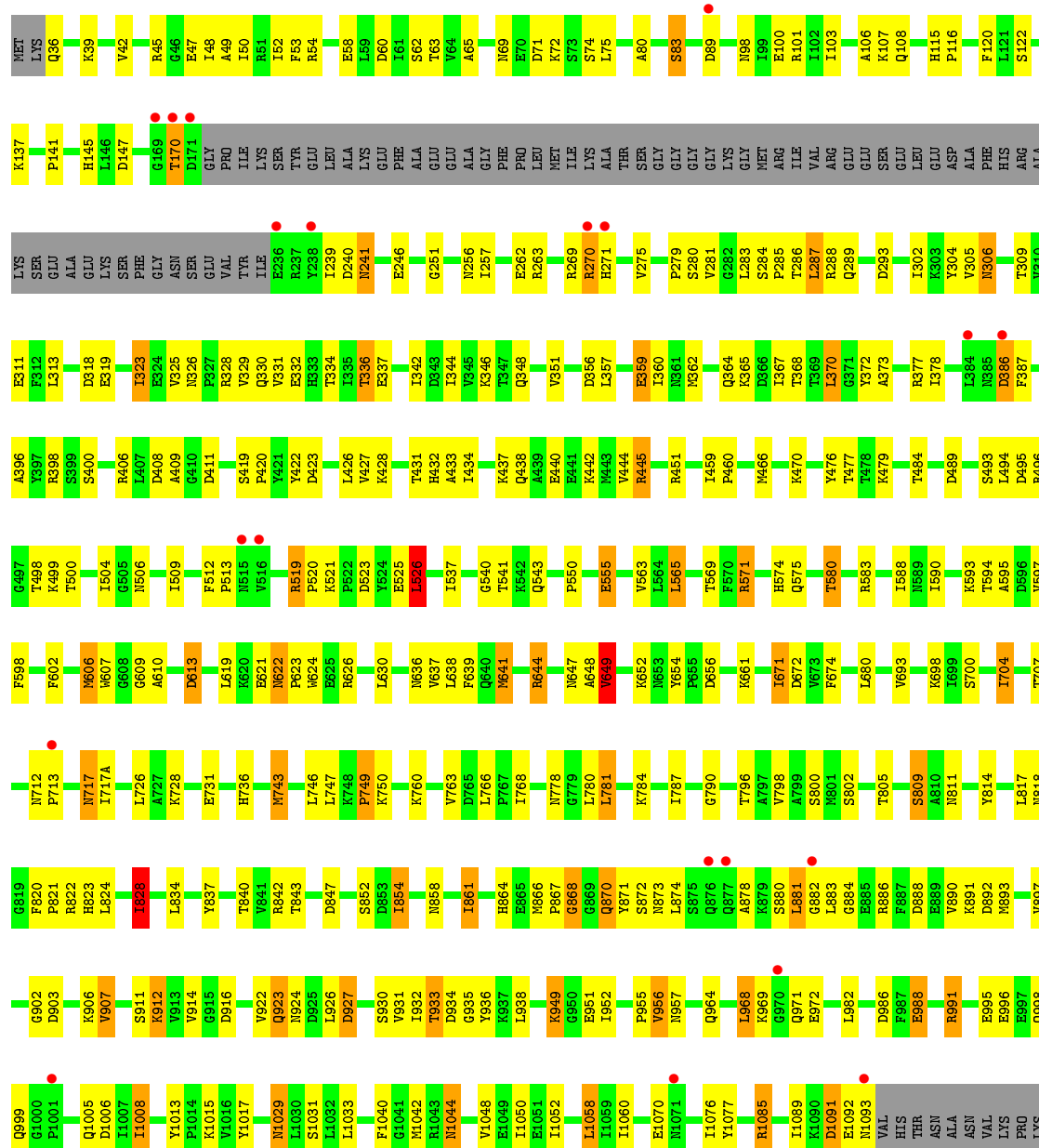


• Molecule 1: Pyruvate carboxylase





• Molecule 1: Pyruvate carboxylase



ALA	ASP	LYS	SER	ASN	PRO	SER	HIS	ILE	GLY	ALA	GLN	MET	PRO	GLY	SER	VAL	THR	GLU	VAL	LYS	VAL	SER	VAL	GLY	GLU	THR	THR	VAL	LYS	ALA	ASN	GLN	GLN	PRO	LEU	LEU	ILE	THR	GLU	ALA	ALA	MET	LYS	MET	GLU	THR	THR	ILE	GLN	ALA	PRO	PHE	ASP	GLY	VAL	ILE	LYS	GLN	VAL	THR	VAL	ASN
ASN	GLY	ASP	THR	ILE	ALA	ALA	THR	GLY	ASP	LEU	ILE	GLU	ILE	GLU	GLY	LYS	ALA	THR	THR	ASP																																										

• Molecule 1: Pyruvate carboxylase



VAL	R1043	S930	I828	K725	L638	G540	K428	V339	D264	SER	Y118	MET
GLY	N1044	V931	E829	L726	F639	T541	L429	C265	C266	GLY	G119	LYS
THR	E4049	I932	G830	I736	G640	K542	S430	I342	S266	GLY	F120	Q36
VAL	D942	T933	K831	H737	M641	Q543	T431	T267	V267	GLY	L121	K39
LYS	D1083	G935	E832	I738	R644	E547	H432	V245	Q268	LYS	S122	L40
ALA	I1059	L938	H836	A739	A645	P550	I434	K346	K269	GLY	Q126	L41
ASN	I1060	L938	H836	M743	N647	P550	S435	Q348	R270	MET	H271	V42
GLN	I1065	V944	S839	L747	V649	W556	K442	A352	Q272	ARG	R129	A43
LEU	I1076	V945	D847	I747	V649	W557	K462	A353	V275	VAL	C131	R45
ILE	E1070	I952	I854	A751	G650	K558	L462	G354	A278	ARG	I139	A49
THR	N1071	N957	K855	A752	K652	K559	K469	F357A	P279	GLU	I50	E51
ALA	I1076	N960	S856	E758	D656	D657	S473	T369	S280	SER	H142	E52
MET	Y1077	R961	R857	K760	N658	D562	D563	L370	V281	GLU	L143	E53
LYS	N1080	I962	I858	I769	L659	F570	T477	T379	G282	LEU	E144	E54
MET	N1081	L963	E860	L766	H680	R571	K479	T379	L283	GLU	H145	E55
THR	R1086	T975	I861	P767	K661	D572	F480	A373	G286	ASP	E148	
THR		A976	H862	I768	A573	E574	K491	C376	L287	PHS	D151	E58
ILE		A976	Q863	I768	S666	H574	P492	R377	R288	PHS	D151	E59
GLN	I1089	R977	E864	H773	A667	Q575	S493	T378	L384	ARG	K152	E60
GLN		P978	E865	H773	D774	T580	L494	T379	Q289	ALA	E156	E61
PRO	E1092	N1093	K866	T775	D672	R581	D495	T380	L290	LYS	R156	S62
PHS	VAL		G868	T775	V673	R581	R496	E381	A294	SER	D163	T63
ASP			G869	N778	G674	I588	R496	E381	A295	ALA	L164	A65
GLY	THR		Q870	N778	R674	N589		L384	L296	GLU	P165	
VAL			K871	L781	R675		I504	P389	Q297	LYS	V166	N69
ILE	ASN		S872	L782	L676	S592	G505	P389	L298	SER	I167	
LYS	ALA	L994	N873	L782	D684	K593	V507	T391		PHS	P168	K72
GLN	ASN		L874	K784				G392		THR	G17	
VAL	LYS	E997			V693	D596		T393		GLY	THR	
THR			K879	I787		V597	G511	T393		ASN	ASP	
VAL	PRO	G1000			A696		F512	T393		SER	THR	
ASN	LYS	P1001			G697	E605	S511	G392		GLY	ASP	E82
ASN	LYS	I1002	G884	I794	K698	N515	P513	T394		GLU	PRO	S83
GLY	ASP	T1003			G698	N515	R306			VAL	ILE	Y84
ASP	LYS	E1004	D888	T796	L699	G606	V516	A307		THR	ILE	L85
THR	SER	Q1005			I699	W607	E517	S399		GLU	LYS	E86
ILE	ASN	D1006	K891	A799	E701	K518	E517	S400		ARG	SER	G87
PRO	PRO	I1007				A610	K518	F403		THR	GLU	S88
THR	SER	I1008	N898	S802	I704	V614	R519	L407		T129	GLU	R89
GLY	HIS	S1009				A615	K521	L407		D240	ALA	L90
ASP	ILE	Y1010	F901	S806	G708	E623	P522	D408		N241	LYS	
LEU	GLY	Y1011				F618	E524	A409		P242	GLU	E94
ILE	ALA		K906	S809	L711	L619	E525	G410		T245	PHS	
LEU	GLN	Y1017	T907	A810	R715	L619	E525	D411			ALA	L97
ILE	MET	E1018	T908	N811	R716	N622	L526	G412		T245	GLU	N98
ILE	PRO	Q1019			S716	N622	L526	F413		I250	GLU	I99
GLU	GLY		K917	Y814	N717	W624		R327		G251	ALA	E100
LYS	SER	Q1022	K918	Y815	I717A	W624	P530	R327		D252	GLY	R101
VAL	VAL		L919	A816	I717A	E625	T531	G415		E253	PHS	
ASP	THR	N1029	N921	L817	T719	R626				I253	PRO	V111
THR	GLU	T1035	N921	F820	L720	L630	K536	D423		N257	LEU	D112
ASP	LYS	P1036	D927		E721	R631	A538	L335		I257	MET	A113
	VAL		E928	R825	I722	S538A	L425	T336		G258	ILE	H114
							P538B	L426		H259	LYS	H115
											ALA	P116

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.59Å 164.47Å 373.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.90 29.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.97-2.90) 89.8 (29.98-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.264 , 0.328 0.266 , 0.322	Depositor DCC
R_{free} test set	5969 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	3 of 118418 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	31229	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.90 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.1935e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: COA, MN, BTI

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	0.43	0/8033	0.60	1/10868 (0.0%)
1	B	0.49	0/7990	0.64	0/10810
1	C	0.50	0/8042	0.65	2/10880 (0.0%)
1	D	0.43	0/7537	0.60	0/10192
All	All	0.47	0/31602	0.62	3/42750 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	526	LEU	CA-CB-CG	5.56	128.09	115.30
1	C	828	ILE	CB-CA-C	-5.22	101.16	111.60
1	C	526	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	880	SER	Peptide

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	7880	0	7807	199	0
1	B	7838	0	7771	292	0
1	C	7889	0	7813	232	0
1	D	7396	0	7347	158	0
2	A	48	0	32	0	0
2	B	48	0	32	1	0
2	C	48	0	32	2	0
2	D	48	0	32	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	15	0	16	0	0
4	C	15	0	16	3	0
All	All	31229	0	30898	870	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 14.

All (870) 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:C:504:ILE:HG21	1:C:1042:MET:HE2	1.18	1.12
1:C:704:ILE:HG12	1:C:726:LEU:HD23	1.22	1.12
1:A:304:TYR:HE2	1:A:307:ALA:O	1.35	1.10
1:A:1085:ARG:HG2	1:A:1085:ARG:HH11	1.12	1.06
1:C:743:MET:HG3	1:C:907:VAL:HG13	1.38	1.04
1:B:825:ARG:HG2	1:B:825:ARG:HH11	1.20	1.02
1:D:451:ARG:HH22	2:D:2001:COA:H62	1.27	0.99
1:D:496:ARG:HE	1:D:1052:ILE:HG21	1.26	0.99
1:B:516:VAL:HG12	1:B:517:GLU:H	1.22	0.97
1:C:364:GLN:HA	1:C:367:ILE:HD12	1.46	0.96
1:A:44:ASN:HD22	1:A:45:ARG:H	1.13	0.96
1:A:304:TYR:CE2	1:A:307:ALA:O	2.17	0.95
1:B:288:ARG:HH11	1:B:288:ARG:HG3	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:MET:HE2	1:C:639:PHE:HB3	1.49	0.94
1:B:700:SER:H	1:B:736:HIS:HD2	1.17	0.91
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.34	0.91
1:D:43:ALA:HA	1:D:66:ILE:HD11	1.49	0.90
1:C:864:HIS:HD2	1:C:866:MET:H	1.19	0.90
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.36	0.89
1:B:644:ARG:HH11	1:B:647:ASN:HD21	1.15	0.89
1:D:277:VAL:HG22	1:D:374:ILE:HG22	1.54	0.88
1:C:506:ASN:OD1	4:C:2000:BTI:H92	1.73	0.88
1:C:870:GLN:HE22	1:C:911:SER:HB2	1.38	0.87
1:B:898:ASN:ND2	1:B:906:LYS:HE3	1.88	0.87
1:B:570:PHE:O	1:B:574:HIS:HE1	1.58	0.86
1:B:719:THR:HG22	1:B:721:GLU:H	1.40	0.86
1:C:574:HIS:HD2	1:C:580:THR:HA	1.41	0.85
1:B:1092:GLU:O	1:B:1093:ASN:HB2	1.77	0.85
1:B:917:MET:HG2	1:B:944:VAL:HG21	1.58	0.84
1:C:866:MET:CE	1:C:871:TYR:HA	2.07	0.83
1:A:442:LYS:O	1:A:446:SER:HB2	1.78	0.83
1:C:1044:ASN:N	1:C:1044:ASN:HD22	1.77	0.83
1:B:864:HIS:HD2	1:B:866:MET:H	1.28	0.81
1:B:516:VAL:HG12	1:B:517:GLU:N	1.95	0.81
1:C:743:MET:CG	1:C:907:VAL:HG13	2.10	0.80
1:C:704:ILE:CG1	1:C:726:LEU:HD23	2.09	0.80
1:A:418:ILE:HD12	1:A:418:ILE:H	1.47	0.80
1:D:162:ALA:O	1:D:163:ASP:HB2	1.82	0.80
1:A:1085:ARG:HG2	1:A:1085:ARG:NH1	1.88	0.79
1:C:626:ARG:O	1:C:630:LEU:HB2	1.82	0.79
1:B:866:MET:HG2	1:B:870:GLN:HB3	1.65	0.79
1:C:866:MET:HE2	1:C:871:TYR:HA	1.65	0.79
1:B:901:PHE:HZ	1:B:917:MET:HG3	1.48	0.79
1:A:1058:LEU:HD12	1:A:1060:ILE:HD11	1.66	0.78
1:B:329:VAL:HG22	1:B:348:GLN:HE22	1.49	0.77
1:C:512:PHE:CZ	4:C:2000:BTI:H5	2.20	0.76
1:D:288:ARG:HA	1:D:291:ILE:HD12	1.64	0.76
1:A:313:LEU:HB2	1:A:323:ILE:HD11	1.67	0.76
1:A:543:GLN:HE22	1:A:636:ASN:HA	1.51	0.76
1:B:306:ASN:HD21	1:B:348:GLN:HG3	1.49	0.75
1:B:409:ALA:HA	1:B:427:VAL:HG12	1.68	0.75
1:B:516:VAL:CG1	1:B:517:GLU:H	1.98	0.75
1:C:606:MET:CE	1:C:639:PHE:HB3	2.15	0.75
1:A:306:ASN:OD1	1:A:348:GLN:HG2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ARG:HH11	1:C:1052:ILE:HD12	1.52	0.74
1:C:858:ASN:O	1:C:861:ILE:HG12	1.87	0.74
1:B:54:ARG:O	1:B:58:GLU:HG2	1.87	0.74
1:C:743:MET:HG3	1:C:907:VAL:CG1	2.16	0.74
1:B:873:ASN:ND2	1:B:873:ASN:H	1.86	0.74
1:A:44:ASN:HD22	1:A:45:ARG:N	1.84	0.73
1:C:717(A):ILE:HG12	1:C:957:ASN:HD21	1.53	0.73
1:B:901:PHE:CZ	1:B:917:MET:HG3	2.21	0.73
1:B:825:ARG:HG2	1:B:825:ARG:NH1	1.92	0.73
1:A:570:PHE:HB2	1:A:606:MET:HB3	1.71	0.73
1:D:677:PHE:HB3	1:D:703:THR:HB	1.69	0.73
1:C:1044:ASN:HD22	1:C:1044:ASN:H	1.33	0.73
1:C:357:LEU:O	1:C:362:MET:HB3	1.88	0.73
1:B:700:SER:H	1:B:736:HIS:CD2	2.06	0.72
1:D:277:VAL:HG22	1:D:374:ILE:CG2	2.19	0.72
1:A:658:VAL:HG11	1:A:1011:VAL:HG11	1.71	0.72
1:C:571:ARG:C	1:C:571:ARG:HD2	2.10	0.72
1:C:870:GLN:NE2	1:C:911:SER:HB2	2.05	0.72
1:B:379:THR:HG22	1:B:425:LEU:HA	1.72	0.71
1:C:555:GLU:HA	1:C:555:GLU:OE1	1.90	0.71
1:D:279:PRO:HD3	1:D:339:VAL:HG11	1.72	0.71
1:D:622:ASN:HB3	1:D:625:GLU:HB2	1.71	0.71
1:C:145:HIS:HE1	1:C:302:ILE:O	1.73	0.71
1:A:731:GLU:HG3	1:A:766:LEU:HD21	1.73	0.71
1:A:259:HIS:HB3	1:A:296:ILE:HD11	1.70	0.71
1:B:286:THR:O	1:B:290:ARG:HG3	1.91	0.70
1:C:924:ASN:HB2	1:C:926:LEU:CD2	2.20	0.70
1:C:563:VAL:HG21	1:C:787:ILE:HG12	1.74	0.70
1:D:283:LEU:HD23	1:D:288:ARG:HB2	1.73	0.70
1:D:337:GLU:HG2	1:D:344:ILE:HD12	1.74	0.70
1:C:396:ALA:HB2	1:C:1085:ARG:HD2	1.73	0.70
1:C:500:THR:O	1:C:504:ILE:HD12	1.91	0.70
1:B:717:ASN:HD22	1:B:717:ASN:H	1.40	0.70
1:C:504:ILE:HG21	1:C:1042:MET:CE	2.10	0.69
1:C:823:HIS:HD2	1:C:824:LEU:N	1.90	0.69
1:B:644:ARG:HH11	1:B:647:ASN:ND2	1.89	0.69
1:B:869:GLY:O	1:B:871:TYR:N	2.26	0.69
1:C:334:THR:HG23	1:C:406:ARG:CZ	2.22	0.69
1:B:540:GLY:H	1:B:543:GLN:HE21	1.40	0.68
1:B:864:HIS:CD2	1:B:866:MET:H	2.09	0.68
1:A:335:ILE:HD11	1:A:374:ILE:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:LEU:HD23	1:C:496:ARG:HE	1.58	0.68
1:B:775:THR:HG23	1:B:861:ILE:HD13	1.75	0.68
1:B:719:THR:HG22	1:B:721:GLU:N	2.07	0.68
1:C:53:PHE:CD2	1:C:63:THR:HB	2.29	0.68
1:D:156:ARG:HG2	1:D:166:VAL:HG11	1.76	0.68
1:D:453:ARG:NE	2:D:2001:COA:O8A	2.27	0.67
1:C:823:HIS:HD2	1:C:824:LEU:H	1.42	0.67
1:C:311:GLU:HB2	1:C:323:ILE:HG22	1.75	0.67
1:B:1049:GLU:HG2	1:B:1059:ILE:HG13	1.76	0.67
1:C:309:THR:HG21	1:C:330:GLN:NE2	2.09	0.67
1:D:252:ASP:HA	1:D:351:VAL:HG13	1.77	0.67
1:D:408:ASP:HB2	1:D:428:LYS:HB3	1.77	0.67
1:D:335:ILE:O	1:D:339:VAL:HG23	1.95	0.67
1:B:917:MET:HG2	1:B:944:VAL:CG2	2.25	0.66
1:A:44:ASN:ND2	1:A:45:ARG:H	1.90	0.66
1:B:960:ASN:HD22	1:B:963:LEU:H	1.43	0.66
1:C:569:THR:OG1	1:C:798:VAL:HG23	1.95	0.66
1:B:873:ASN:HD22	1:B:873:ASN:H	1.43	0.66
1:D:1032:LEU:HD13	1:D:1052:ILE:HA	1.78	0.66
1:A:309:THR:HB	1:A:326:ASN:ND2	2.09	0.66
1:C:731:GLU:OE1	1:C:763:VAL:HB	1.95	0.66
1:B:719:THR:CG2	1:B:721:GLU:H	2.08	0.66
1:D:44:ASN:HD22	1:D:45:ARG:H	1.42	0.66
1:A:250:ILE:HD11	1:A:344:ILE:HG23	1.78	0.66
1:B:644:ARG:HD2	1:B:647:ASN:HD21	1.61	0.65
1:B:284:SER:HB2	1:B:285:PRO:HD2	1.78	0.65
1:C:864:HIS:CD2	1:C:866:MET:H	2.08	0.65
1:A:525:GLU:HB3	1:A:840:THR:HG23	1.79	0.65
1:D:116:PRO:HB2	1:D:122:SER:HA	1.78	0.65
1:A:249:VAL:HG11	1:A:299:MET:HG2	1.76	0.65
1:C:241:ASN:HB2	1:C:477:THR:OG1	1.95	0.65
1:C:866:MET:HE1	1:C:871:TYR:HA	1.77	0.65
1:C:1044:ASN:ND2	1:C:1044:ASN:H	1.92	0.65
1:D:651:TYR:HD2	1:D:651:TYR:H	1.43	0.65
1:D:949:LYS:HB3	1:D:951:GLU:HG2	1.78	0.64
1:B:641:MET:HE2	1:B:671:ILE:HG13	1.77	0.64
1:A:898:ASN:HD21	1:A:904:ILE:H	1.43	0.64
2:D:2001:COA:H10	2:D:2001:COA:O2A	1.97	0.64
1:B:1000:GLY:H	1:B:1001:PRO:HD3	1.62	0.64
1:B:575:GLN:HG3	1:B:580:THR:OG1	1.98	0.64
1:A:783:TYR:CE1	1:A:808:PRO:HG2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:HIS:H	1:B:145:HIS:HD2	1.45	0.64
1:D:58:GLU:OE1	1:D:346:LYS:NZ	2.30	0.64
1:B:543:GLN:HE22	1:B:636:ASN:CA	2.08	0.64
1:B:570:PHE:O	1:B:574:HIS:CE1	2.47	0.63
1:A:69:ASN:HD22	1:A:72:LYS:HE2	1.63	0.63
1:A:363:GLN:O	1:A:366:ASP:HB2	1.98	0.63
1:A:1044:ASN:HA	1:A:1062:LEU:CD2	2.27	0.63
1:A:1044:ASN:HA	1:A:1062:LEU:HD23	1.81	0.63
1:B:802:SER:OG	1:B:809:SER:HB2	1.98	0.63
1:C:309:THR:HG21	1:C:330:GLN:HE22	1.63	0.63
1:A:675:ARG:HA	1:A:701:GLU:HB3	1.81	0.63
1:D:451:ARG:NH2	2:D:2001:COA:H62	2.08	0.63
1:C:263:ARG:HH11	1:C:336:THR:HB	1.61	0.63
1:C:680:LEU:HD11	1:C:952:ILE:HG22	1.81	0.63
1:D:334:THR:HG21	1:D:430:SER:OG	1.98	0.63
1:B:720:LEU:HD11	1:B:758:GLU:HG3	1.80	0.63
1:B:493:SER:O	1:B:495:ASP:N	2.31	0.63
1:B:306:ASN:HD22	1:B:307:ALA:N	1.97	0.63
1:A:879:LYS:HG2	1:A:884:GLY:HA3	1.79	0.63
1:A:251:GLY:HA3	1:A:257:ILE:HG13	1.81	0.63
1:C:881:LEU:HD12	1:C:882:GLY:H	1.63	0.63
1:D:567:ASP:OD2	1:D:569:THR:OG1	2.16	0.63
1:B:288:ARG:NH1	1:B:288:ARG:HG3	2.09	0.62
1:D:42:VAL:HG11	1:D:49:ALA:HA	1.79	0.62
1:C:927:ASP:H	1:C:930:SER:HB3	1.63	0.62
1:C:575:GLN:HG3	1:C:580:THR:OG1	1.99	0.62
1:B:306:ASN:HD22	1:B:307:ALA:H	1.46	0.62
1:A:309:THR:HB	1:A:326:ASN:HD21	1.64	0.62
1:A:130:ARG:HH12	1:A:134:GLU:HG2	1.63	0.62
1:B:814:TYR:CE2	1:B:828:ILE:HG12	2.35	0.62
1:B:377:ARG:HH11	1:B:377:ARG:HG3	1.64	0.62
1:B:543:GLN:NE2	1:B:636:ASN:HA	2.11	0.62
1:D:513:PRO:O	1:D:515:ASN:HB2	1.98	0.62
1:A:615:ALA:HA	1:A:619:LEU:HD12	1.82	0.61
1:B:263:ARG:HG2	1:B:278:ALA:HB2	1.81	0.61
1:B:269:ARG:NH1	1:B:269:ARG:HB2	2.14	0.61
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.12	0.61
1:C:924:ASN:HB2	1:C:926:LEU:HD21	1.81	0.61
1:C:811:ASN:H	1:C:811:ASN:HD22	1.46	0.61
1:D:730:LEU:HA	1:D:733:GLU:HB2	1.83	0.61
1:B:536:LYS:O	1:B:538(A):SER:OG	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HD11	1:A:298:LEU:HB2	1.82	0.61
1:D:701:GLU:HG3	1:D:737:ILE:HB	1.81	0.61
1:A:394:ILE:O	1:A:415:GLY:HA2	2.00	0.61
1:C:63:THR:OG1	1:C:80:ALA:HA	2.00	0.61
1:C:593:LYS:O	1:C:597:VAL:HG23	2.00	0.61
1:B:376:CYS:HB3	1:B:462:LEU:HD13	1.82	0.61
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.36	0.61
1:C:509:ILE:HG21	1:C:1091:ASP:HB2	1.83	0.61
1:C:823:HIS:CD2	1:C:824:LEU:N	2.68	0.60
1:B:403:PHE:O	1:B:442:LYS:HE3	2.01	0.60
1:B:143:LEU:H	1:B:143:LEU:HD12	1.66	0.60
1:B:644:ARG:NH1	1:B:647:ASN:HD21	1.95	0.60
1:B:828:ILE:O	1:B:832:GLU:HG2	2.01	0.60
1:A:331:VAL:HG12	1:A:428:LYS:HD2	1.83	0.60
1:D:335:ILE:HG23	1:D:373:ALA:HB3	1.84	0.60
1:B:537:ILE:HA	1:B:538(B):PHE:CD1	2.37	0.60
1:C:805:THR:HG23	1:C:854:ILE:HD13	1.83	0.60
1:A:662:PHE:HA	1:A:1008:ILE:HD13	1.84	0.60
1:C:870:GLN:O	1:C:871:TYR:C	2.40	0.60
1:B:306:ASN:ND2	1:B:348:GLN:HG3	2.17	0.60
1:C:438:GLN:O	1:C:442:LYS:HG3	2.02	0.60
1:C:378:ILE:HG22	1:C:426:LEU:HD12	1.82	0.60
1:A:917:MET:HG2	1:A:944:VAL:HG21	1.84	0.60
1:A:960:ASN:HB3	1:A:963:LEU:HB3	1.83	0.60
1:C:823:HIS:CD2	1:C:824:LEU:H	2.19	0.59
1:D:517:GLU:HB2	1:D:847:ASP:OD1	2.02	0.59
1:D:404:GLY:O	1:D:431:THR:HA	2.02	0.59
1:B:69:ASN:O	1:B:72:LYS:HG2	2.03	0.59
1:B:606:MET:HE1	1:B:671:ILE:CD1	2.31	0.59
1:D:86:VAL:O	1:D:87:GLY:O	2.21	0.59
1:D:700:SER:H	1:D:736:HIS:HD2	1.50	0.59
1:B:1092:GLU:O	1:B:1093:ASN:CB	2.49	0.59
1:A:335:ILE:HD11	1:A:374:ILE:CA	2.33	0.59
1:B:772:THR:HG22	1:B:783:TYR:CE2	2.38	0.59
1:B:537:ILE:C	1:B:538(A):SER:H	2.05	0.59
1:A:99:ILE:HG12	1:A:127:PHE:HB2	1.85	0.59
1:A:626:ARG:O	1:A:630:LEU:HB2	2.03	0.58
1:B:952:ILE:HG22	1:B:952:ILE:O	2.03	0.58
1:B:512:PHE:CD2	1:B:513:PRO:HD2	2.38	0.58
1:B:251:GLY:O	1:B:306:ASN:N	2.33	0.58
1:C:337:GLU:HG2	1:C:342:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ASN:HB3	1:B:357(A):PHE:HE1	1.69	0.58
1:A:116:PRO:HB2	1:A:122:SER:HA	1.85	0.58
1:D:600:ASP:HB3	1:D:825:ARG:HD3	1.85	0.58
1:B:917:MET:SD	1:B:921:MET:CE	2.92	0.58
1:A:527:ALA:HB2	1:A:840:THR:HB	1.84	0.58
1:B:606:MET:HE1	1:B:671:ILE:HD11	1.86	0.58
1:D:385:ASN:O	1:D:388:MET:HG2	2.03	0.58
1:D:104:ASP:O	1:D:108:GLN:HG2	2.03	0.58
1:B:743:MET:HG3	1:B:907:VAL:HG13	1.86	0.58
1:A:494:LEU:H	1:A:494:LEU:HD12	1.68	0.58
1:B:856:SER:HB2	1:B:857:PRO:HD2	1.86	0.58
1:B:1000:GLY:N	1:B:1001:PRO:HD3	2.19	0.58
1:B:51:ARG:HH12	1:B:55:ALA:HB2	1.68	0.57
1:A:517:GLU:HB3	1:A:519:ARG:HH21	1.69	0.57
1:C:116:PRO:HB2	1:C:122:SER:HA	1.85	0.57
1:B:825:ARG:CG	1:B:825:ARG:HH11	2.05	0.57
1:C:626:ARG:HG2	1:C:630:LEU:HD12	1.86	0.57
1:D:278:ALA:HB3	1:D:335:ILE:HG22	1.85	0.57
1:B:537:ILE:O	1:B:538(A):SER:N	2.37	0.57
1:D:710:ILE:HD13	1:D:720:LEU:HD13	1.85	0.57
1:C:852:SER:OG	1:C:854:ILE:HG12	2.04	0.57
1:C:932:ILE:O	1:C:936:TYR:CE2	2.57	0.57
1:C:495:ASP:O	1:C:499:LYS:HD2	2.03	0.57
1:B:622:ASN:HD22	1:B:623:PRO:CD	2.17	0.57
1:B:773:HIS:C	1:B:775:THR:H	2.07	0.57
1:A:244:HIS:HD2	1:A:265:CYS:HB2	1.69	0.57
1:B:701:GLU:HG2	1:B:739:ALA:HB2	1.86	0.57
1:A:543:GLN:HA	1:A:546:ASP:HB2	1.87	0.57
1:B:164:LEU:HD21	1:B:294:ALA:HB1	1.85	0.57
1:B:960:ASN:ND2	1:B:963:LEU:H	2.02	0.57
1:C:991:ARG:O	1:C:995:GLU:HG2	2.05	0.57
1:A:920:TYR:O	1:A:924:ASN:ND2	2.37	0.57
1:A:445:ARG:HH21	1:C:54:ARG:HB3	1.70	0.56
1:C:513:PRO:HD3	4:C:2000:BTI:H11	1.86	0.56
1:A:438:GLN:O	1:A:442:LYS:HG3	2.05	0.56
1:B:1005:GLN:O	1:B:1009:SER:HB2	2.05	0.56
1:B:331:VAL:HG23	1:B:332:GLU:OE1	2.05	0.56
1:B:64:VAL:HG22	1:B:82:GLU:HB2	1.86	0.56
1:C:241:ASN:HB3	1:C:479:LYS:HD3	1.87	0.56
1:B:269:ARG:HH11	1:B:269:ARG:HB2	1.69	0.56
1:A:578:LEU:HD11	1:A:842:ARG:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:820:PHE:HB3	1:C:821:PRO:HD2	1.87	0.56
1:B:41:LEU:HB2	1:B:111:VAL:HG11	1.86	0.56
1:C:700:SER:H	1:C:736:HIS:HD2	1.52	0.56
1:D:448:ARG:HB2	2:D:2001:COA:H21	1.88	0.56
1:A:685:GLN:HA	1:A:977:ARG:HD2	1.87	0.56
1:C:496:ARG:HH11	1:C:1052:ILE:CD1	2.17	0.56
1:B:288:ARG:CG	1:B:288:ARG:HH11	2.12	0.56
1:C:881:LEU:HB2	1:C:884:GLY:H	1.71	0.55
1:B:917:MET:SD	1:B:921:MET:HE1	2.46	0.55
1:B:811:ASN:H	1:B:811:ASN:HD22	1.52	0.55
1:D:783:TYR:CE1	1:D:808:PRO:HG2	2.41	0.55
1:D:783:TYR:O	1:D:786:ALA:N	2.35	0.55
1:A:144:GLU:CD	1:A:144:GLU:H	2.09	0.55
1:B:879:LYS:HG3	1:B:884:GLY:HA2	1.89	0.55
1:A:391:THR:HG23	1:A:418:ILE:O	2.06	0.55
1:B:638:LEU:HD22	1:B:672:ASP:HB3	1.87	0.55
1:B:661:LYS:NZ	1:B:1004:GLU:OE2	2.32	0.55
1:C:357:LEU:HA	1:C:360:ILE:HD12	1.89	0.55
1:C:311:GLU:OE1	1:C:326:ASN:ND2	2.30	0.55
1:B:672:ASP:HA	1:B:698:LYS:HD2	1.87	0.55
1:C:780:LEU:HD13	1:B:778:ASN:ND2	2.22	0.55
1:D:496:ARG:NE	1:D:1052:ILE:HG21	2.09	0.55
1:C:39:LYS:HG3	1:C:62:SER:HB3	1.87	0.55
1:D:240:ASP:C	1:D:242:PRO:HD3	2.26	0.55
1:A:968:LEU:C	1:A:970:GLY:H	2.08	0.55
1:D:533:SER:HB3	1:D:536:LYS:HB2	1.89	0.55
1:A:440:GLU:O	1:A:444:VAL:HG13	2.07	0.54
1:A:525:GLU:HB3	1:A:840:THR:CG2	2.37	0.54
1:C:760:LYS:CD	1:C:768:ILE:HD12	2.37	0.54
1:C:284:SER:HB2	1:C:285:PRO:HD2	1.89	0.54
1:D:468:ASN:OD1	1:D:470:LYS:HG2	2.07	0.54
1:B:556:TRP:HA	1:B:559:LYS:HD3	1.88	0.54
1:C:672:ASP:HA	1:C:698:LYS:HD2	1.90	0.54
1:C:519:ARG:HB2	1:C:520:PRO:HD2	1.88	0.54
1:B:622:ASN:HD22	1:B:623:PRO:HD2	1.71	0.54
1:C:370:LEU:O	1:C:432:HIS:HE1	1.91	0.54
1:A:252:ASP:O	1:A:305:VAL:HG22	2.07	0.54
1:A:145:HIS:CE1	1:A:304:TYR:HA	2.42	0.54
1:B:720:LEU:O	1:B:724:VAL:HG23	2.07	0.54
1:B:1081:ASN:N	1:B:1081:ASN:HD22	2.04	0.54
1:D:679:SER:HB3	1:D:909:PRO:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:ARG:HD2	1:B:647:ASN:ND2	2.22	0.54
1:C:924:ASN:HB2	1:C:926:LEU:HD22	1.90	0.54
1:B:522:PRO:HA	1:B:524:TYR:HE1	1.72	0.54
1:D:330:GLN:O	1:D:333:HIS:ND1	2.32	0.54
1:B:563:VAL:HG21	1:B:787:ILE:HG12	1.89	0.54
1:C:359:GLU:CD	1:C:359:GLU:H	2.10	0.54
1:A:938:LEU:O	1:A:939:ASP:O	2.25	0.54
1:C:931:VAL:O	1:C:935:GLY:HA3	2.08	0.53
1:A:586:ASP:OD1	1:A:1035:THR:OG1	2.25	0.53
1:C:622:ASN:HD22	1:C:623:PRO:HD2	1.74	0.53
1:A:574:HIS:HD2	1:A:580:THR:HA	1.73	0.53
1:B:45:ARG:NH2	1:B:411:ASP:OD2	2.40	0.53
1:B:675:ARG:HA	1:B:701:GLU:HB3	1.89	0.53
1:B:239:ILE:HG21	1:B:313:LEU:HD23	1.89	0.53
1:D:541:THR:HA	1:D:544:LEU:HB2	1.89	0.53
1:B:960:ASN:HD21	1:B:962:ASP:HB2	1.73	0.53
1:B:898:ASN:HD22	1:B:906:LYS:HE3	1.67	0.53
1:D:572:ASP:OD1	1:D:807:GLN:NE2	2.41	0.53
1:D:496:ARG:HE	1:D:1052:ILE:CG2	2.12	0.53
1:B:575:GLN:NE2	1:B:610:ALA:H	2.07	0.53
1:D:704:ILE:HD11	1:D:727:ALA:HB2	1.91	0.53
1:D:44:ASN:HD22	1:D:45:ARG:N	2.04	0.53
1:D:243:LYS:O	1:D:313:LEU:HA	2.09	0.53
1:D:414:GLN:O	1:D:414:GLN:HG3	2.09	0.53
1:C:52:ILE:HG12	1:C:115:HIS:CG	2.44	0.53
1:C:48:ILE:O	1:C:52:ILE:HD12	2.08	0.53
1:B:328:ARG:HD3	1:B:329:VAL:O	2.09	0.53
1:B:504:ILE:HD13	1:B:1042:MET:HE2	1.91	0.53
1:A:246:GLU:HG2	1:A:311:GLU:HG2	1.90	0.53
1:D:571:ARG:HH11	1:D:575:GLN:NE2	2.06	0.53
1:D:810:ALA:HB3	1:D:831:MET:HE3	1.90	0.53
1:B:866:MET:SD	1:B:874:LEU:HD22	2.49	0.52
1:C:280:SER:OG	1:C:283:LEU:HG	2.08	0.52
1:D:445:ARG:NH1	1:B:54:ARG:HB3	2.25	0.52
1:C:263:ARG:HH21	1:C:330:GLN:HE21	1.56	0.52
1:A:444:VAL:HG12	1:A:466:MET:HB3	1.91	0.52
1:C:746:LEU:HD23	1:C:861:ILE:HG22	1.90	0.52
1:B:263:ARG:HH21	1:B:330:GLN:HE22	1.58	0.52
1:C:598:PHE:O	1:C:637:VAL:HG21	2.09	0.52
1:D:641:MET:HE2	1:D:671:ILE:HG13	1.91	0.52
1:C:1006:ASP:HB3	1:C:1017:TYR:OH	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:HG22	1:A:374:ILE:HG23	1.91	0.52
1:C:897:VAL:HG23	1:C:914:VAL:HG13	1.92	0.52
1:D:94:GLU:HA	1:D:97:LEU:HB2	1.91	0.52
1:A:418:ILE:HD12	1:A:418:ILE:N	2.21	0.52
1:C:48:ILE:O	1:C:52:ILE:CD1	2.57	0.52
1:B:263:ARG:NH2	1:B:330:GLN:NE2	2.58	0.52
1:C:949:LYS:HB3	1:C:951:GLU:HG3	1.91	0.52
1:B:281:VAL:HG22	1:B:372:TYR:CE2	2.45	0.52
1:D:661:LYS:HB3	1:D:1008:ILE:HD13	1.92	0.52
1:D:339:VAL:O	1:D:369:THR:HA	2.09	0.52
1:B:118:TYR:CE2	1:B:331:VAL:HG12	2.45	0.52
1:B:930:SER:HA	1:B:933:THR:HB	1.91	0.52
1:D:360:ILE:O	1:D:361:ASN:C	2.47	0.52
1:C:239:ILE:HD12	1:C:313:LEU:HD23	1.91	0.52
1:C:935:GLY:HA2	1:C:938:LEU:HD12	1.92	0.52
1:C:328:ARG:HD2	1:C:329:VAL:O	2.10	0.52
1:C:986:ASP:OD1	1:C:988:GLU:HG2	2.10	0.52
1:C:802:SER:OG	1:C:809:SER:HB2	2.10	0.52
1:D:484:THR:HB	1:D:487:LEU:HD22	1.92	0.52
1:C:864:HIS:CD2	1:C:866:MET:HB2	2.45	0.51
1:B:541:THR:HB	1:B:638:LEU:HG	1.92	0.51
1:C:638:LEU:HD22	1:C:672:ASP:HB3	1.93	0.51
2:D:2001:COA:H2A	1:B:77:ARG:NH2	2.26	0.51
1:D:1052:ILE:HD11	1:D:1058:LEU:HD13	1.92	0.51
1:B:1060:ILE:HG12	1:B:1080:MET:HG3	1.93	0.51
1:A:90:LEU:HD21	1:A:101:ARG:HD2	1.92	0.51
1:D:162:ALA:O	1:D:163:ASP:CB	2.55	0.51
1:A:1004:GLU:HA	1:A:1007:ILE:HD12	1.93	0.51
1:A:690:ASN:HB2	1:A:735:PHE:CZ	2.46	0.51
1:C:661:LYS:HG2	1:C:1008:ILE:HG23	1.92	0.51
1:C:781:LEU:HD13	1:B:816:ALA:HB1	1.93	0.51
1:D:274:VAL:HG12	1:D:275:VAL:HG23	1.92	0.51
1:B:377:ARG:HD2	1:B:425:LEU:HD11	1.93	0.51
1:B:507:VAL:O	1:B:511:GLY:HA2	2.11	0.51
1:C:624:TRP:CD2	1:C:1005:GLN:HG2	2.46	0.51
1:B:519:ARG:NH2	1:B:847:ASP:OD2	2.44	0.51
1:A:357:LEU:HD22	1:A:362:MET:HG3	1.92	0.51
1:A:654:TYR:HB3	1:A:658:VAL:CG2	2.41	0.51
1:A:858:ASN:OD1	1:A:860:GLU:HG2	2.11	0.51
1:B:1059:ILE:H	1:B:1081:ASN:HD21	1.59	0.51
1:B:263:ARG:NH2	1:B:330:GLN:HE22	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:LEU:HD12	1:A:1076:ILE:HG23	1.93	0.51
1:D:568:THR:HG22	1:D:605:GLU:HB3	1.92	0.51
1:C:661:LYS:HG2	1:C:1008:ILE:CG2	2.41	0.51
1:B:252:ASP:HB3	1:B:357:LEU:HD13	1.92	0.51
1:B:267:VAL:HG11	1:B:275:VAL:HB	1.93	0.51
1:A:853:ASP:OD2	1:A:872:SER:HB2	2.12	0.51
1:C:65:ALA:HB3	1:C:83:SER:HB3	1.92	0.50
1:C:263:ARG:HH21	1:C:330:GLN:NE2	2.09	0.50
1:B:994:LEU:HD21	1:B:1017:TYR:HE2	1.75	0.50
1:C:504:ILE:CG2	1:C:1042:MET:HE2	2.13	0.50
1:B:562:ASP:OD2	1:B:825:ARG:HD3	2.10	0.50
1:B:408:ASP:HB2	1:B:428:LYS:HG3	1.92	0.50
1:A:42:VAL:HG11	1:A:49:ALA:HA	1.93	0.50
1:D:621:GLU:HB2	1:D:1031:SER:HB2	1.93	0.50
1:C:574:HIS:CD2	1:C:580:THR:HA	2.32	0.50
1:D:445:ARG:HD3	1:B:54:ARG:HA	1.92	0.50
1:D:999:GLN:HG2	1:D:1001:PRO:HD2	1.93	0.50
1:C:269:ARG:HG3	1:C:270:ARG:HG2	1.93	0.50
1:C:641:MET:HG2	1:C:671:ILE:HD12	1.94	0.50
1:A:898:ASN:ND2	1:A:904:ILE:H	2.09	0.50
1:D:1013:TYR:HB3	1:D:1016:VAL:HB	1.94	0.50
1:B:512:PHE:CG	1:B:513:PRO:HD2	2.46	0.50
1:C:541:THR:HG21	1:C:602:PHE:HA	1.92	0.50
1:B:418:ILE:N	1:B:418:ILE:HD12	2.27	0.50
1:C:42:VAL:HG11	1:C:49:ALA:HA	1.92	0.50
1:B:266:SER:O	1:B:478:THR:HA	2.11	0.50
1:C:873:ASN:HD22	1:C:873:ASN:H	1.59	0.50
1:B:269:ARG:HG3	1:B:270:ARG:N	2.27	0.50
1:A:441:GLU:OE2	1:C:58:GLU:HB3	2.12	0.50
1:A:641:MET:HB3	1:A:671:ILE:HD12	1.94	0.50
1:C:867:PRO:HD2	1:C:870:GLN:HE21	1.76	0.50
1:A:90:LEU:HD11	1:A:101:ARG:HD3	1.92	0.50
1:B:337:GLU:HG2	1:B:342:ILE:O	2.11	0.50
1:D:442:LYS:HE3	1:B:58:GLU:OE2	2.12	0.50
1:B:381:GLU:HA	1:B:389:PRO:HA	1.94	0.50
1:C:1033:LEU:HD22	1:C:1050:ILE:HG12	1.94	0.50
1:C:717:ASN:HD22	1:C:717:ASN:H	1.59	0.50
1:A:70:GLU:HG3	1:A:92:PRO:HB3	1.93	0.50
1:D:50:ILE:O	1:D:54:ARG:HG3	2.11	0.50
1:B:1065:ILE:HG12	1:B:1076:ILE:HG12	1.95	0.49
1:C:1052:ILE:HD13	1:C:1058:LEU:HD21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ALA:HA	1:C:431:THR:O	2.12	0.49
1:B:506:ASN:HD22	1:B:1089:ILE:HG23	1.77	0.49
1:A:130:ARG:NH1	1:A:134:GLU:HG2	2.27	0.49
1:A:314:VAL:HG22	1:A:320:PHE:HB2	1.94	0.49
1:B:743:MET:CG	1:B:907:VAL:HG13	2.41	0.49
1:A:540:GLY:H	1:A:543:GLN:HE21	1.58	0.49
1:A:53:PHE:CZ	1:A:80:ALA:HB2	2.47	0.49
1:C:1076:ILE:HD11	1:C:1089:ILE:HG13	1.95	0.49
1:D:501:LEU:HB3	1:D:1078:TYR:CE1	2.47	0.49
1:C:652:LYS:O	1:C:654:TYR:CE1	2.66	0.49
1:D:651:TYR:N	1:D:651:TYR:CD2	2.79	0.49
1:A:1013:TYR:HB3	1:A:1016:VAL:HB	1.95	0.49
1:C:717(A):ILE:HG21	1:C:956:VAL:HG11	1.95	0.49
1:D:343:ASP:CG	1:D:346:LYS:HB2	2.33	0.49
1:D:701:GLU:HG2	1:D:739:ALA:HB2	1.94	0.49
1:B:434:ILE:HD12	1:B:435:SER:H	1.78	0.49
1:A:394:ILE:HG13	1:A:418:ILE:HD11	1.94	0.49
1:B:622:ASN:HD22	1:B:623:PRO:N	2.10	0.49
1:B:888:ASP:HA	1:B:891:LYS:HE3	1.93	0.49
1:B:542:LYS:HG3	1:B:631:ARG:HH12	1.77	0.49
1:A:278:ALA:CB	1:A:335:ILE:HG23	2.42	0.48
1:A:332:GLU:HA	1:A:375:GLN:NE2	2.27	0.48
1:A:664:GLN:O	1:A:668:LYS:HB2	2.13	0.48
1:B:259:HIS:HB3	1:B:296:ILE:HD11	1.94	0.48
1:A:90:LEU:HD21	1:A:101:ARG:CD	2.42	0.48
1:B:434:ILE:HD12	1:B:435:SER:N	2.28	0.48
1:B:370:LEU:O	1:B:432:HIS:CE1	2.66	0.48
1:D:251:GLY:HA2	1:D:256:ASN:O	2.14	0.48
1:C:289:GLN:OE1	1:C:293:ASP:OD2	2.31	0.48
1:B:641:MET:HE2	1:B:671:ILE:CG1	2.43	0.48
1:C:893:MET:O	1:C:897:VAL:HG22	2.12	0.48
1:D:379:THR:HG22	1:D:425:LEU:HA	1.95	0.48
1:B:1018:GLU:O	1:B:1022:GLN:HG2	2.14	0.48
1:D:1051:GLU:HB3	1:D:1057:ARG:HG2	1.96	0.48
1:B:646:SER:O	1:B:659:ILE:HD11	2.13	0.48
1:A:624:TRP:CZ2	1:A:1008:ILE:HD11	2.48	0.48
1:C:337:GLU:HG3	1:C:344:ILE:HG12	1.96	0.48
1:A:755:LEU:HD12	1:A:759:LEU:HD11	1.95	0.48
1:C:537:ILE:HD12	1:C:595:ALA:HB3	1.96	0.48
1:B:144:GLU:CD	1:B:144:GLU:H	2.17	0.48
1:B:85:LEU:HD21	1:B:88:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:LEU:HD13	1:D:323:ILE:HG13	1.95	0.48
1:A:371:GLY:HA3	1:A:434:ILE:HA	1.96	0.48
1:A:266:SER:HB2	1:A:476:TYR:HD2	1.77	0.48
1:B:606:MET:CE	1:B:607:TRP:HB2	2.44	0.48
1:B:145:HIS:CE1	1:B:304:TYR:HA	2.49	0.48
1:B:864:HIS:CD2	1:B:866:MET:HB2	2.49	0.48
1:C:621:GLU:HB2	1:C:1031:SER:HB3	1.95	0.48
1:D:143:LEU:H	1:D:143:LEU:HD23	1.79	0.48
1:D:606:MET:SD	1:D:606:MET:C	2.92	0.48
1:C:287:LEU:C	1:C:289:GLN:H	2.18	0.47
1:A:501:LEU:HB3	1:A:1078:TYR:CE1	2.49	0.47
1:B:614:VAL:HG13	1:B:618:PHE:HD1	1.79	0.47
1:A:83:SER:HB2	2:C:2001:COA:H61A	1.79	0.47
1:A:883:LEU:HD13	1:A:922:VAL:HG12	1.95	0.47
1:B:817:LEU:O	1:B:820:PHE:HB2	2.14	0.47
1:B:40:LEU:HB2	1:B:61:ILE:HG21	1.96	0.47
1:A:394:ILE:O	1:A:414:GLN:O	2.32	0.47
1:C:360:ILE:C	1:C:362:MET:H	2.18	0.47
1:B:993:LEU:O	1:B:997:GLU:HG3	2.14	0.47
1:C:526:LEU:HD13	1:C:526:LEU:O	2.14	0.47
1:A:817:LEU:HD12	1:A:824:LEU:HB2	1.95	0.47
1:C:814:TYR:CE2	1:C:828:ILE:HG23	2.49	0.47
1:B:72:LYS:O	1:B:77:ARG:HD3	2.15	0.47
1:D:571:ARG:HH11	1:D:575:GLN:HE22	1.59	0.47
1:C:927:ASP:OD1	1:C:927:ASP:N	2.48	0.47
1:A:999:GLN:HG2	1:A:1001:PRO:HD2	1.97	0.47
1:A:376:CYS:HB3	1:A:462:LEU:HD13	1.97	0.47
1:B:864:HIS:HD2	1:B:866:MET:N	2.06	0.47
1:C:760:LYS:HD2	1:C:768:ILE:HD12	1.96	0.47
1:C:47:GLU:OE1	1:C:428:LYS:NZ	2.47	0.47
1:B:747:LEU:HG	1:B:752:ALA:HB2	1.94	0.47
1:C:890:VAL:HG22	1:C:922:VAL:HG21	1.96	0.47
1:A:435:SER:OG	1:A:438:GLN:HG2	2.15	0.47
1:B:116:PRO:HB3	1:B:122:SER:HA	1.96	0.47
1:B:245:ILE:HD13	1:B:264:ASP:HA	1.97	0.47
1:C:543:GLN:OE1	1:C:636:ASN:HA	2.15	0.47
1:B:65:ALA:O	1:B:83:SER:HA	2.14	0.47
1:C:704:ILE:HD11	1:C:726:LEU:HB3	1.96	0.47
1:C:811:ASN:H	1:C:811:ASN:ND2	2.12	0.47
1:B:394:ILE:HD11	1:B:426:LEU:HD22	1.96	0.47
1:C:47:GLU:HA	1:C:50:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ILE:CD1	1:C:409:ALA:O	2.63	0.47
1:C:279:PRO:HD2	1:C:372:TYR:CD2	2.49	0.47
1:A:870:GLN:O	1:A:874:LEU:HB3	2.14	0.47
1:C:571:ARG:HH11	1:C:575:GLN:NE2	2.12	0.46
1:B:256:ASN:HB3	1:B:357(A):PHE:CE1	2.48	0.46
1:B:400:SER:O	1:B:407:LEU:HD11	2.15	0.46
1:D:390:ASP:OD1	1:D:456:LYS:HD2	2.15	0.46
1:A:136:ILE:CG2	1:A:137:LYS:N	2.79	0.46
1:C:622:ASN:HD21	1:C:624:TRP:HD1	1.63	0.46
1:C:398:ARG:NH2	1:C:451:ARG:NH1	2.63	0.46
1:D:88:SER:C	1:D:90:LEU:H	2.18	0.46
1:D:142:HIS:HB2	1:D:145:HIS:CD2	2.51	0.46
1:A:940:PHE:CE2	1:A:967:ILE:HA	2.50	0.46
1:B:345:VAL:O	1:B:348:GLN:HB3	2.14	0.46
1:D:70:GLU:HG3	1:D:92:PRO:HB3	1.96	0.46
1:C:870:GLN:O	1:C:873:ASN:N	2.48	0.46
1:B:571:ARG:HE	1:B:605:GLU:CD	2.18	0.46
1:B:373:ALA:HA	1:B:431:THR:O	2.14	0.46
1:C:53:PHE:HD2	1:C:63:THR:HB	1.79	0.46
1:A:690:ASN:O	1:A:694:GLN:HG2	2.15	0.46
1:D:566:THR:OG1	1:D:769:HIS:CE1	2.69	0.46
1:A:680:LEU:HD22	1:A:955:PRO:HB3	1.98	0.46
1:A:250:ILE:HD12	1:A:260:LEU:HD11	1.97	0.46
1:A:673:VAL:HG12	1:A:673:VAL:O	2.15	0.46
1:D:1078:TYR:HB2	1:D:1085:ARG:HB3	1.98	0.46
1:B:370:LEU:O	1:B:432:HIS:HE1	1.99	0.46
1:C:141:PRO:HB3	1:C:305:VAL:O	2.14	0.46
1:A:504:ILE:HG21	1:A:1042:MET:CE	2.45	0.46
1:C:881:LEU:C	1:C:883:LEU:H	2.18	0.46
1:A:149:PHE:HA	1:A:155:ALA:HB2	1.98	0.46
1:A:281:VAL:HB	1:A:474:GLY:HA3	1.98	0.46
1:A:597:VAL:HG13	1:A:827:ASP:HB3	1.97	0.46
1:B:647:ASN:HD22	1:B:647:ASN:H	1.64	0.46
1:A:738:LEU:HD21	1:A:759:LEU:HD13	1.97	0.46
1:D:266:SER:O	1:D:478:THR:HA	2.16	0.46
1:D:1024:ARG:HH21	1:D:1025:ASN:HD21	1.64	0.46
1:C:613:ASP:HB2	1:C:1013:TYR:CE2	2.51	0.46
1:B:55:ALA:HA	1:B:58:GLU:HG3	1.97	0.46
1:C:955:PRO:O	1:C:956:VAL:C	2.53	0.46
1:C:700:SER:N	1:C:736:HIS:HD2	2.14	0.46
1:A:329:VAL:HG22	1:A:348:GLN:HE22	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1058:LEU:HB2	1:C:1060:ILE:HD11	1.97	0.45
1:B:717:ASN:N	1:B:717:ASN:HD22	2.10	0.45
1:C:269:ARG:O	1:C:270:ARG:C	2.55	0.45
1:A:755:LEU:CD1	1:A:759:LEU:HD11	2.46	0.45
1:C:69:ASN:HD22	1:C:72:LYS:HE3	1.81	0.45
1:A:98:ASN:HD22	1:A:101:ARG:H	1.63	0.45
1:B:593:LYS:O	1:B:597:VAL:HG23	2.16	0.45
1:A:170:THR:HG22	1:A:171:ASP:H	1.81	0.45
1:B:279:PRO:HD3	1:B:369:THR:HG21	1.99	0.45
1:D:951:GLU:HB2	1:D:952:ILE:HD12	1.97	0.45
1:C:287:LEU:C	1:C:289:GLN:N	2.70	0.45
1:C:408:ASP:HB2	1:C:428:LYS:HB2	1.98	0.45
1:D:753:TYR:CD1	1:D:789:ALA:HB2	2.51	0.45
1:C:912:LYS:HD3	1:C:916:ASP:OD2	2.15	0.45
1:D:861:ILE:H	1:D:861:ILE:HG13	1.61	0.45
1:B:54:ARG:O	1:B:58:GLU:CG	2.61	0.45
1:D:567:ASP:O	1:D:605:GLU:N	2.44	0.45
1:B:371:GLY:HA2	1:B:434:ILE:O	2.16	0.45
1:D:590:ILE:HD11	1:D:838:TRP:CZ2	2.51	0.45
1:B:251:GLY:HA3	1:B:257:ILE:HG12	1.98	0.45
1:A:322:PHE:CE2	1:A:325:VAL:HG23	2.50	0.45
1:B:676:ILE:HD11	1:B:693:VAL:HG21	1.98	0.45
1:D:643:LEU:O	1:D:676:ILE:HA	2.16	0.45
1:B:529:ILE:HG21	1:B:589:ASN:O	2.17	0.45
1:B:241:ASN:HB3	1:B:477:THR:HG21	1.98	0.45
1:D:677:PHE:CB	1:D:703:THR:HB	2.41	0.45
1:B:537:ILE:C	1:B:538(A):SER:N	2.70	0.45
1:B:794:ILE:HD12	1:B:796:THR:HG23	1.98	0.45
1:A:479:LYS:HA	1:A:482:GLU:OE1	2.17	0.45
1:D:802:SER:OG	1:D:809:SER:HB2	2.17	0.45
1:A:1061:LYS:HB3	1:A:1079:ALA:HB3	1.97	0.45
1:B:615:ALA:HA	1:B:619:LEU:HB2	1.99	0.45
1:A:58:GLU:HG3	1:C:445:ARG:HG3	1.99	0.45
1:A:643:LEU:HD22	1:A:676:ILE:HG12	1.99	0.45
1:D:952:ILE:O	1:D:952:ILE:HG22	2.17	0.45
1:C:306:ASN:HA	1:C:351:VAL:HG11	1.98	0.45
1:B:39:LYS:CD	1:B:62:SER:HB2	2.47	0.45
1:A:283:LEU:HD22	1:A:287:LEU:HG	1.99	0.45
1:B:543:GLN:O	1:B:547:GLU:HG2	2.17	0.45
1:D:335:ILE:CG2	1:D:373:ALA:HB3	2.47	0.45
1:A:322:PHE:HE2	1:A:325:VAL:HG23	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1035:THR:HB	1:B:1036:PRO:HD3	1.99	0.45
1:A:590:ILE:HG12	1:A:837:TYR:CE2	2.52	0.45
1:A:638:LEU:HD22	1:A:672:ASP:HB2	1.99	0.45
1:D:555:GLU:O	1:D:559:LYS:HG3	2.17	0.45
1:D:335:ILE:HG23	1:D:373:ALA:CB	2.46	0.45
1:A:309:THR:HG21	1:A:330:GLN:HE22	1.81	0.45
1:A:346:LYS:HZ2	1:C:438:GLN:HE21	1.64	0.45
1:A:116:PRO:HG3	1:A:138:PHE:CZ	2.52	0.45
1:C:778:ASN:ND2	1:B:816:ALA:HB2	2.33	0.45
1:D:50:ILE:HG12	1:D:79:LYS:HG3	2.00	0.45
1:B:265:CYS:O	1:B:268:GLN:NE2	2.49	0.45
1:D:125:GLU:O	1:D:125:GLU:HG2	2.17	0.45
1:C:866:MET:HE2	1:C:871:TYR:CA	2.40	0.44
1:B:773:HIS:O	1:B:775:THR:N	2.50	0.44
1:C:693:VAL:CG1	1:C:700:SER:OG	2.65	0.44
1:A:504:ILE:HD13	1:A:1042:MET:CE	2.47	0.44
1:C:1070:GLU:HG3	1:C:1070:GLU:H	1.59	0.44
1:B:606:MET:SD	1:B:639:PHE:CD2	3.10	0.44
1:C:700:SER:H	1:C:736:HIS:CD2	2.33	0.44
1:D:993:LEU:C	1:D:995:GLU:H	2.20	0.44
1:A:435:SER:OG	1:A:438:GLN:CG	2.66	0.44
1:B:641:MET:CE	1:B:666:SER:HB3	2.48	0.44
1:D:568:THR:OG1	1:D:807:GLN:HG3	2.18	0.44
1:C:828:ILE:H	1:C:828:ILE:HG13	1.59	0.44
1:A:59:LEU:HD21	1:A:350:LEU:HD11	1.99	0.44
1:C:251:GLY:HA2	1:C:256:ASN:O	2.17	0.44
1:B:1007:ILE:O	1:B:1011:VAL:HG23	2.18	0.44
1:C:108:GLN:HG3	1:C:108:GLN:O	2.16	0.44
1:B:494:LEU:HB2	1:B:496:ARG:NH2	2.32	0.44
1:A:753:TYR:HB2	1:A:785:GLN:HB3	1.99	0.44
1:C:575:GLN:NE2	1:C:610:ALA:H	2.14	0.44
1:C:927:ASP:O	1:C:931:VAL:HG23	2.16	0.44
1:C:638:LEU:HD22	1:C:672:ASP:CB	2.47	0.44
1:D:501:LEU:HD22	1:D:1078:TYR:CD2	2.52	0.44
1:B:935:GLY:HA2	1:B:938:LEU:HD12	1.99	0.44
1:B:626:ARG:HG2	1:B:630:LEU:HD12	1.98	0.44
1:B:42:VAL:HG12	1:B:44:ASN:H	1.82	0.44
1:A:243:LYS:HG3	1:A:266:SER:OG	2.17	0.44
1:A:339:VAL:HG23	1:A:340:THR:HG23	1.98	0.44
1:A:248:GLN:HB2	1:A:263:ARG:HH12	1.81	0.44
1:D:68:SER:HB3	1:D:95:SER:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:LYS:HE2	1:B:767:PRO:HD3	1.97	0.44
1:A:550:PRO:HB2	1:A:736:HIS:CE1	2.53	0.44
1:A:901:PHE:HZ	1:A:917:MET:HG3	1.83	0.44
1:A:266:SER:HB2	1:A:476:TYR:CD2	2.52	0.44
1:A:242:PRO:O	1:A:477:THR:HB	2.18	0.44
1:C:422:TYR:O	1:C:423:ASP:C	2.56	0.44
1:C:496:ARG:HD2	1:C:1052:ILE:HD12	1.99	0.44
1:C:878:ALA:O	1:C:881:LEU:HA	2.18	0.44
1:A:968:LEU:C	1:A:970:GLY:N	2.71	0.44
1:C:71:ASP:HB3	1:C:74:SER:HB3	1.99	0.44
1:D:464:ASN:OD1	1:D:491:GLN:NE2	2.51	0.44
1:A:861:ILE:HD11	1:A:866:MET:O	2.18	0.44
1:B:560:GLN:OE1	1:B:825:ARG:NH2	2.51	0.44
1:B:550:PRO:HB2	1:B:736:HIS:CE1	2.52	0.44
1:C:874:LEU:O	1:C:878:ALA:HB2	2.17	0.44
1:B:493:SER:O	1:B:493:SER:OG	2.29	0.44
1:C:597:VAL:HG21	1:C:834:LEU:HG	2.00	0.44
1:D:241:ASN:N	1:D:242:PRO:CD	2.81	0.44
1:B:708:GLY:HA2	1:B:715:ARG:NH1	2.33	0.44
1:A:798:VAL:CG1	1:A:835:SER:HA	2.48	0.44
1:B:1059:ILE:N	1:B:1081:ASN:HD21	2.16	0.43
1:C:263:ARG:NH1	1:C:336:THR:HB	2.29	0.43
1:D:47:GLU:HG2	1:D:425:LEU:HD21	2.00	0.43
1:C:583:ARG:HG2	1:C:619:LEU:HD13	2.00	0.43
1:D:241:ASN:N	1:D:242:PRO:HD3	2.32	0.43
1:D:655:PRO:HG2	1:D:985:VAL:HG23	2.00	0.43
1:D:977:ARG:HH21	1:D:979:GLY:HA3	1.83	0.43
1:B:760:LYS:HG2	1:B:768:ILE:HD12	1.99	0.43
1:B:380:THR:HG23	1:B:426:LEU:HD21	2.00	0.43
1:B:94:GLU:HA	1:B:97:LEU:HD12	2.00	0.43
1:D:248:GLN:NE2	1:D:308:GLY:O	2.51	0.43
1:B:167:ILE:HG13	1:B:168:PRO:HD2	2.00	0.43
1:C:470:LYS:O	1:C:476:TYR:HB3	2.18	0.43
1:B:516:VAL:CG1	1:B:517:GLU:N	2.65	0.43
1:A:346:LYS:NZ	1:C:438:GLN:HE21	2.16	0.43
1:A:90:LEU:HD22	1:A:94:GLU:CG	2.48	0.43
1:A:781:LEU:HD12	1:D:780:LEU:HD12	2.00	0.43
1:B:377:ARG:NH1	1:B:377:ARG:HG3	2.31	0.43
1:C:313:LEU:HB2	1:C:323:ILE:HD13	1.99	0.43
1:B:142:HIS:CE1	1:B:305:VAL:HG21	2.53	0.43
1:B:394:ILE:HG13	1:B:418:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:THR:HB	1:B:326:ASN:HB2	1.99	0.43
1:C:743:MET:SD	1:C:907:VAL:HG13	2.58	0.43
1:C:540:GLY:H	1:C:543:GLN:HG2	1.83	0.43
1:A:500:THR:HG22	1:A:504:ILE:HD11	2.01	0.43
1:B:927:ASP:O	1:B:931:VAL:HG23	2.18	0.43
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.99	0.43
1:B:513:PRO:O	1:B:515:ASN:HB2	2.19	0.43
1:B:977:ARG:HA	1:B:978:PRO:HD3	1.91	0.43
1:D:673:VAL:HG22	1:D:699:ILE:HD12	2.00	0.43
1:B:624:TRP:HB3	1:B:1005:GLN:HE22	1.83	0.43
1:B:118:TYR:CZ	1:B:331:VAL:HG12	2.54	0.43
1:A:710:ILE:HD13	1:A:755:LEU:HD23	2.01	0.43
1:D:90:LEU:HD21	1:D:101:ARG:NH2	2.34	0.43
1:B:413:PHE:O	1:B:415:GLY:N	2.52	0.43
1:B:711:LEU:HG	1:B:751:ALA:HB2	2.01	0.43
1:A:771:HIS:CD2	1:A:771:HIS:C	2.91	0.43
1:A:380:THR:HG22	1:A:426:LEU:HD11	2.01	0.43
1:B:606:MET:HE1	1:B:671:ILE:HD13	1.99	0.43
1:A:1076:ILE:O	1:A:1086:ARG:HA	2.18	0.43
1:B:115:HIS:HA	1:B:116:PRO:HD3	1.72	0.43
1:B:126:GLN:HA	1:B:129:ARG:HH11	1.84	0.43
1:C:964:GLN:O	1:C:968:LEU:HG	2.19	0.43
1:C:800:SER:O	1:C:842:ARG:NH1	2.52	0.43
1:A:294:ALA:HA	1:A:297:GLN:HB2	2.00	0.43
1:A:399:SER:HA	1:A:450:MET:SD	2.59	0.43
1:A:755:LEU:O	1:A:759:LEU:HG	2.18	0.43
1:B:309:THR:O	1:B:325:VAL:HA	2.19	0.43
1:A:38:LYS:HB2	1:A:112:ASP:OD1	2.19	0.43
1:C:609:GLY:HA2	1:C:644:ARG:NH1	2.34	0.43
1:A:1002:VAL:HG13	1:A:1006:ASP:HB2	2.01	0.43
1:C:902:GLY:O	1:C:903:ASP:HB3	2.19	0.43
1:A:239:ILE:HG21	1:A:313:LEU:HD21	2.01	0.42
1:B:541:THR:CB	1:B:638:LEU:HG	2.49	0.42
1:B:44:ASN:HD22	1:B:45:ARG:H	1.67	0.42
1:B:860:GLU:HA	1:B:863:GLN:NE2	2.34	0.42
1:D:620:LYS:HD3	1:D:1023:THR:HG21	2.00	0.42
1:B:531:THR:HA	1:B:592:SER:OG	2.19	0.42
1:B:716:SER:OG	1:B:717(A):ILE:HD12	2.18	0.42
1:B:49:ALA:O	1:B:53:PHE:CD1	2.72	0.42
1:C:565:LEU:O	1:C:565:LEU:HD23	2.20	0.42
1:A:444:VAL:HG12	1:A:466:MET:CB	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:VAL:HG12	1:D:274:VAL:HB	2.00	0.42
1:D:490:ILE:O	1:D:491:GLN:C	2.58	0.42
1:D:742:ASP:HB3	1:D:771:HIS:O	2.19	0.42
1:D:787:ILE:HA	1:D:822:ARG:HH21	1.84	0.42
1:D:645:ALA:HB1	1:D:685:GLN:O	2.19	0.42
1:A:570:PHE:HB2	1:A:606:MET:CB	2.45	0.42
1:A:287:LEU:HD22	1:A:318:ASP:OD1	2.18	0.42
1:B:738:LEU:HD23	1:B:768:ILE:HG12	2.01	0.42
1:A:889:GLU:O	1:A:893:MET:HB2	2.20	0.42
1:B:651:TYR:CZ	1:B:652:LYS:HD3	2.54	0.42
1:A:766:LEU:HA	1:A:767:PRO:HD2	1.87	0.42
1:B:802:SER:HA	1:B:806:SER:HB3	2.02	0.42
1:D:783:TYR:O	1:D:784:LYS:C	2.57	0.42
1:B:45:ARG:HH22	1:B:411:ASP:CG	2.22	0.42
1:B:281:VAL:HG22	1:B:372:TYR:HE2	1.84	0.42
1:C:647:ASN:O	1:C:649:VAL:N	2.47	0.42
1:D:276:GLU:OE2	1:D:332:GLU:HB3	2.19	0.42
1:A:326:ASN:HA	1:A:327:PRO:HD3	1.76	0.42
1:D:360:ILE:O	1:D:362:MET:N	2.53	0.42
1:C:750:LYS:HE2	1:B:820:PHE:CE2	2.54	0.42
1:B:571:ARG:NE	1:B:605:GLU:OE2	2.52	0.42
1:A:334:THR:HA	1:A:337:GLU:OE2	2.20	0.42
1:D:522:PRO:HG2	1:D:524:TYR:CZ	2.55	0.42
1:B:1000:GLY:N	1:B:1001:PRO:CD	2.76	0.42
1:C:883:LEU:HA	1:C:886:ARG:HB2	2.02	0.42
1:C:594:THR:HG23	1:C:598:PHE:HD1	1.83	0.42
1:C:444:VAL:CG1	1:C:445:ARG:N	2.82	0.42
1:C:867:PRO:O	1:C:868:GLY:O	2.37	0.42
1:B:379:THR:OG1	1:B:381:GLU:HG2	2.19	0.42
1:A:615:ALA:HB3	1:A:623:PRO:HG3	2.00	0.42
1:C:671:ILE:HG22	1:C:674:PHE:CE2	2.54	0.42
1:B:434:ILE:HG13	1:B:434:ILE:H	1.68	0.42
1:D:1058:LEU:HD23	1:D:1060:ILE:HD11	2.01	0.42
1:B:288:ARG:H	1:B:288:ARG:HG2	1.71	0.42
1:B:775:THR:CG2	1:B:861:ILE:HD13	2.47	0.42
1:A:445:ARG:NH2	1:C:54:ARG:HB3	2.34	0.42
1:A:90:LEU:HD22	1:A:94:GLU:HG3	2.00	0.42
1:D:633:ALA:O	1:D:635:PRO:HD3	2.20	0.42
1:C:494:LEU:HD23	1:C:496:ARG:NE	2.31	0.42
1:B:284:SER:CB	1:B:285:PRO:HD2	2.48	0.42
1:B:656:ASP:O	1:B:659:ILE:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:VAL:HG22	1:A:830:GLY:HA3	2.02	0.42
1:C:53:PHE:CZ	1:C:65:ALA:HB2	2.55	0.41
1:B:145:HIS:HA	1:B:148:MET:HE2	2.02	0.41
1:A:440:GLU:O	1:A:443:MET:HB3	2.20	0.41
1:B:118:TYR:CE2	1:B:331:VAL:CG1	3.03	0.41
1:B:667:ALA:HB1	1:B:698:LYS:HG3	2.02	0.41
1:B:572:ASP:HB2	1:B:605:GLU:OE1	2.20	0.41
1:A:422:TYR:O	1:A:423:ASP:C	2.57	0.41
1:A:588:ILE:HD13	1:A:588:ILE:O	2.20	0.41
1:D:273:LYS:O	1:D:377:ARG:NH2	2.53	0.41
1:A:731:GLU:HG3	1:A:766:LEU:CD2	2.46	0.41
1:A:701:GLU:OE1	1:A:739:ALA:HB2	2.20	0.41
1:D:772:THR:HG22	1:D:783:TYR:CZ	2.55	0.41
1:D:251:GLY:O	1:D:306:ASN:N	2.51	0.41
1:C:289:GLN:O	1:C:293:ASP:OD2	2.38	0.41
1:B:264:ASP:HB2	1:B:280:SER:HB2	2.02	0.41
1:C:398:ARG:HH21	1:C:451:ARG:NH1	2.18	0.41
1:C:459:ILE:HB	1:C:460:PRO:HD3	2.02	0.41
1:B:811:ASN:ND2	1:B:811:ASN:H	2.18	0.41
1:B:854:ILE:H	1:B:854:ILE:HD12	1.86	0.41
1:D:242:PRO:HB2	1:D:313:LEU:HG	2.02	0.41
1:B:335:ILE:O	1:B:339:VAL:HG22	2.21	0.41
1:B:139:ILE:HG23	1:B:352:ALA:HB2	2.02	0.41
1:D:65:ALA:HB3	1:D:83:SER:HB3	2.02	0.41
1:D:614:VAL:HG13	1:D:618:PHE:HB2	2.03	0.41
1:D:711:LEU:O	1:D:713:PRO:HD3	2.20	0.41
1:D:642:LEU:HD12	1:D:675:ARG:HB3	2.01	0.41
1:A:277:VAL:HG11	1:A:436:PHE:HE1	1.85	0.41
1:B:828:ILE:HD12	1:B:829:GLU:H	1.86	0.41
1:C:433:ALA:HB3	1:C:438:GLN:HB3	2.03	0.41
1:C:329:VAL:HG13	1:C:348:GLN:NE2	2.35	0.41
1:B:339:VAL:HG12	1:B:432:HIS:CE1	2.55	0.41
1:D:845:TYR:O	1:D:846:SER:C	2.58	0.41
1:D:760:LYS:HG2	1:D:768:ILE:HD12	2.02	0.41
1:C:923:GLN:HE21	1:C:923:GLN:HB2	1.66	0.41
1:B:719:THR:CG2	1:B:720:LEU:N	2.83	0.41
1:B:743:MET:SD	1:B:907:VAL:HG13	2.60	0.41
1:C:760:LYS:HE2	1:C:790:GLY:O	2.21	0.41
1:C:906:LYS:HD3	1:C:914:VAL:HG21	2.02	0.41
1:B:717(A):ILE:O	1:B:722:TYR:HB2	2.21	0.41
1:A:1059:ILE:H	1:A:1081:ASN:ND2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:GLU:OE2	1:C:466:MET:HB3	2.20	0.41
1:B:647:ASN:O	1:B:649:VAL:N	2.52	0.41
1:B:641:MET:HE3	1:B:674:PHE:CE1	2.55	0.41
1:D:59:LEU:HG	1:D:346:LYS:HD2	2.02	0.41
1:A:444:VAL:HG23	1:A:445:ARG:N	2.36	0.41
1:B:45:ARG:HG3	1:B:45:ARG:HH11	1.85	0.41
1:B:994:LEU:HB3	1:B:1002:VAL:HG21	2.02	0.41
1:D:145:HIS:CE1	1:D:304:TYR:HA	2.55	0.41
1:D:41:LEU:HD12	1:D:64:VAL:HG11	2.03	0.41
1:A:909:PRO:HD2	1:A:952:ILE:HD11	2.03	0.41
1:D:255:GLY:O	1:D:257:ILE:HG13	2.21	0.41
1:D:864:HIS:O	1:D:864:HIS:CD2	2.74	0.41
1:C:145:HIS:CE1	1:C:302:ILE:O	2.63	0.41
1:C:309:THR:O	1:C:325:VAL:HA	2.21	0.41
1:B:622:ASN:HD21	1:B:624:TRP:HB2	1.85	0.41
1:B:701:GLU:CG	1:B:739:ALA:HB2	2.49	0.41
1:D:641:MET:HE2	1:D:671:ILE:HG21	2.03	0.41
1:C:890:VAL:O	1:C:891:LYS:C	2.59	0.41
1:B:704:ILE:HG23	1:B:726:LEU:HD23	2.01	0.41
1:C:712:ASN:HA	1:C:713:PRO:HD2	1.90	0.41
1:A:496:ARG:HH22	1:A:1029:ASN:HB2	1.86	0.41
1:A:494:LEU:CD1	1:A:494:LEU:H	2.33	0.41
1:B:242:PRO:HB2	1:B:313:LEU:HG	2.02	0.41
1:C:749:PRO:HG3	1:C:781:LEU:HB3	2.03	0.41
1:C:331:VAL:HG22	1:C:428:LYS:HD3	2.03	0.41
1:B:39:LYS:O	1:B:112:ASP:OD1	2.37	0.41
1:B:867:PRO:O	1:B:868:GLY:C	2.59	0.41
1:C:246:GLU:OE1	1:C:332:GLU:OE2	2.38	0.41
1:D:286:THR:O	1:D:287:LEU:C	2.58	0.41
1:A:881:LEU:HD12	1:A:919:LEU:HD12	2.03	0.41
1:A:582:VAL:HA	1:A:845:TYR:CZ	2.55	0.41
2:B:2001:COA:H8A	2:B:2001:COA:C9P	2.51	0.41
1:C:817:LEU:HD13	1:C:822:ARG:O	2.21	0.41
1:D:553:VAL:O	1:D:557:VAL:HG23	2.21	0.41
1:D:465:VAL:HG13	1:D:480:PHE:HE2	1.86	0.41
1:B:606:MET:HE3	1:B:607:TRP:HB2	2.01	0.41
1:B:811:ASN:ND2	1:B:831:MET:HG2	2.36	0.41
1:C:717:ASN:HD22	1:C:717:ASN:N	2.18	0.41
1:C:419:SER:HA	1:C:420:PRO:HD3	1.94	0.41
1:C:840:THR:O	1:C:843:THR:HB	2.21	0.41
1:B:799:ALA:H	1:B:811:ASN:ND2	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:622:ASN:HD22	1:C:623:PRO:CD	2.33	0.40
1:C:287:LEU:O	1:C:289:GLN:N	2.54	0.40
1:A:504:ILE:HG21	1:A:1042:MET:HE2	2.03	0.40
1:A:278:ALA:HA	1:A:279:PRO:HA	1.85	0.40
1:A:626:ARG:HG2	1:A:630:LEU:HD12	2.03	0.40
1:B:622:ASN:ND2	1:B:624:TRP:H	2.19	0.40
1:D:679:SER:HA	1:D:907:VAL:CG2	2.51	0.40
1:A:590:ILE:H	1:A:590:ILE:HG13	1.71	0.40
1:D:747:LEU:HD23	1:D:770:LEU:HD11	2.03	0.40
1:D:683:VAL:HG12	1:D:687:LYS:HE3	2.02	0.40
1:A:667:ALA:HB1	1:A:698:LYS:HG3	2.02	0.40
1:B:870:GLN:O	1:B:874:LEU:HB2	2.21	0.40
1:A:738:LEU:HD23	1:A:768:ILE:HG12	2.04	0.40
1:A:760:LYS:HG2	1:A:768:ILE:HD12	2.01	0.40
1:A:770:LEU:HD12	1:A:771:HIS:H	1.87	0.40
1:C:521:LYS:HD3	1:C:1040:PHE:HB2	2.04	0.40
1:B:624:TRP:HB3	1:B:1005:GLN:NE2	2.37	0.40
1:A:1035:THR:HB	1:A:1036:PRO:HD3	2.03	0.40
1:D:796:THR:OG1	1:D:810:ALA:HB2	2.21	0.40
1:B:391:THR:OG1	1:B:418:ILE:O	2.37	0.40
1:C:1029:ASN:ND2	1:C:1031:SER:OG	2.53	0.40
1:A:74:SER:OG	1:A:75:LEU:N	2.54	0.40
1:B:59:LEU:HD11	1:B:346:LYS:HG3	2.03	0.40
1:A:681:ASN:HD21	1:A:705:CYS:N	2.20	0.40
1:A:452:ILE:HD12	1:A:459:ILE:HD11	2.04	0.40
1:B:836:HIS:O	1:B:839:SER:HB3	2.21	0.40
1:B:1077:TYR:CD1	1:B:1077:TYR:N	2.89	0.40
1:C:1077:TYR:N	1:C:1077:TYR:CD1	2.90	0.40
1:A:736:HIS:O	1:A:766:LEU:HD12	2.21	0.40
1:B:521:LYS:HA	1:B:522:PRO:HD3	1.88	0.40
1:B:313:LEU:HB2	1:B:323:ILE:HD11	2.04	0.40
2:C:2001:COA:O2A	2:C:2001:COA:H10	2.20	0.40
1:C:141:PRO:HG3	1:C:304:TYR:OH	2.22	0.40
1:A:947:PHE:HD2	1:A:952:ILE:HG21	1.87	0.40
1:B:151:ASP:OD1	1:B:152:LYS:N	2.55	0.40
1:B:298:LEU:O	1:B:302:ILE:HG13	2.21	0.40
1:B:114:ILE:HD12	1:B:131:CYS:SG	2.62	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	990/1150 (86%)	862 (87%)	105 (11%)	23 (2%)	8	30
1	B	985/1150 (86%)	875 (89%)	89 (9%)	21 (2%)	9	32
1	C	991/1150 (86%)	887 (90%)	79 (8%)	25 (2%)	7	27
1	D	924/1150 (80%)	777 (84%)	123 (13%)	24 (3%)	7	26
All	All	3890/4600 (85%)	3401 (87%)	396 (10%)	93 (2%)	7	29

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	868	GLY
1	A	939	ASP
1	D	87	GLY
1	D	163	ASP
1	D	272	GLN
1	D	361	ASN
1	C	170	THR
1	C	386	ASP
1	C	387	PHE
1	C	828	ILE
1	C	870	GLN
1	B	414	GLN
1	B	423	ASP
1	B	494	LEU
1	B	520	PRO
1	B	522	PRO
1	B	868	GLY
1	B	870	GLN
1	B	1001	PRO
1	A	148	MET
1	A	434	ILE
1	A	674	PHE

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Mol	Chain	Res	Type
1	A	925	ASP
1	A	1026	GLN
1	D	99	ILE
1	D	274	VAL
1	D	424	SER
1	D	515	ASN
1	D	959	PHE
1	C	89	ASP
1	C	747	LEU
1	C	854	ILE
1	C	868	GLY
1	C	881	LEU
1	B	538	ALA
1	B	1053	ASP
1	B	1070	GLU
1	A	366	ASP
1	A	416	ALA
1	A	648	ALA
1	A	761	SER
1	A	854	ILE
1	D	60	ASP
1	D	256	ASN
1	D	414	GLN
1	C	270	ARG
1	B	120	PHE
1	B	648	ALA
1	B	696	ALA
1	A	120	PHE
1	A	307	ALA
1	A	424	SER
1	A	480	PHE
1	D	241	ASN
1	D	271	HIS
1	D	648	ALA
1	C	106	ALA
1	C	288	ARG
1	C	648	ALA
1	C	649	VAL
1	C	933	THR
1	B	1002	VAL
1	A	433	ALA
1	A	494	LEU

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Mol	Chain	Res	Type
1	A	620	LYS
1	A	826	THR
1	D	491	GLN
1	D	886	ARG
1	C	120	PHE
1	C	241	ASN
1	C	306	ASN
1	C	400	SER
1	C	934	ASP
1	B	480	PHE
1	A	1014	PRO
1	B	869	GLY
1	A	1072	GLY
1	D	635	PRO
1	C	956	VAL
1	B	87	GLY
1	B	166	VAL
1	B	354	GLY
1	D	649	VAL
1	D	749	PRO
1	D	1000	GLY
1	C	550	PRO
1	C	749	PRO
1	D	434	ILE
1	D	485	PRO
1	D	828	ILE
1	C	861	ILE
1	A	1000	GLY
1	B	516	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	860/987 (87%)	783 (91%)	77 (9%)	12	34
1	B	856/987 (87%)	762 (89%)	94 (11%)	8	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	861/987 (87%)	759 (88%)	102 (12%)	6	19
1	D	806/987 (82%)	711 (88%)	95 (12%)	6	19
All	All	3383/3948 (86%)	3015 (89%)	368 (11%)	8	23

All (368) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	83	SER
1	A	98	ASN
1	A	108	GLN
1	A	123	GLU
1	A	126	GLN
1	A	151	ASP
1	A	170	THR
1	A	241	ASN
1	A	269	ARG
1	A	274	VAL
1	A	284	SER
1	A	287	LEU
1	A	299	MET
1	A	326	ASN
1	A	329	VAL
1	A	331	VAL
1	A	366	ASP
1	A	375	GLN
1	A	393	THR
1	A	418	ILE
1	A	427	VAL
1	A	440	GLU
1	A	445	ARG
1	A	446	SER
1	A	455	VAL
1	A	472	THR
1	A	486	GLU
1	A	491	GLN
1	A	493	SER
1	A	506	ASN
1	A	518	LYS
1	A	523	ASP
1	A	526	LEU

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Mol	Chain	Res	Type
1	A	548	VAL
1	A	565	LEU
1	A	567	ASP
1	A	580	THR
1	A	588	ILE
1	A	606	MET
1	A	607	TRP
1	A	630	LEU
1	A	632	LYS
1	A	657	ASN
1	A	661	LYS
1	A	668	LYS
1	A	672	ASP
1	A	685	GLN
1	A	714	GLU
1	A	715	ARG
1	A	725	LYS
1	A	743	MET
1	A	750	LYS
1	A	755	LEU
1	A	780	LEU
1	A	784	LYS
1	A	793	ILE
1	A	805	THR
1	A	807	GLN
1	A	813	LEU
1	A	828	ILE
1	A	839	SER
1	A	861	ILE
1	A	870	GLN
1	A	907	VAL
1	A	924	ASN
1	A	934	ASP
1	A	952	ILE
1	A	962	ASP
1	A	969	LYS
1	A	989	LYS
1	A	991	ARG
1	A	1048	VAL
1	A	1058	LEU
1	A	1062	LEU
1	A	1064	THR

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Mol	Chain	Res	Type
1	A	1085	ARG
1	D	36	GLN
1	D	44	ASN
1	D	69	ASN
1	D	99	ILE
1	D	101	ARG
1	D	125	GLU
1	D	131	CYS
1	D	137	LYS
1	D	143	LEU
1	D	144	GLU
1	D	147	ASP
1	D	158	THR
1	D	166	VAL
1	D	262	GLU
1	D	283	LEU
1	D	288	ARG
1	D	290	ARG
1	D	296	ILE
1	D	298	LEU
1	D	300	GLU
1	D	301	ASN
1	D	303	LYS
1	D	306	ASN
1	D	329	VAL
1	D	331	VAL
1	D	339	VAL
1	D	346	LYS
1	D	357(A)	PHE
1	D	358	GLU
1	D	360	ILE
1	D	362	MET
1	D	365	LYS
1	D	368	THR
1	D	374	ILE
1	D	375	GLN
1	D	417	GLU
1	D	434	ILE
1	D	440	GLU
1	D	442	LYS
1	D	445	ARG
1	D	451	ARG

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Mol	Chain	Res	Type
1	D	456	LYS
1	D	482	GLU
1	D	517	GLU
1	D	525	GLU
1	D	541	THR
1	D	543	GLN
1	D	544	LEU
1	D	551	LYS
1	D	569	THR
1	D	575	GLN
1	D	580	THR
1	D	588	ILE
1	D	592	SER
1	D	606	MET
1	D	607	TRP
1	D	631	ARG
1	D	636	ASN
1	D	644	ARG
1	D	651	TYR
1	D	661	LYS
1	D	685	GLN
1	D	691	GLU
1	D	707	THR
1	D	715	ARG
1	D	719	THR
1	D	743	MET
1	D	747	LEU
1	D	760	LYS
1	D	766	LEU
1	D	780	LEU
1	D	781	LEU
1	D	792	ASP
1	D	818	ASN
1	D	822	ARG
1	D	827	ASP
1	D	839	SER
1	D	840	THR
1	D	856	SER
1	D	891	LYS
1	D	892	ASP
1	D	949	LYS
1	D	956	VAL

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Mol	Chain	Res	Type
1	D	971	GLN
1	D	983	GLU
1	D	1003	THR
1	D	1019	GLN
1	D	1044	ASN
1	D	1048	VAL
1	D	1052	ILE
1	D	1059	ILE
1	D	1061	LYS
1	D	1064	THR
1	D	1083	GLN
1	D	1086	ARG
1	C	36	GLN
1	C	45	ARG
1	C	60	ASP
1	C	75	LEU
1	C	83	SER
1	C	98	ASN
1	C	100	GLU
1	C	101	ARG
1	C	103	ILE
1	C	107	LYS
1	C	137	LYS
1	C	147	ASP
1	C	170	THR
1	C	240	ASP
1	C	257	ILE
1	C	262	GLU
1	C	271	HIS
1	C	275	VAL
1	C	281	VAL
1	C	286	THR
1	C	287	LEU
1	C	318	ASP
1	C	319	GLU
1	C	323	ILE
1	C	336	THR
1	C	346	LYS
1	C	356	ASP
1	C	359	GLU
1	C	365	LYS
1	C	368	THR

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Mol	Chain	Res	Type
1	C	370	LEU
1	C	377	ARG
1	C	386	ASP
1	C	411	ASP
1	C	427	VAL
1	C	434	ILE
1	C	437	LYS
1	C	445	ARG
1	C	484	THR
1	C	489	ASP
1	C	493	SER
1	C	498	THR
1	C	519	ARG
1	C	523	ASP
1	C	525	GLU
1	C	526	LEU
1	C	555	GLU
1	C	565	LEU
1	C	571	ARG
1	C	580	THR
1	C	588	ILE
1	C	606	MET
1	C	607	TRP
1	C	613	ASP
1	C	622	ASN
1	C	641	MET
1	C	644	ARG
1	C	649	VAL
1	C	656	ASP
1	C	671	ILE
1	C	704	ILE
1	C	707	THR
1	C	717	ASN
1	C	728	LYS
1	C	743	MET
1	C	766	LEU
1	C	781	LEU
1	C	784	LYS
1	C	796	THR
1	C	809	SER
1	C	818	ASN
1	C	828	ILE

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Mol	Chain	Res	Type
1	C	847	ASP
1	C	872	SER
1	C	888	ASP
1	C	892	ASP
1	C	907	VAL
1	C	912	LYS
1	C	923	GLN
1	C	927	ASP
1	C	933	THR
1	C	949	LYS
1	C	968	LEU
1	C	969	LYS
1	C	971	GLN
1	C	972	GLU
1	C	982	LEU
1	C	988	GLU
1	C	991	ARG
1	C	996	GLU
1	C	998	GLN
1	C	999	GLN
1	C	1008	ILE
1	C	1015	LYS
1	C	1029	ASN
1	C	1044	ASN
1	C	1048	VAL
1	C	1058	LEU
1	C	1085	ARG
1	C	1091	ASP
1	C	1092	GLU
1	C	1093	ASN
1	B	39	LYS
1	B	40	LEU
1	B	44	ASN
1	B	58	GLU
1	B	89	ASP
1	B	90	LEU
1	B	98	ASN
1	B	101	ARG
1	B	144	GLU
1	B	156	ARG
1	B	163	ASP
1	B	239	ILE

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Mol	Chain	Res	Type
1	B	250	ILE
1	B	253	GLU
1	B	269	ARG
1	B	270	ARG
1	B	272	GLN
1	B	286	THR
1	B	287	LEU
1	B	288	ARG
1	B	306	ASN
1	B	318	ASP
1	B	329	VAL
1	B	384	LEU
1	B	393	THR
1	B	399	SER
1	B	426	LEU
1	B	427	VAL
1	B	429	LEU
1	B	435	SER
1	B	469	LYS
1	B	473	SER
1	B	479	LYS
1	B	491	GLN
1	B	518	LYS
1	B	525	GLU
1	B	526	LEU
1	B	536	LYS
1	B	537	ILE
1	B	547	GLU
1	B	580	THR
1	B	581	ARG
1	B	588	ILE
1	B	596	ASP
1	B	605	GLU
1	B	606	MET
1	B	607	TRP
1	B	622	ASN
1	B	631	ARG
1	B	647	ASN
1	B	649	VAL
1	B	657	ASN
1	B	684	ASP
1	B	715	ARG

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Mol	Chain	Res	Type
1	B	717	ASN
1	B	717(A)	ILE
1	B	719	THR
1	B	743	MET
1	B	766	LEU
1	B	781	LEU
1	B	784	LYS
1	B	806	SER
1	B	809	SER
1	B	825	ARG
1	B	828	ILE
1	B	833	SER
1	B	858	ASN
1	B	863	GLN
1	B	866	MET
1	B	871	TYR
1	B	872	SER
1	B	873	ASN
1	B	888	ASP
1	B	907	VAL
1	B	908	THR
1	B	917	MET
1	B	919	LEU
1	B	928	GLU
1	B	945	VAL
1	B	957	ASN
1	B	975	THR
1	B	977	ARG
1	B	989	LYS
1	B	1008	ILE
1	B	1009	SER
1	B	1019	GLN
1	B	1029	ASN
1	B	1044	ASN
1	B	1053	ASP
1	B	1077	TYR
1	B	1081	ASN
1	B	1086	ARG
1	B	1092	GLU
1	B	1093	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	69	ASN
1	A	98	ASN
1	A	126	GLN
1	A	241	ASN
1	A	244	HIS
1	A	254	HIS
1	A	326	ASN
1	A	330	GLN
1	A	375	GLN
1	A	414	GLN
1	A	506	ASN
1	A	543	GLN
1	A	574	HIS
1	A	575	GLN
1	A	664	GLN
1	A	685	GLN
1	A	736	HIS
1	A	778	ASN
1	A	811	ASN
1	A	898	ASN
1	A	924	ASN
1	A	960	ASN
1	A	1025	ASN
1	A	1081	ASN
1	D	44	ASN
1	D	145	HIS
1	D	289	GLN
1	D	330	GLN
1	D	364	GLN
1	D	414	GLN
1	D	464	ASN
1	D	491	GLN
1	D	506	ASN
1	D	543	GLN
1	D	574	HIS
1	D	575	GLN
1	D	653	ASN
1	D	694	GLN
1	D	736	HIS
1	D	778	ASN
1	D	811	ASN
1	D	818	ASN

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Mol	Chain	Res	Type
1	D	864	HIS
1	D	1005	GLN
1	D	1025	ASN
1	D	1026	GLN
1	D	1029	ASN
1	D	1044	ASN
1	C	44	ASN
1	C	69	ASN
1	C	98	ASN
1	C	126	GLN
1	C	145	HIS
1	C	271	HIS
1	C	297	GLN
1	C	326	ASN
1	C	330	GLN
1	C	432	HIS
1	C	438	GLN
1	C	464	ASN
1	C	574	HIS
1	C	575	GLN
1	C	622	ASN
1	C	717	ASN
1	C	736	HIS
1	C	778	ASN
1	C	811	ASN
1	C	818	ASN
1	C	823	HIS
1	C	864	HIS
1	C	870	GLN
1	C	873	ASN
1	C	876	GLN
1	C	898	ASN
1	C	923	GLN
1	C	957	ASN
1	C	1005	GLN
1	C	1025	ASN
1	C	1029	ASN
1	C	1044	ASN
1	C	1083	GLN
1	B	44	ASN
1	B	142	HIS
1	B	145	HIS

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Mol	Chain	Res	Type
1	B	241	ASN
1	B	297	GLN
1	B	306	ASN
1	B	326	ASN
1	B	330	GLN
1	B	333	HIS
1	B	348	GLN
1	B	414	GLN
1	B	438	GLN
1	B	491	GLN
1	B	543	GLN
1	B	574	HIS
1	B	575	GLN
1	B	589	ASN
1	B	617	ASN
1	B	622	ASN
1	B	647	ASN
1	B	657	ASN
1	B	717	ASN
1	B	736	HIS
1	B	771	HIS
1	B	778	ASN
1	B	811	ASN
1	B	858	ASN
1	B	864	HIS
1	B	873	ASN
1	B	877	GLN
1	B	898	ASN
1	B	923	GLN
1	B	960	ASN
1	B	999	GLN
1	B	1005	GLN
1	B	1019	GLN
1	B	1025	ASN
1	B	1029	ASN
1	B	1044	ASN
1	B	1081	ASN

5.3.3 RNA ⓘ

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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	COA	A	2001	-	40,50,50	0.96	2 (5%)	50,75,75	2.00	7 (14%)
4	BTI	B	2000	-	14,16,16	1.81	3 (21%)	13,21,21	1.53	1 (7%)
2	COA	B	2001	-	40,50,50	1.10	2 (5%)	50,75,75	2.04	10 (20%)
4	BTI	C	2000	-	14,16,16	1.86	2 (14%)	13,21,21	1.77	2 (15%)
2	COA	C	2001	-	40,50,50	1.03	1 (2%)	50,75,75	1.95	8 (16%)
2	COA	D	2001	-	40,50,50	1.00	1 (2%)	50,75,75	1.99	5 (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
2	COA	A	2001	-	-	0/44/64/64	0/3/3/3
4	BTI	B	2000	-	-	0/5/27/27	0/2/2/2
2	COA	B	2001	-	-	0/44/64/64	0/3/3/3
4	BTI	C	2000	-	-	0/5/27/27	0/2/2/2
2	COA	C	2001	-	-	0/44/64/64	0/3/3/3
2	COA	D	2001	-	-	0/44/64/64	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2000	BTI	C2-S1	-3.62	1.76	1.82
4	B	2000	BTI	C2-S1	-3.36	1.77	1.82
2	B	2001	COA	P3B-O9A	-2.09	1.47	1.54
4	B	2000	BTI	C3-N3	-2.08	1.32	1.35
2	A	2001	COA	P3B-O8A	2.04	1.62	1.54
2	D	2001	COA	P3B-O7A	2.66	1.59	1.51
2	A	2001	COA	P3B-O7A	2.90	1.60	1.51
2	C	2001	COA	P3B-O7A	3.00	1.61	1.51
2	B	2001	COA	P3B-O7A	3.19	1.61	1.51
4	B	2000	BTI	O3-C3	4.59	1.32	1.23
4	C	2000	BTI	O3-C3	4.91	1.33	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	COA	N3A-C2A-N1A	-9.84	121.36	128.89
2	A	2001	COA	N3A-C2A-N1A	-9.59	121.55	128.89
2	C	2001	COA	N3A-C2A-N1A	-9.12	121.91	128.89
2	B	2001	COA	N3A-C2A-N1A	-8.46	122.42	128.89
2	B	2001	COA	P2A-O3A-P1A	-5.72	116.67	132.73
2	D	2001	COA	P2A-O3A-P1A	-5.53	117.21	132.73
2	C	2001	COA	C4B-O4B-C1B	-4.75	104.50	109.72
2	D	2001	COA	O4B-C1B-N9A	-4.70	98.26	108.10
2	B	2001	COA	C4B-O4B-C1B	-4.50	104.78	109.72
2	C	2001	COA	P2A-O3A-P1A	-4.27	120.74	132.73
2	A	2001	COA	C4B-O4B-C1B	-3.83	105.51	109.72
2	A	2001	COA	P2A-O3A-P1A	-3.68	122.41	132.73
2	A	2001	COA	O4B-C1B-N9A	-3.61	100.54	108.10
2	B	2001	COA	O4B-C4B-C5B	-3.31	97.48	109.32
2	B	2001	COA	O4B-C1B-N9A	-3.26	101.27	108.10
4	C	2000	BTI	C5-N3-C3	-3.18	110.11	112.49
2	A	2001	COA	O8A-P3B-O7A	-3.13	100.52	110.58
2	C	2001	COA	C4A-C5A-N7A	-3.06	106.67	109.48
2	C	2001	COA	O4B-C1B-N9A	-2.76	102.32	108.10
2	D	2001	COA	C4B-O4B-C1B	-2.66	106.80	109.72
2	B	2001	COA	O8A-P3B-O7A	-2.59	102.23	110.58
2	C	2001	COA	O8A-P3B-O7A	-2.46	102.68	110.58
2	D	2001	COA	O8A-P3B-O7A	-2.38	102.92	110.58
2	C	2001	COA	C2B-C1B-N9A	-2.15	111.01	114.29
2	A	2001	COA	C6P-C7P-N8P	2.02	116.31	111.88
2	B	2001	COA	C2B-C1B-N9A	2.14	117.57	114.29
2	C	2001	COA	O9A-P3B-O7A	2.34	118.11	110.58
2	B	2001	COA	CEP-CBP-CCP	2.68	111.97	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	COA	O9A-P3B-O7A	2.72	119.33	110.58
2	B	2001	COA	CDP-CBP-CAP	2.91	114.65	109.34
2	A	2001	COA	C7P-N8P-C9P	3.15	128.77	122.53
4	B	2000	BTI	N2-C3-N3	3.93	111.59	108.88
4	C	2000	BTI	N2-C3-N3	4.14	111.74	108.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	COA	1	0
4	C	2000	BTI	3	0
2	C	2001	COA	2	0
2	D	2001	COA	6	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	994/1150 (86%)	0.23	48 (4%) 34 28	39, 76, 117, 151	0
1	B	989/1150 (86%)	-0.19	12 (1%) 81 78	26, 52, 83, 102	0
1	C	995/1150 (86%)	-0.16	20 (2%) 68 64	29, 52, 83, 107	0
1	D	934/1150 (81%)	0.43	71 (7%) 17 11	41, 83, 128, 173	0
All	All	3912/4600 (85%)	0.07	151 (3%) 43 36	26, 64, 111, 173	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	962	ASP	10.0
1	D	965	ALA	6.8
1	D	981	TYR	6.6
1	D	975	THR	5.7
1	D	959	PHE	5.1
1	D	966	VAL	5.1
1	D	153	VAL	5.0
1	A	713	PRO	4.8
1	D	885	GLU	4.5
1	D	892	ASP	4.5
1	D	272	GLN	4.4
1	A	993	LEU	4.4
1	D	883	LEU	4.3
1	D	961	LYS	4.2
1	C	970	GLY	4.2
1	A	929	GLN	4.2
1	A	282	GLY	4.1
1	A	933	THR	4.0
1	D	684	ASP	4.0
1	D	999	GLN	3.9
1	D	958	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	876	GLN	3.8
1	C	236	GLU	3.8
1	A	999	GLN	3.7
1	A	538(A)	SER	3.6
1	A	489	ASP	3.5
1	D	537	ILE	3.5
1	C	238	TYR	3.5
1	D	994	LEU	3.5
1	A	932	ILE	3.5
1	A	970	GLY	3.5
1	A	714	GLU	3.5
1	D	490	ILE	3.4
1	D	533	SER	3.4
1	D	988	GLU	3.3
1	D	893	MET	3.3
1	B	282	GLY	3.3
1	A	1001	PRO	3.3
1	A	888	ASP	3.2
1	A	965	ALA	3.2
1	D	971	GLN	3.2
1	D	790	GLY	3.2
1	C	877	GLN	3.2
1	D	886	ARG	3.2
1	D	1000	GLY	3.2
1	D	641	MET	3.2
1	D	1001	PRO	3.1
1	D	890	VAL	3.1
1	A	875	SER	3.1
1	C	89	ASP	3.1
1	C	882	GLY	3.0
1	A	940	PHE	3.0
1	C	515	ASN	3.0
1	B	163	ASP	3.0
1	A	238	TYR	3.0
1	D	963	LEU	2.9
1	D	989	LYS	2.9
1	A	240	ASP	2.8
1	B	494	LEU	2.8
1	A	168	PRO	2.8
1	A	603	SER	2.8
1	A	170	THR	2.8
1	C	876	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	879	LYS	2.8
1	A	931	VAL	2.8
1	A	877	GLN	2.8
1	A	885	GLU	2.7
1	D	888	ASP	2.7
1	A	821	PRO	2.7
1	A	927	ASP	2.7
1	D	734	GLY	2.7
1	C	1093	ASN	2.7
1	D	603	SER	2.7
1	D	960	ASN	2.7
1	D	969	LYS	2.7
1	A	618	PHE	2.6
1	C	384	LEU	2.6
1	D	882	GLY	2.6
1	A	880	SER	2.6
1	A	872	SER	2.6
1	B	271	HIS	2.6
1	A	537	ILE	2.6
1	D	683	VAL	2.6
1	A	934	ASP	2.5
1	D	388	MET	2.5
1	A	919	LEU	2.5
1	C	1071	ASN	2.5
1	C	169	GLY	2.5
1	D	864	HIS	2.5
1	D	1019	GLN	2.5
1	D	863	GLN	2.5
1	D	992	GLU	2.5
1	A	938	LEU	2.5
1	B	168	PRO	2.4
1	D	682	TRP	2.4
1	C	271	HIS	2.4
1	A	994	LEU	2.4
1	D	761	SER	2.4
1	B	981	TYR	2.4
1	C	171	ASP	2.4
1	D	884	GLY	2.4
1	B	270	ARG	2.4
1	D	608	GLY	2.3
1	D	160	ILE	2.3
1	A	1090	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	524	TYR	2.3
1	A	538	ALA	2.3
1	C	270	ARG	2.3
1	D	954	GLN	2.3
1	C	386	ASP	2.3
1	C	1001	PRO	2.3
1	D	673	VAL	2.3
1	D	762	ALA	2.3
1	A	886	ARG	2.2
1	D	1088	TYR	2.2
1	A	515	ASN	2.2
1	B	1071	ASN	2.2
1	D	119	GLY	2.2
1	D	387	PHE	2.2
1	D	997	GLU	2.2
1	B	99	ILE	2.2
1	A	966	VAL	2.2
1	D	315	SER	2.2
1	B	167	ILE	2.2
1	D	980	GLU	2.2
1	A	526	LEU	2.2
1	C	713	PRO	2.1
1	D	532	VAL	2.1
1	D	993	LEU	2.1
1	D	793	ILE	2.1
1	D	955	PRO	2.1
1	A	981	TYR	2.1
1	D	881	LEU	2.1
1	D	685	GLN	2.1
1	D	714	GLU	2.1
1	A	978	PRO	2.1
1	C	516	VAL	2.1
1	D	675	ARG	2.1
1	D	1014	PRO	2.1
1	D	912	LYS	2.0
1	A	840	THR	2.0
1	C	170	THR	2.0
1	D	967	ILE	2.0
1	A	416	ALA	2.0
1	D	303	LYS	2.0
1	D	745	GLY	2.0
1	A	823	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	722	TYR	2.0
1	B	515	ASN	2.0
1	D	909	PRO	2.0
1	A	889	GLU	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	COA	B	2001	48/48	0.96	0.14	-0.46	37,40,43,45	0
2	COA	D	2001	48/48	0.94	0.15	-0.91	45,51,55,56	0
2	COA	C	2001	48/48	0.97	0.13	-0.92	32,36,48,51	0
4	BTI	B	2000	15/15	0.94	0.13	-1.26	47,53,54,55	0
2	COA	A	2001	48/48	0.97	0.13	-1.49	44,48,57,59	0
4	BTI	C	2000	15/15	0.96	0.12	-1.83	36,40,42,43	0
3	MN	D	2002	1/1	0.97	0.10	-3.41	65,65,65,65	0
3	MN	C	2002	1/1	0.96	0.06	-3.92	65,65,65,65	0
3	MN	B	2002	1/1	0.94	0.08	-4.06	60,60,60,60	0
3	MN	A	2002	1/1	0.92	0.08	-	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.