



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 08:27 PM EDT

PDB ID : 3R05
Title : Structure of neurexin 1 alpha (domains LNS1-LNS6), with splice insert SS3
Authors : Venugopal, V.; Rudenko, G.
Deposited on : unknown
Resolution : 2.95 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

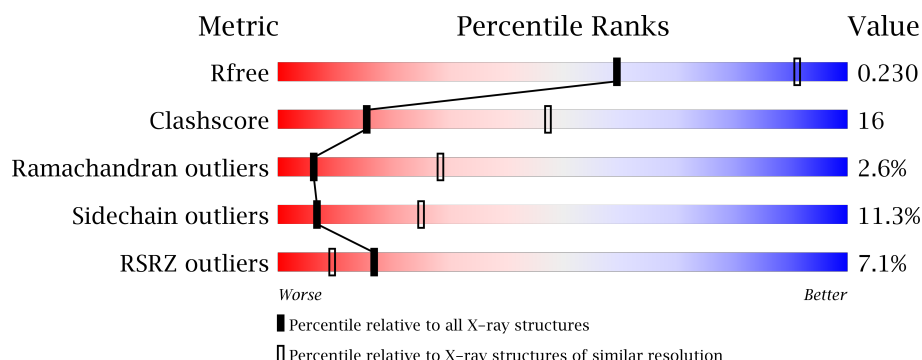
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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	1254	
1	B	1254	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15522 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 Neurexin-1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1008	Total	C	N	O	S	0	0	0
			7733	4857	1334	1499	43			
1	B	1008	Total	C	N	O	S	0	0	0
			7733	4857	1334	1499	43			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1340	ALA	-	EXPRESSION TAG	UNP Q28146
A	1341	SER	-	EXPRESSION TAG	UNP Q28146
A	1342	THR	-	EXPRESSION TAG	UNP Q28146
A	1343	SER	-	EXPRESSION TAG	UNP Q28146
A	1344	HIS	-	EXPRESSION TAG	UNP Q28146
A	1345	HIS	-	EXPRESSION TAG	UNP Q28146
A	1346	HIS	-	EXPRESSION TAG	UNP Q28146
A	1347	HIS	-	EXPRESSION TAG	UNP Q28146
A	1348	HIS	-	EXPRESSION TAG	UNP Q28146
A	1349	HIS	-	EXPRESSION TAG	UNP Q28146
B	1340	ALA	-	EXPRESSION TAG	UNP Q28146
B	1341	SER	-	EXPRESSION TAG	UNP Q28146
B	1342	THR	-	EXPRESSION TAG	UNP Q28146
B	1343	SER	-	EXPRESSION TAG	UNP Q28146
B	1344	HIS	-	EXPRESSION TAG	UNP Q28146
B	1345	HIS	-	EXPRESSION TAG	UNP Q28146
B	1346	HIS	-	EXPRESSION TAG	UNP Q28146
B	1347	HIS	-	EXPRESSION TAG	UNP Q28146
B	1348	HIS	-	EXPRESSION TAG	UNP Q28146
B	1349	HIS	-	EXPRESSION TAG	UNP Q28146

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).

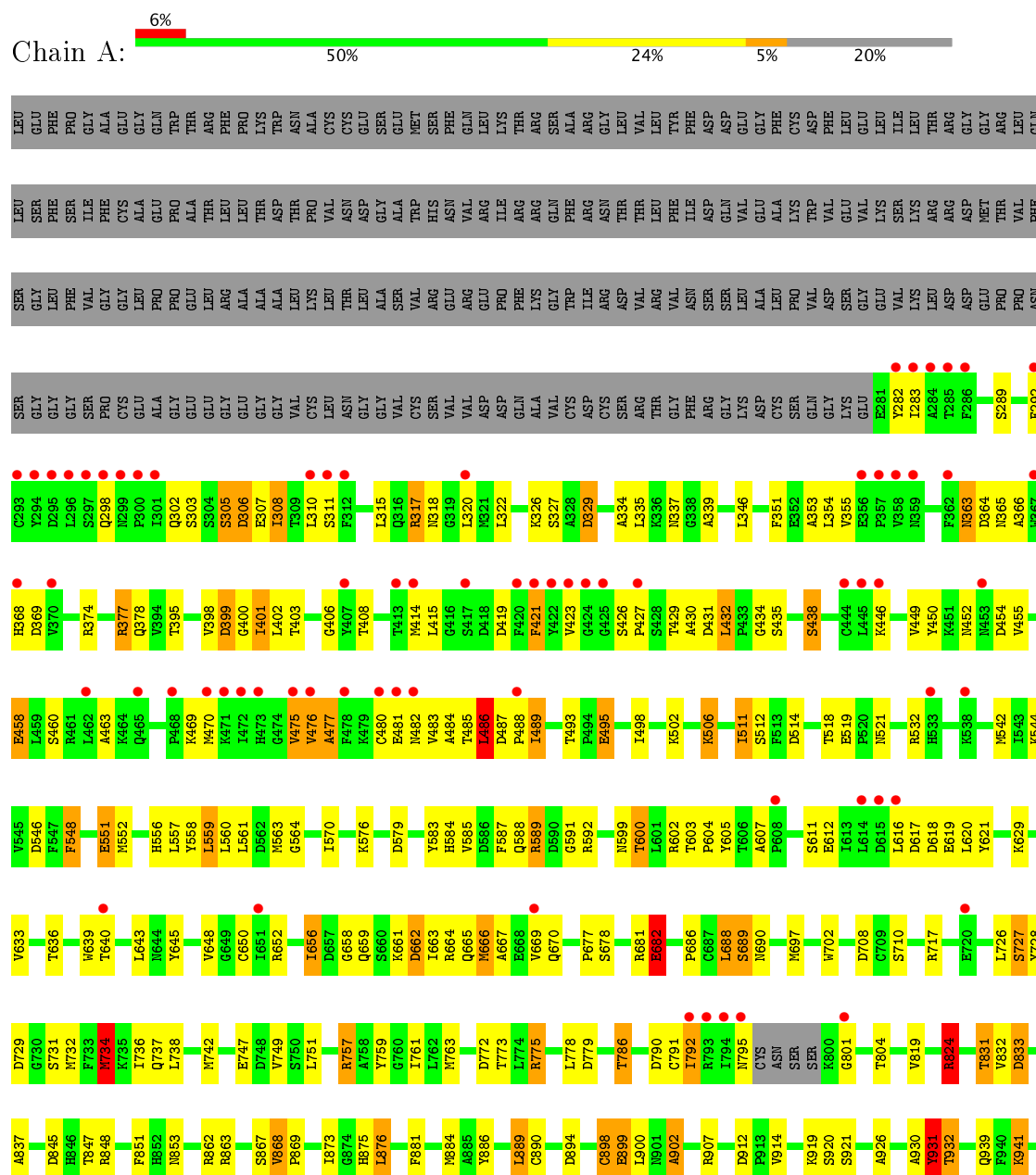


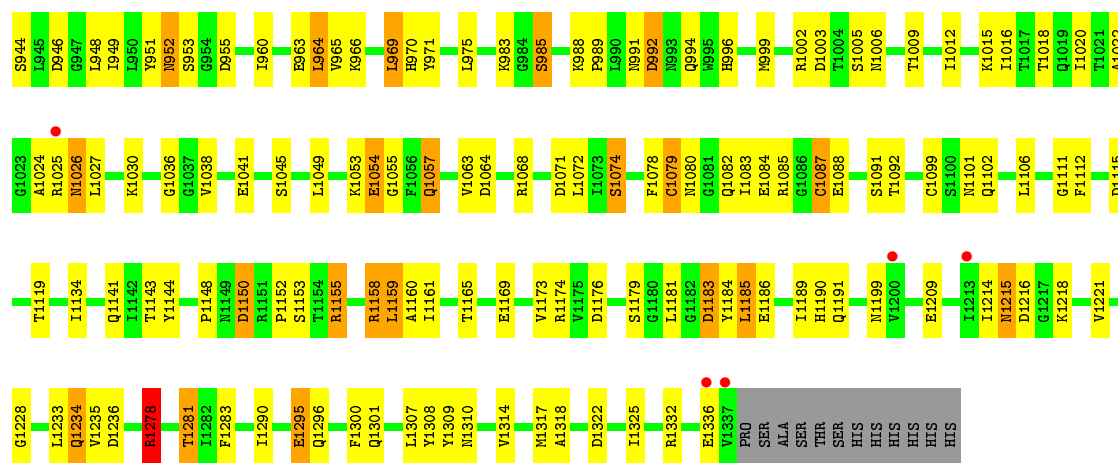
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

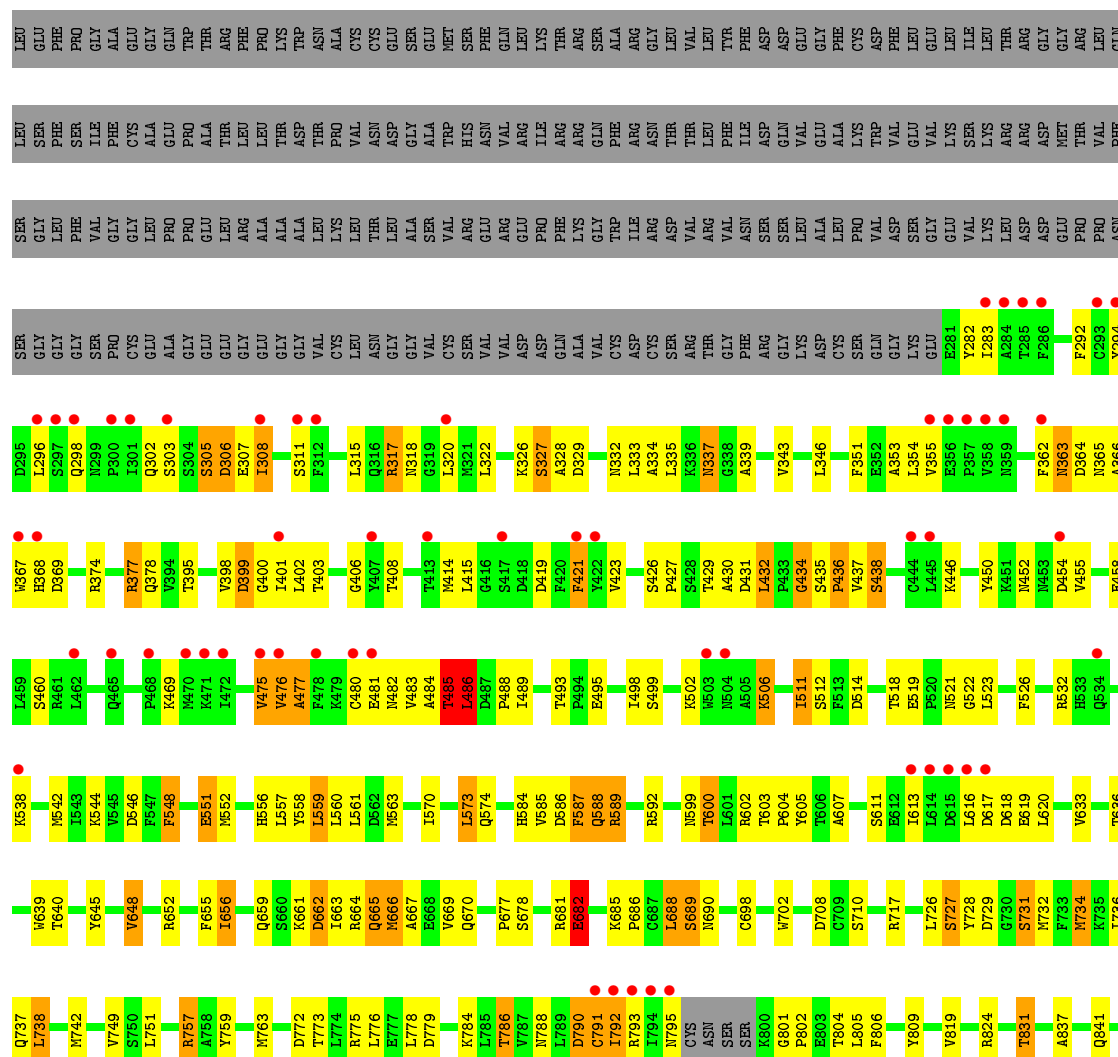
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Neurexin-1-alpha





● Molecule 1: Neurexin-1-alpha



F1283	Y1144	P1047	K941	D845
I1290	P1148	K1048	S944	H846
K1294	M1149	L1049	I949	T847
E1295	D1150	V1050	H051	R848
Q1296	R1151	A1051	H052	F851
Q1301	P1152	K1052	S953	H852
	S1153	K1053	G954	H853
	T1154	E1054	D955	
	R1155	G1055	F1056	R862
Q1302		Q1057	F959	R863
Q1303	R1158	V1063	I960	R867
L1304	L1159	D1064	I961	S867
S1305	A1160	L1065	V962	H868
G1306	I1161	L1069	E963	P869
L1307	T1165	P1070	L964	
L1308	E1169	D1071	V965	F872
Y1309	V1173	L1072	K966	L873
Y1310	R1174	S1074	L969	H874
V1314		F1078	H970	H875
A1318	L1181	C1079	Y971	L876
A1319	G1182	N1080		Q877
I1325	D1183	G1081	K988	S878
A1326	Y1184	Q1082		F881
I1327	E1185	I1083	H991	H884
R1332	L1187	E1084	D992	A885
	H1188	R1085	N993	Y886
G1335	I1189	G1086	Q994	L889
E1336	H1190	E1087	H995	C890
V1337	Q1191	E1088	H996	
PRO	V1196		M999	D894
SER	K1197		R1002	E899
ALA	F1198	T1092	D1003	L900
SER	F1198	T1093	T1004	H901
THR	N1199	C1094	S1005	A902
SER			M1006	
HIS	I1205	C1099	T1009	H907
HIS	A1206	S1100	N1101	V914
HIS	I1207	Q1102	I1012	
HIS	M1215			K919
HIS	D1216	W1109	I1016	S920
	G1217	D1110	T1017	S921
	K1218	G1111	T1018	
		F1112	Q1019	A926
	V1221		I1020	T927
	V1222	T1119		L928
				H929
	G1228	T1132	A1024	A930
		V1133	R1025	H931
	Q1234		N1026	T932
		K1137		
	R1278		K1030	L936
		Q1141	L1033	
	T1281	I1142		Q939
	I1282	T1143	G1036	F940

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.03Å 114.57Å 160.13Å 89.60° 89.98° 87.96°	Depositor
Resolution (Å)	44.29 – 2.95 44.29 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.29-2.95) 97.6 (44.29-2.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.96Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.235 0.202 , 0.230	Depositor DCC
R_{free} test set	4655 reflections (5.48%)	DCC
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-l 0.004 for -h,k,-l 0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15522	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: NAG

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	1.19	32/7886 (0.4%)	1.12	25/10691 (0.2%)
1	B	1.19	29/7886 (0.4%)	1.13	28/10691 (0.3%)
All	All	1.19	61/15772 (0.4%)	1.13	53/21382 (0.2%)

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	A	0	3
1	B	0	3
All	All	0	6

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1057	GLN	CG-CD	14.07	1.83	1.51
1	B	1057	GLN	CG-CD	13.73	1.82	1.51
1	A	898	CYS	CB-SG	10.65	2.00	1.82
1	B	868	VAL	CB-CG2	-9.30	1.33	1.52
1	B	963	GLU	CD-OE2	9.26	1.35	1.25
1	A	963	GLU	CD-OE2	8.43	1.34	1.25
1	B	1054	GLU	CG-CD	8.29	1.64	1.51
1	A	1054	GLU	CG-CD	8.18	1.64	1.51
1	A	868	VAL	CB-CG2	-8.06	1.35	1.52
1	A	1036	GLY	C-O	7.79	1.36	1.23
1	A	1084	GLU	CD-OE1	7.48	1.33	1.25
1	A	899	GLU	CD-OE1	7.46	1.33	1.25
1	B	1094	CYS	CB-SG	-7.43	1.69	1.82
1	B	551	GLU	CG-CD	7.14	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1084	GLU	CD-OE1	7.07	1.33	1.25
1	A	1078	PHE	CE1-CZ	7.05	1.50	1.37
1	B	1295	GLU	CG-CD	6.99	1.62	1.51
1	A	1054	GLU	CD-OE1	6.87	1.33	1.25
1	B	931	TYR	CE2-CZ	6.84	1.47	1.38
1	B	1084	GLU	CD-OE2	6.83	1.33	1.25
1	A	551	GLU	CG-CD	6.68	1.61	1.51
1	A	931	TYR	CG-CD1	6.58	1.47	1.39
1	A	931	TYR	CE1-CZ	6.56	1.47	1.38
1	B	931	TYR	CE1-CZ	6.40	1.46	1.38
1	A	931	TYR	CE2-CZ	6.33	1.46	1.38
1	A	1038	VAL	CB-CG2	-6.30	1.39	1.52
1	A	1308	TYR	CD1-CE1	6.17	1.48	1.39
1	B	931	TYR	CG-CD1	6.16	1.47	1.39
1	A	963	GLU	CG-CD	6.15	1.61	1.51
1	A	1078	PHE	CB-CG	-6.15	1.40	1.51
1	B	1036	GLY	C-O	6.12	1.33	1.23
1	B	931	TYR	CD2-CE2	5.93	1.48	1.39
1	A	1057	GLN	CB-CG	5.89	1.68	1.52
1	B	1078	PHE	CD1-CE1	5.87	1.50	1.39
1	B	899	GLU	CD-OE1	5.85	1.32	1.25
1	B	1078	PHE	CE1-CZ	5.84	1.48	1.37
1	A	902	ALA	CA-CB	-5.80	1.40	1.52
1	A	1054	GLU	CD-OE2	5.77	1.31	1.25
1	A	951	TYR	CE1-CZ	-5.62	1.31	1.38
1	A	1099	CYS	CB-SG	5.62	1.91	1.82
1	B	890	CYS	CB-SG	-5.61	1.72	1.81
1	B	902	ALA	CA-CB	-5.61	1.40	1.52
1	B	872	PHE	CD1-CE1	-5.60	1.28	1.39
1	B	1054	GLU	CD-OE1	5.58	1.31	1.25
1	A	983	LYS	CD-CE	5.55	1.65	1.51
1	B	1109	TRP	CB-CG	-5.54	1.40	1.50
1	B	1057	GLN	CB-CG	5.51	1.67	1.52
1	B	926	ALA	CA-CB	-5.51	1.40	1.52
1	A	931	TYR	CD2-CE2	5.50	1.47	1.39
1	B	1099	CYS	CB-SG	5.50	1.91	1.82
1	B	1084	GLU	CG-CD	5.49	1.60	1.51
1	A	1084	GLU	CD-OE2	5.48	1.31	1.25
1	A	926	ALA	CA-CB	-5.40	1.41	1.52
1	B	1071	ASP	CB-CG	5.36	1.62	1.51
1	A	931	TYR	CD1-CE1	5.34	1.47	1.39
1	A	775	ARG	CG-CD	5.29	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	809	TYR	CB-CG	-5.29	1.43	1.51
1	A	1079	CYS	CB-SG	-5.28	1.73	1.81
1	A	931	TYR	CG-CD2	5.27	1.46	1.39
1	B	992	ASP	CB-CG	5.22	1.62	1.51
1	A	761	ILE	C-O	5.10	1.33	1.23

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1071	ASP	CB-CG-OD1	10.07	127.37	118.30
1	A	824	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	B	1053	LYS	CD-CE-NZ	-9.41	90.05	111.70
1	A	941	LYS	CD-CE-NZ	-8.72	91.65	111.70
1	A	824	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	B	941	LYS	CD-CE-NZ	-8.52	92.11	111.70
1	B	306	ASP	CB-CG-OD2	8.51	125.95	118.30
1	A	1053	LYS	CD-CE-NZ	-8.16	92.92	111.70
1	A	876	LEU	CB-CG-CD1	-7.89	97.59	111.00
1	A	1087	CYS	CA-CB-SG	-7.59	100.33	114.00
1	B	486	LEU	CA-CB-CG	6.88	131.13	115.30
1	A	486	LEU	CA-CB-CG	6.82	130.99	115.30
1	A	999	MET	CG-SD-CE	6.72	110.95	100.20
1	A	559	LEU	CA-CB-CG	-6.50	100.34	115.30
1	A	1119	THR	C-N-CA	-6.47	105.52	121.70
1	B	863	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	B	698	CYS	CA-CB-SG	-6.19	102.85	114.00
1	A	890	CYS	CA-CB-SG	-6.18	102.87	114.00
1	B	801	GLY	N-CA-C	-6.11	97.82	113.10
1	B	757	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	890	CYS	CA-CB-SG	-5.92	103.34	114.00
1	B	960	ILE	CG1-CB-CG2	-5.89	98.44	111.40
1	A	757	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	964	LEU	CA-CB-CG	-5.83	101.90	115.30
1	B	775	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	819	VAL	CB-CA-C	-5.79	100.40	111.40
1	B	1158	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	B	1119	THR	C-N-CA	-5.64	107.59	121.70
1	A	1064	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	1278	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	1003	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	960	ILE	CG1-CB-CG2	-5.57	99.14	111.40
1	B	889	LEU	CA-CB-CG	-5.53	102.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	738	LEU	CA-CB-CG	-5.51	102.62	115.30
1	A	975	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	B	969	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	A	964	LEU	CA-CB-CG	-5.38	102.94	115.30
1	B	999	MET	CG-SD-CE	5.36	108.78	100.20
1	A	889	LEU	CA-CB-CG	-5.36	102.98	115.30
1	B	992	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	485	THR	N-CA-C	5.34	125.43	111.00
1	B	889	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	A	992	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	1158	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	863	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	B	1278	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	912	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	801	GLY	N-CA-C	-5.18	100.14	113.10
1	B	949	ILE	CG1-CB-CG2	-5.18	100.00	111.40
1	A	734	MET	CG-SD-CE	5.18	108.48	100.20
1	B	779	ASP	CB-CG-OD1	5.15	122.93	118.30
1	B	819	VAL	CB-CA-C	-5.08	101.74	111.40
1	B	559	LEU	CA-CB-CG	-5.07	103.64	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1215	ASN	Peptide
1	A	484	ALA	Peptide
1	A	747	GLU	Peptide
1	B	1215	ASN	Peptide
1	B	484	ALA	Peptide
1	B	790	ASP	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	7733	0	7482	253	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7733	0	7482	260	0
2	A	28	0	25	0	0
2	B	28	0	25	4	0
All	All	15522	0	15014	503	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 16.

All (503) 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:1057:GLN:CG	1:B:1057:GLN:CD	1.82	1.46
1:A:1057:GLN:CG	1:A:1057:GLN:CD	1.83	1.44
1:B:519:GLU:HG3	1:B:648:VAL:HG22	1.40	1.02
1:A:988:LYS:HG3	1:B:731:SER:HB3	1.41	1.02
1:A:727:SER:HB2	1:A:875:HIS:CD2	1.94	1.01
1:A:519:GLU:HG3	1:A:648:VAL:HG22	1.42	0.99
1:B:1278:ARG:HB3	1:B:1278:ARG:HH11	1.26	0.99
1:B:727:SER:HB2	1:B:875:HIS:CD2	1.96	0.99
1:A:1024:ALA:O	1:A:1026:ASN:ND2	1.96	0.98
1:A:1278:ARG:HB3	1:A:1278:ARG:HH11	1.24	0.97
1:B:667:ALA:HA	1:B:670:GLN:HB2	1.47	0.94
1:A:486:LEU:HG	1:A:662:ASP:HB2	1.49	0.94
1:A:599:ASN:O	1:A:600:THR:HB	1.65	0.93
1:A:618:ASP:HB3	1:A:619:GLU:OE2	1.69	0.91
1:B:1155:ARG:HH11	1:B:1155:ARG:HG3	1.37	0.89
1:A:667:ALA:HA	1:A:670:GLN:HB2	1.53	0.89
1:B:1228:GLY:HA3	1:B:1281:THR:HG22	1.56	0.86
1:A:1278:ARG:HB3	1:A:1278:ARG:NH1	1.90	0.86
1:B:1071:ASP:OD2	1:B:1074:SER:HB2	1.75	0.85
1:B:618:ASP:HB3	1:B:619:GLU:OE2	1.75	0.85
1:B:738:LEU:H	1:B:738:LEU:HD12	1.42	0.84
1:A:519:GLU:HG3	1:A:648:VAL:CG2	2.06	0.84
1:A:1183:ASP:HA	1:A:1199:ASN:O	1.79	0.82
1:A:1025:ARG:HD2	2:B:2000:NAG:H83	1.62	0.82
1:B:751:LEU:C	1:B:751:LEU:HD12	2.00	0.82
1:A:599:ASN:O	1:A:600:THR:CB	2.28	0.81
1:B:599:ASN:O	1:B:600:THR:HB	1.82	0.80
1:B:952:ASN:HD22	1:B:953:SER:N	1.78	0.80
1:B:1155:ARG:HG3	1:B:1155:ARG:NH1	1.95	0.80
1:B:519:GLU:HG3	1:B:648:VAL:CG2	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LEU:H	1:A:738:LEU:HD12	1.48	0.79
1:A:1101:ASN:O	1:A:1102:GLN:HB2	1.83	0.79
1:B:1278:ARG:HB3	1:B:1278:ARG:NH1	1.97	0.79
1:B:751:LEU:O	1:B:751:LEU:HD12	1.82	0.79
1:B:1174:ARG:HD3	1:B:1296:GLN:HE21	1.47	0.79
1:A:728:TYR:CE2	1:A:876:LEU:HD12	2.18	0.79
1:A:1228:GLY:HA3	1:A:1281:THR:HG22	1.65	0.78
1:B:738:LEU:HD12	1:B:738:LEU:N	1.99	0.77
1:B:1024:ALA:O	1:B:1026:ASN:ND2	2.17	0.77
1:A:988:LYS:CG	1:B:731:SER:HB3	2.14	0.77
1:B:667:ALA:HA	1:B:670:GLN:CB	2.14	0.76
1:A:688:LEU:C	1:A:690:ASN:H	1.89	0.75
1:A:305:SER:O	1:A:306:ASP:HB3	1.87	0.74
1:A:1161:ILE:HD12	1:A:1307:LEU:HB2	1.68	0.74
1:B:1101:ASN:O	1:B:1102:GLN:HB2	1.88	0.73
1:A:726:LEU:HD22	1:A:902:ALA:CB	2.18	0.73
1:A:488:PRO:HB3	1:A:652:ARG:HB3	1.71	0.73
1:A:667:ALA:HA	1:A:670:GLN:CB	2.18	0.73
1:B:426:SER:HB2	1:B:427:PRO:HD2	1.71	0.73
1:B:452:ASN:ND2	1:B:454:ASP:H	1.87	0.72
1:A:1174:ARG:HD3	1:A:1296:GLN:HE21	1.54	0.72
1:B:305:SER:O	1:B:306:ASP:HB3	1.88	0.72
1:B:353:ALA:O	1:B:354:LEU:HD12	1.90	0.72
1:A:548:PHE:O	1:A:548:PHE:CD2	2.43	0.71
1:A:738:LEU:HD12	1:A:738:LEU:N	2.05	0.71
1:A:452:ASN:ND2	1:A:454:ASP:H	1.88	0.70
1:B:318:ASN:HA	1:B:335:LEU:O	1.91	0.70
1:A:430:ALA:HB2	1:A:438:SER:HB3	1.71	0.70
1:B:431:ASP:O	1:B:432:LEU:C	2.29	0.70
1:A:353:ALA:O	1:A:354:LEU:HD12	1.92	0.69
1:B:475:VAL:O	1:B:476:VAL:HB	1.93	0.69
1:A:563:MET:CE	1:A:607:ALA:HB3	2.22	0.69
1:B:686:PRO:O	1:B:689:SER:HB3	1.93	0.69
1:A:738:LEU:HD22	1:A:742:MET:HG2	1.76	0.68
1:A:952:ASN:HD22	1:A:953:SER:N	1.92	0.68
1:B:429:THR:HG22	1:B:438:SER:HA	1.75	0.68
1:A:559:LEU:HG	1:A:560:LEU:N	2.09	0.67
1:A:751:LEU:C	1:A:751:LEU:HD12	2.15	0.67
1:B:306:ASP:OD2	1:B:374:ARG:HD3	1.95	0.67
1:B:587:PHE:CD1	1:B:587:PHE:C	2.66	0.67
1:A:302:GLN:HA	1:A:415:LEU:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLN:HA	1:B:415:LEU:O	1.94	0.66
1:B:688:LEU:C	1:B:690:ASN:H	1.96	0.66
1:A:688:LEU:C	1:A:690:ASN:N	2.47	0.66
1:B:587:PHE:C	1:B:587:PHE:HD1	1.99	0.66
1:B:292:PHE:HB2	1:B:423:VAL:HB	1.78	0.66
1:A:1155:ARG:NH1	1:A:1155:ARG:HG3	2.11	0.65
1:A:1155:ARG:HG3	1:A:1155:ARG:HH11	1.62	0.65
1:A:589:ARG:HB3	1:A:605:TYR:OH	1.96	0.65
1:B:488:PRO:HB3	1:B:652:ARG:HB3	1.77	0.65
1:A:292:PHE:HB2	1:A:423:VAL:HB	1.79	0.65
1:B:1174:ARG:HD3	1:B:1296:GLN:NE2	2.12	0.65
1:A:751:LEU:HD12	1:A:751:LEU:O	1.96	0.65
1:A:426:SER:HB2	1:A:427:PRO:HD2	1.79	0.65
1:A:306:ASP:OD2	1:A:374:ARG:HD3	1.98	0.64
1:A:921:SER:HA	1:A:1080:ASN:O	1.97	0.64
1:A:1020:ILE:O	1:A:1020:ILE:HG23	1.98	0.64
1:A:618:ASP:CB	1:A:619:GLU:OE2	2.45	0.64
1:B:1020:ILE:HG23	1:B:1020:ILE:O	1.96	0.64
1:B:589:ARG:HB3	1:B:605:TYR:OH	1.97	0.64
1:A:1071:ASP:OD2	1:A:1074:SER:HB2	1.98	0.64
1:A:351:PHE:CE1	1:A:406:GLY:HA3	2.33	0.64
1:A:311:SER:HB2	1:A:446:LYS:HB3	1.79	0.63
1:A:686:PRO:O	1:A:689:SER:HB3	1.98	0.63
1:A:688:LEU:O	1:A:690:ASN:N	2.32	0.63
1:B:1150:ASP:O	1:B:1152:PRO:HD3	1.98	0.63
1:A:727:SER:HB2	1:A:875:HIS:HD2	1.55	0.63
1:B:1159:LEU:C	1:B:1159:LEU:HD23	2.19	0.63
1:A:431:ASP:O	1:A:432:LEU:C	2.35	0.62
1:A:429:THR:HG22	1:A:438:SER:HA	1.79	0.62
1:B:538:LYS:HD2	1:B:792:ILE:HD13	1.82	0.62
1:A:432:LEU:HD12	1:A:435:SER:HB2	1.82	0.62
1:A:726:LEU:HD22	1:A:902:ALA:HB1	1.81	0.62
1:B:1216:ASP:OD2	1:B:1218:LYS:HB2	2.00	0.62
1:B:563:MET:CE	1:B:607:ALA:HB3	2.30	0.62
1:B:602:ARG:HH11	1:B:602:ARG:HB2	1.65	0.61
1:A:318:ASN:HA	1:A:335:LEU:O	2.01	0.61
1:A:969:LEU:HG	1:A:970:HIS:N	2.14	0.61
1:B:688:LEU:C	1:B:690:ASN:N	2.52	0.61
1:A:369:ASP:HB2	1:A:399:ASP:HA	1.83	0.61
1:B:311:SER:HB2	1:B:446:LYS:HB3	1.82	0.61
1:B:952:ASN:C	1:B:952:ASN:HD22	2.04	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:ARG:HH11	2:B:2000:NAG:H83	1.65	0.60
1:A:1183:ASP:N	1:A:1183:ASP:OD2	2.33	0.60
1:B:1184:TYR:CD1	1:B:1184:TYR:C	2.74	0.60
1:A:502:LYS:HE2	1:A:618:ASP:H	1.66	0.60
1:A:708:ASP:OD1	1:A:710:SER:OG	2.17	0.60
1:B:738:LEU:HD22	1:B:742:MET:HG2	1.84	0.60
1:B:351:PHE:CE1	1:B:406:GLY:HA3	2.37	0.60
1:A:548:PHE:C	1:A:548:PHE:CD2	2.71	0.59
1:A:757:ARG:HD2	1:A:873:ILE:HD12	1.84	0.59
1:B:1141:GLN:HE22	1:B:1295:GLU:HG2	1.68	0.59
1:B:512:SER:HA	1:B:585:VAL:O	2.02	0.59
1:B:751:LEU:CD1	1:B:751:LEU:C	2.71	0.59
1:B:884:MET:HB2	1:B:886:TYR:CE1	2.37	0.59
1:B:900:LEU:N	1:B:900:LEU:HD23	2.18	0.59
1:A:663:ILE:C	1:A:665:GLN:H	2.06	0.58
1:B:548:PHE:HA	1:B:560:LEU:O	2.03	0.58
1:B:727:SER:HB2	1:B:875:HIS:HD2	1.60	0.58
1:A:563:MET:HE1	1:A:607:ALA:HB3	1.85	0.58
1:B:1183:ASP:HA	1:B:1199:ASN:O	2.02	0.58
1:A:1150:ASP:O	1:A:1152:PRO:HD3	2.03	0.58
1:B:346:LEU:CD2	1:B:415:LEU:HB2	2.34	0.58
1:B:618:ASP:CB	1:B:619:GLU:OE2	2.51	0.58
1:B:346:LEU:HD23	1:B:415:LEU:HB2	1.85	0.58
1:B:476:VAL:O	1:B:477:ALA:HB2	2.04	0.58
1:A:514:ASP:OD1	1:A:584:HIS:HA	2.04	0.58
1:A:726:LEU:HD22	1:A:902:ALA:HB3	1.85	0.58
1:A:476:VAL:O	1:A:477:ALA:HB2	2.04	0.57
1:B:559:LEU:HG	1:B:560:LEU:N	2.20	0.57
1:B:599:ASN:O	1:B:600:THR:CB	2.51	0.57
1:A:311:SER:HB2	1:A:446:LYS:HE2	1.86	0.57
1:B:889:LEU:CD2	1:B:894:ASP:HB2	2.35	0.57
1:A:1025:ARG:HD2	2:B:2000:NAG:C8	2.32	0.57
1:A:1174:ARG:HD3	1:A:1296:GLN:NE2	2.20	0.57
1:A:1296:GLN:CD	1:A:1296:GLN:H	2.08	0.57
1:A:1022:ALA:HB2	1:B:1158:ARG:HD3	1.85	0.57
1:B:1161:ILE:HD12	1:B:1307:LEU:HB2	1.86	0.57
1:A:305:SER:O	1:A:306:ASP:CB	2.53	0.56
1:B:757:ARG:HD2	1:B:873:ILE:HD12	1.87	0.56
1:A:1009:THR:HG23	1:A:1018:THR:HG22	1.87	0.56
1:B:1137:LYS:HA	1:B:1301:GLN:HE21	1.70	0.56
1:A:1159:LEU:HD23	1:A:1159:LEU:C	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:LEU:CD2	1:A:894:ASP:HB2	2.35	0.56
1:A:1184:TYR:C	1:A:1184:TYR:CD1	2.79	0.56
1:B:302:GLN:HG3	1:B:302:GLN:O	2.05	0.56
1:B:305:SER:O	1:B:306:ASP:CB	2.54	0.56
1:A:548:PHE:HA	1:A:560:LEU:O	2.06	0.56
1:B:831:THR:HB	1:B:837:ALA:HA	1.87	0.56
1:B:551:GLU:OE1	1:B:640:THR:HG23	2.06	0.55
1:A:1190:HIS:ND1	1:A:1191:GLN:HG3	2.21	0.55
1:A:475:VAL:O	1:A:476:VAL:HB	2.07	0.55
1:A:884:MET:HB2	1:A:886:TYR:CE1	2.41	0.55
1:B:1005:SER:O	1:B:1006:ASN:HB2	2.07	0.55
1:A:377:ARG:CB	1:A:408:THR:OG1	2.55	0.55
1:B:663:ILE:C	1:B:665:GLN:H	2.09	0.55
1:A:302:GLN:HG3	1:A:302:GLN:O	2.06	0.55
1:B:1183:ASP:N	1:B:1183:ASP:OD2	2.40	0.55
1:A:322:LEU:HD12	1:A:421:PHE:CE1	2.43	0.54
1:A:570:ILE:CD1	1:A:605:TYR:HB3	2.37	0.54
1:A:570:ILE:HD13	1:A:605:TYR:HB3	1.88	0.54
1:B:949:ILE:O	1:B:949:ILE:HG22	2.04	0.54
1:A:1143:THR:HG23	1:A:1290:ILE:HG12	1.88	0.54
1:A:1216:ASP:OD2	1:A:1218:LYS:HB2	2.08	0.54
1:A:364:ASP:OD2	1:A:366:ALA:HB3	2.08	0.54
1:A:532:ARG:HH21	1:A:544:LYS:HB3	1.71	0.54
1:B:426:SER:CB	1:B:427:PRO:HD2	2.36	0.54
1:A:931:TYR:HD1	1:A:932:THR:H	1.55	0.54
1:A:1025:ARG:CD	2:B:2000:NAG:H83	2.35	0.54
1:B:430:ALA:HB2	1:B:438:SER:HB3	1.88	0.54
1:A:665:GLN:HA	1:A:669:VAL:HG23	1.89	0.54
1:B:311:SER:HB2	1:B:446:LYS:HE2	1.88	0.54
1:B:969:LEU:HD23	1:B:1012:ILE:HD11	1.89	0.54
1:B:726:LEU:HD22	1:B:902:ALA:CB	2.38	0.54
1:A:791:CYS:O	1:A:792:ILE:HD12	2.08	0.54
1:B:486:LEU:HG	1:B:662:ASP:HB2	1.91	0.53
1:B:432:LEU:HD12	1:B:435:SER:HB2	1.89	0.53
1:B:728:TYR:CE2	1:B:876:LEU:HD12	2.44	0.53
1:B:377:ARG:CB	1:B:408:THR:OG1	2.57	0.53
1:B:786:THR:HG23	1:B:804:THR:HG22	1.89	0.53
1:A:1159:LEU:HD23	1:A:1160:ALA:N	2.24	0.53
1:A:900:LEU:HD23	1:A:900:LEU:N	2.22	0.53
1:A:1083:ILE:N	1:A:1083:ILE:HD12	2.24	0.53
1:A:889:LEU:HD23	1:A:894:ASP:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1159:LEU:HD23	1:B:1160:ALA:N	2.22	0.53
1:B:639:TRP:CZ3	1:B:824:ARG:HB3	2.44	0.53
1:A:487:ASP:HB2	1:A:664:ARG:CB	2.38	0.53
1:A:831:THR:HB	1:A:837:ALA:HA	1.90	0.53
1:B:486:LEU:HG	1:B:662:ASP:CB	2.38	0.53
1:B:315:LEU:HD13	1:B:485:THR:HG22	1.91	0.53
1:B:1165:THR:O	1:B:1215:ASN:HA	2.09	0.52
1:A:1015:LYS:HD3	1:B:1109:TRP:CD2	2.45	0.52
1:B:322:LEU:HD12	1:B:421:PHE:CE1	2.44	0.52
1:A:1087:CYS:SG	1:A:1087:CYS:O	2.66	0.52
1:B:1143:THR:HG23	1:B:1290:ILE:HG12	1.92	0.52
1:A:1112:PHE:CD1	1:A:1112:PHE:C	2.83	0.52
1:B:969:LEU:CD2	1:B:1012:ILE:HD11	2.39	0.52
1:A:463:ALA:HA	1:A:470:MET:HG2	1.91	0.52
1:B:726:LEU:HD22	1:B:902:ALA:HB3	1.92	0.52
1:B:931:TYR:N	1:B:931:TYR:CD1	2.77	0.52
1:A:311:SER:CB	1:A:446:LYS:HE2	2.40	0.52
1:B:1228:GLY:CA	1:B:1281:THR:HG22	2.34	0.52
1:A:512:SER:HA	1:A:585:VAL:O	2.09	0.52
1:A:742:MET:HG3	1:A:851:PHE:CZ	2.45	0.52
1:B:315:LEU:O	1:B:363:ASN:HB2	2.09	0.52
1:B:369:ASP:HB2	1:B:399:ASP:HA	1.92	0.52
1:B:1009:THR:HG23	1:B:1018:THR:HG22	1.92	0.51
1:A:656:ILE:HG13	1:A:661:LYS:HG3	1.92	0.51
1:B:921:SER:HA	1:B:1080:ASN:O	2.10	0.51
1:B:742:MET:HG3	1:B:851:PHE:CZ	2.46	0.51
1:A:845:ASP:OD1	1:A:845:ASP:N	2.43	0.51
1:A:948:LEU:HD12	1:A:949:ILE:H	1.76	0.51
1:A:639:TRP:CZ3	1:A:824:ARG:HB3	2.46	0.51
1:B:1190:HIS:ND1	1:B:1191:GLN:HG3	2.25	0.51
1:B:532:ARG:HH21	1:B:544:LYS:HB3	1.76	0.51
1:B:570:ILE:HD13	1:B:605:TYR:HB3	1.92	0.51
1:B:889:LEU:HD23	1:B:894:ASP:HB2	1.92	0.51
1:A:308:ILE:HD13	1:A:450:TYR:HD1	1.76	0.51
1:B:772:ASP:OD1	1:B:790:ASP:HB2	2.11	0.51
1:A:1169:GLU:OE1	1:A:1190:HIS:HA	2.11	0.51
1:A:663:ILE:C	1:A:665:GLN:N	2.64	0.51
1:A:1020:ILE:O	1:A:1020:ILE:CG2	2.58	0.50
1:A:374:ARG:HA	1:A:378:GLN:O	2.11	0.50
1:B:738:LEU:H	1:B:738:LEU:CD1	2.20	0.50
1:B:548:PHE:CD2	1:B:548:PHE:O	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:VAL:O	1:A:477:ALA:CB	2.59	0.50
1:B:519:GLU:CG	1:B:648:VAL:HG22	2.27	0.50
1:A:322:LEU:HD12	1:A:421:PHE:HE1	1.76	0.50
1:A:438:SER:O	1:A:658:GLY:HA2	2.10	0.50
1:A:775:ARG:HG3	1:A:786:THR:OG1	2.12	0.50
1:A:346:LEU:CD2	1:A:415:LEU:HB2	2.41	0.50
1:B:502:LYS:HE2	1:B:618:ASP:H	1.77	0.50
1:A:426:SER:CB	1:A:427:PRO:HD2	2.40	0.50
1:B:431:ASP:O	1:B:432:LEU:O	2.29	0.50
1:B:452:ASN:HD21	1:B:454:ASP:HB2	1.77	0.50
1:B:1318:ALA:HA	1:B:1325:ILE:HG21	1.93	0.49
1:B:311:SER:CB	1:B:446:LYS:HE2	2.42	0.49
1:A:1317:MET:CE	1:A:1322:ASP:OD1	2.60	0.49
1:B:1020:ILE:CG2	1:B:1020:ILE:O	2.60	0.49
1:B:1112:PHE:CD1	1:B:1112:PHE:C	2.86	0.49
1:B:959:PHE:CD1	1:B:959:PHE:C	2.84	0.49
1:A:955:ASP:OD1	1:A:1030:LYS:HG3	2.12	0.49
1:A:521:ASN:HB3	1:A:645:TYR:CD2	2.48	0.49
1:B:475:VAL:O	1:B:476:VAL:CB	2.60	0.49
1:B:613:ILE:N	1:B:613:ILE:HD12	2.27	0.49
1:B:1137:LYS:HA	1:B:1301:GLN:NE2	2.28	0.49
1:B:329:ASP:OD1	1:B:414:MET:O	2.31	0.49
1:B:663:ILE:C	1:B:665:GLN:N	2.66	0.49
1:B:656:ILE:HG13	1:B:661:LYS:HG3	1.94	0.49
1:B:734:MET:HE3	1:B:736:ILE:HD12	1.93	0.49
1:B:1222:VAL:HG13	1:B:1222:VAL:O	2.12	0.49
1:A:1186:GLU:HG2	1:A:1186:GLU:O	2.12	0.49
1:B:955:ASP:OD1	1:B:1030:LYS:HG3	2.11	0.49
1:A:493:THR:C	1:A:648:VAL:HG12	2.33	0.49
1:B:729:ASP:OD1	1:B:732:MET:HG3	2.13	0.48
1:A:480:CYS:SG	1:A:481:GLU:N	2.83	0.48
1:A:737:GLN:O	1:A:738:LEU:C	2.51	0.48
1:B:665:GLN:HA	1:B:669:VAL:HG23	1.94	0.48
1:B:686:PRO:O	1:B:689:SER:CB	2.60	0.48
1:A:298:GLN:HG2	1:A:469:LYS:HE3	1.95	0.48
1:A:946:ASP:HA	1:A:964:LEU:O	2.13	0.48
1:A:1022:ALA:CB	1:B:1158:ARG:HD3	2.42	0.48
1:A:1063:VAL:HG21	1:A:1072:LEU:HD11	1.94	0.48
1:B:364:ASP:OD2	1:B:366:ALA:HB3	2.13	0.48
1:B:587:PHE:HD1	1:B:588:GLN:N	2.11	0.48
1:B:784:LYS:HG3	1:B:806:PHE:CE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:THR:O	1:A:1215:ASN:HA	2.14	0.48
1:B:965:VAL:O	1:B:966:LYS:HB2	2.13	0.48
1:A:511:ILE:CG2	1:A:587:PHE:HB3	2.43	0.48
1:A:681:ARG:HG3	1:A:702:TRP:CH2	2.48	0.48
1:B:320:LEU:HA	1:B:334:ALA:HB2	1.95	0.48
1:A:1002:ARG:NH1	1:A:1026:ASN:OD1	2.46	0.48
1:A:1144:TYR:HA	1:A:1325:ILE:HD13	1.96	0.48
1:B:1296:GLN:CD	1:B:1296:GLN:H	2.17	0.48
1:A:751:LEU:C	1:A:751:LEU:CD1	2.81	0.48
1:A:728:TYR:HE2	1:A:876:LEU:HD12	1.75	0.48
1:A:952:ASN:HD22	1:A:952:ASN:C	2.17	0.48
1:B:476:VAL:O	1:B:477:ALA:CB	2.62	0.48
1:B:480:CYS:SG	1:B:481:GLU:N	2.83	0.48
1:B:919:LYS:HG2	1:B:1055:GLY:O	2.13	0.48
1:B:949:ILE:CG2	1:B:949:ILE:O	2.59	0.48
1:B:688:LEU:O	1:B:690:ASN:N	2.47	0.48
1:B:791:CYS:O	1:B:792:ILE:HB	2.14	0.47
1:A:519:GLU:CG	1:A:648:VAL:HG22	2.30	0.47
1:A:964:LEU:HA	1:A:964:LEU:HD12	1.50	0.47
1:A:315:LEU:O	1:A:363:ASN:HB2	2.13	0.47
1:A:1015:LYS:HD3	1:B:1109:TRP:CE2	2.49	0.47
1:A:1101:ASN:O	1:A:1102:GLN:CB	2.55	0.47
1:A:919:LYS:HG2	1:A:1055:GLY:O	2.15	0.47
1:A:1027:LEU:HD12	1:B:1155:ARG:NE	2.29	0.47
1:B:1159:LEU:C	1:B:1159:LEU:CD2	2.83	0.47
1:A:311:SER:HA	1:A:368:HIS:O	2.15	0.47
1:A:587:PHE:C	1:A:587:PHE:CD1	2.83	0.47
1:B:1197:LYS:HA	1:B:1205:ILE:O	2.14	0.47
1:B:1207:ILE:O	1:B:1207:ILE:HG23	2.15	0.47
1:A:759:TYR:HA	1:A:778:LEU:O	2.14	0.47
1:A:728:TYR:CZ	1:A:876:LEU:HD12	2.50	0.47
1:B:317:ARG:HH11	1:B:317:ARG:HG3	1.78	0.47
1:B:845:ASP:N	1:B:845:ASP:OD1	2.42	0.47
1:A:1307:LEU:HD23	1:A:1314:VAL:HB	1.96	0.47
1:A:395:THR:HG23	1:A:403:THR:HG23	1.97	0.47
1:A:602:ARG:HH11	1:A:602:ARG:HB2	1.79	0.47
1:B:317:ARG:CG	1:B:317:ARG:HH11	2.28	0.47
1:B:737:GLN:O	1:B:738:LEU:C	2.51	0.47
1:A:965:VAL:O	1:A:966:LYS:HB2	2.15	0.47
1:B:1092:THR:O	1:B:1111:GLY:HA2	2.14	0.47
1:A:339:ALA:HB1	1:A:355:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:LEU:HA	1:B:334:ALA:CB	2.45	0.47
1:B:311:SER:HA	1:B:368:HIS:O	2.15	0.47
1:B:395:THR:HG23	1:B:403:THR:HG23	1.96	0.47
1:A:1141:GLN:HE22	1:A:1295:GLU:HG2	1.80	0.47
1:A:1174:ARG:HG3	1:A:1186:GLU:HB2	1.96	0.47
1:B:1101:ASN:O	1:B:1102:GLN:CB	2.58	0.47
1:B:681:ARG:HG3	1:B:702:TRP:CH2	2.49	0.47
1:B:928:LEU:HD21	1:B:936:LEU:HD21	1.97	0.47
1:A:289:SER:HB3	1:A:659:GLN:OE1	2.14	0.47
1:B:988:LYS:HB2	1:B:988:LYS:HE3	1.58	0.47
1:B:1155:ARG:CG	1:B:1155:ARG:HH11	2.18	0.46
1:A:1003:ASP:OD1	1:A:1003:ASP:C	2.54	0.46
1:A:1296:GLN:CD	1:A:1296:GLN:N	2.68	0.46
1:A:551:GLU:OE1	1:A:640:THR:HG23	2.15	0.46
1:A:317:ARG:HH11	1:A:317:ARG:HG3	1.79	0.46
1:B:655:PHE:HA	1:B:659:GLN:O	2.15	0.46
1:A:1072:LEU:HD23	1:A:1072:LEU:HA	1.53	0.46
1:A:452:ASN:HD21	1:A:454:ASP:HB2	1.80	0.46
1:A:992:ASP:OD2	1:A:994:GLN:NE2	2.48	0.46
1:B:282:TYR:HB3	1:B:460:SER:HB3	1.96	0.46
1:B:469:LYS:HA	1:B:469:LYS:HD3	1.78	0.46
1:B:969:LEU:HG	1:B:970:HIS:N	2.30	0.46
1:A:939:GLN:HA	1:A:996:HIS:O	2.15	0.46
1:B:1072:LEU:HA	1:B:1072:LEU:HD23	1.42	0.46
1:B:339:ALA:HB1	1:B:355:VAL:O	2.15	0.46
1:B:570:ILE:CD1	1:B:605:TYR:HB3	2.46	0.46
1:A:556:HIS:NE2	1:A:576:LYS:HG2	2.31	0.46
1:B:1016:ILE:HG22	1:B:1018:THR:HG23	1.98	0.46
1:A:991:ASN:N	1:A:991:ASN:OD1	2.41	0.46
1:B:1002:ARG:NH1	1:B:1026:ASN:OD1	2.49	0.46
1:B:367:TRP:CZ3	1:B:446:LYS:HB2	2.52	0.45
1:A:282:TYR:HB3	1:A:460:SER:HB3	1.97	0.45
1:A:868:VAL:O	1:A:869:PRO:C	2.53	0.45
1:B:1065:LEU:CD1	1:B:1070:PRO:HG3	2.46	0.45
1:B:514:ASP:OD1	1:B:584:HIS:HA	2.16	0.45
1:B:759:TYR:HA	1:B:778:LEU:O	2.16	0.45
1:B:841:GLN:HA	1:B:841:GLN:OE1	2.16	0.45
1:B:1030:LYS:HD3	1:B:1030:LYS:HA	1.82	0.45
1:B:772:ASP:HA	1:B:788:ASN:O	2.17	0.45
1:B:788:ASN:HD22	1:B:802:PRO:HB3	1.82	0.45
1:A:315:LEU:HD13	1:A:485:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:ASP:OD1	1:A:732:MET:HG3	2.17	0.45
1:B:586:ASP:OD2	1:B:588:GLN:NE2	2.50	0.45
1:A:1005:SER:O	1:A:1006:ASN:HB2	2.17	0.45
1:B:332:ASN:ND2	1:B:435:SER:HA	2.32	0.45
1:B:931:TYR:HD1	1:B:932:THR:H	1.64	0.45
1:A:1317:MET:HE3	1:A:1322:ASP:OD1	2.17	0.45
1:B:322:LEU:HD12	1:B:421:PHE:HE1	1.81	0.45
1:B:952:ASN:HB2	1:B:1033:LEU:HD12	1.97	0.45
1:B:685:LYS:HE3	1:B:685:LYS:HB2	1.88	0.45
1:A:621:TYR:OH	1:A:629:LYS:HD3	2.16	0.45
1:A:786:THR:HG23	1:A:804:THR:HG22	1.98	0.45
1:B:552:MET:HA	1:B:556:HIS:O	2.16	0.45
1:B:991:ASN:OD1	1:B:991:ASN:N	2.43	0.45
1:A:377:ARG:HB3	1:A:408:THR:OG1	2.16	0.44
1:A:317:ARG:HH11	1:A:317:ARG:CG	2.30	0.44
1:B:374:ARG:HA	1:B:378:GLN:O	2.17	0.44
1:A:636:THR:HG21	1:A:848:ARG:HG3	1.98	0.44
1:B:928:LEU:HD13	1:B:1065:LEU:HB3	1.99	0.44
1:B:343:VAL:HG21	1:B:434:GLY:O	2.18	0.44
1:B:308:ILE:HD13	1:B:450:TYR:HD1	1.82	0.44
1:A:1158:ARG:HH11	1:A:1158:ARG:HD2	1.55	0.44
1:B:1003:ASP:C	1:B:1003:ASP:OD1	2.55	0.44
1:A:736:ILE:HG12	1:A:886:TYR:CD2	2.52	0.44
1:A:1185:LEU:HD12	1:A:1186:GLU:N	2.32	0.44
1:A:557:LEU:HG	1:A:558:TYR:N	2.33	0.44
1:A:579:ASP:OD2	1:A:583:TYR:OH	2.36	0.44
1:A:749:VAL:HG22	1:A:881:PHE:CD1	2.53	0.44
1:B:708:ASP:OD1	1:B:710:SER:OG	2.27	0.44
1:B:805:LEU:HA	1:B:805:LEU:HD23	1.79	0.44
1:A:931:TYR:CD1	1:A:931:TYR:N	2.84	0.44
1:B:734:MET:CE	1:B:736:ILE:CD1	2.96	0.44
1:A:489:ILE:CD1	1:A:664:ARG:HA	2.48	0.43
1:A:551:GLU:HG2	1:A:560:LEU:HD13	2.00	0.43
1:A:884:MET:CB	1:A:886:TYR:CE1	3.01	0.43
1:B:1132:THR:HG23	1:B:1305:SER:HB2	2.00	0.43
1:B:1158:ARG:HD2	1:B:1158:ARG:HH11	1.54	0.43
1:B:1169:GLU:HA	1:B:1189:ILE:O	2.18	0.43
1:B:681:ARG:O	1:B:682:GLU:C	2.56	0.43
1:B:1173:VAL:HG13	1:B:1187:LEU:HB3	2.01	0.43
1:B:557:LEU:HG	1:B:558:TYR:N	2.33	0.43
1:B:636:THR:HG21	1:B:848:ARG:HG3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889:LEU:HD23	1:B:889:LEU:HA	1.53	0.43
1:A:1016:ILE:HG22	1:A:1018:THR:HG23	2.00	0.43
1:A:1309:TYR:O	1:A:1310:ASN:C	2.56	0.43
1:A:398:VAL:C	1:A:400:GLY:H	2.21	0.43
1:A:734:MET:HE3	1:A:736:ILE:HD12	2.01	0.43
1:B:298:GLN:HG2	1:B:469:LYS:HE3	2.01	0.43
1:B:436:PRO:HD2	1:B:437:VAL:H	1.83	0.43
1:A:548:PHE:HD1	1:A:587:PHE:HE2	1.64	0.43
1:A:681:ARG:O	1:A:682:GLU:C	2.56	0.43
1:B:727:SER:HB2	1:B:875:HIS:NE2	2.32	0.43
1:A:1159:LEU:CD2	1:A:1159:LEU:C	2.86	0.43
1:A:310:LEU:O	1:A:310:LEU:HD12	2.19	0.43
1:A:329:ASP:OD1	1:A:414:MET:O	2.37	0.43
1:B:1144:TYR:HA	1:B:1325:ILE:HD13	2.01	0.43
1:B:1309:TYR:O	1:B:1310:ASN:C	2.57	0.43
1:B:663:ILE:HA	1:B:666:MET:HB2	2.01	0.43
1:B:961:VAL:CG1	1:B:962:VAL:N	2.82	0.43
1:A:1092:THR:O	1:A:1111:GLY:HA2	2.19	0.43
1:A:1134:ILE:HD12	1:A:1332:ARG:HH22	1.83	0.43
1:B:522:GLY:HA2	1:B:645:TYR:O	2.19	0.43
1:B:734:MET:CE	1:B:736:ILE:HD12	2.49	0.43
1:A:1012:ILE:HD12	1:A:1012:ILE:HG23	1.69	0.43
1:A:772:ASP:OD1	1:A:790:ASP:HB2	2.19	0.43
1:B:1063:VAL:HG21	1:B:1072:LEU:HD11	2.01	0.42
1:B:1307:LEU:HD23	1:B:1314:VAL:HB	2.01	0.42
1:B:573:LEU:HD12	1:B:574:GLN:H	1.84	0.42
1:B:511:ILE:HG23	1:B:587:PHE:HB3	2.01	0.42
1:B:952:ASN:HD22	1:B:953:SER:H	1.62	0.42
1:A:320:LEU:HA	1:A:334:ALA:CB	2.48	0.42
1:A:570:ILE:CD1	1:A:605:TYR:CB	2.97	0.42
1:A:488:PRO:CB	1:A:652:ARG:HB3	2.46	0.42
1:A:988:LYS:CD	1:B:731:SER:HB3	2.49	0.42
1:B:398:VAL:C	1:B:400:GLY:H	2.23	0.42
1:A:791:CYS:O	1:A:792:ILE:HB	2.19	0.42
1:B:521:ASN:HB3	1:B:645:TYR:CD2	2.55	0.42
1:B:532:ARG:NH2	1:B:544:LYS:HB3	2.34	0.42
1:B:793:ARG:HB2	1:B:793:ARG:HE	1.70	0.42
1:B:294:TYR:HD2	1:B:296:LEU:HD23	1.85	0.42
1:B:523:LEU:HD11	1:B:526:PHE:HB2	2.02	0.42
1:B:952:ASN:HB2	1:B:1033:LEU:CD1	2.50	0.42
1:A:1041:GLU:HA	1:A:1041:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LEU:HA	1:A:334:ALA:HB2	2.00	0.42
1:B:327:SER:HB2	1:B:328:ALA:H	1.46	0.42
1:B:1296:GLN:CD	1:B:1296:GLN:N	2.73	0.42
1:A:495:GLU:N	1:A:495:GLU:OE2	2.51	0.42
1:B:1196:VAL:HG12	1:B:1197:LYS:N	2.35	0.41
1:B:551:GLU:HG2	1:B:560:LEU:HD13	2.01	0.41
1:B:749:VAL:HG22	1:B:881:PHE:CD1	2.55	0.41
1:A:308:ILE:CD1	1:A:450:TYR:HD1	2.33	0.41
1:B:603:THR:HA	1:B:604:PRO:HD2	1.90	0.41
1:B:964:LEU:HA	1:B:964:LEU:HD12	1.61	0.41
1:A:832:VAL:O	1:A:833:ASP:HB2	2.19	0.41
1:A:985:SER:HG	1:B:1109:TRP:HE1	1.67	0.41
1:B:900:LEU:H	1:B:900:LEU:HD23	1.83	0.41
1:A:449:VAL:HG13	1:A:458:GLU:HA	2.02	0.41
1:A:486:LEU:HG	1:A:662:ASP:CB	2.35	0.41
1:A:779:ASP:OD1	1:A:779:ASP:C	2.59	0.41
1:B:488:PRO:HB3	1:B:652:ARG:CB	2.46	0.41
1:B:1087:CYS:SG	1:B:1087:CYS:O	2.79	0.41
1:B:322:LEU:CD2	1:B:333:LEU:HD23	2.50	0.41
1:A:488:PRO:HB3	1:A:652:ARG:CB	2.47	0.41
1:A:493:THR:HB	1:A:495:GLU:OE2	2.20	0.41
1:B:1069:LEU:HA	1:B:1070:PRO:HD2	1.91	0.41
1:B:992:ASP:OD2	1:B:994:GLN:NE2	2.54	0.41
1:A:1169:GLU:HA	1:A:1189:ILE:O	2.20	0.41
1:A:1233:LEU:HA	1:A:1233:LEU:HD12	1.65	0.41
1:A:398:VAL:C	1:A:400:GLY:N	2.73	0.41
1:A:532:ARG:NH1	1:A:564:GLY:HA2	2.36	0.41
1:A:591:GLY:HA2	1:A:612:GLU:O	2.20	0.41
1:A:738:LEU:CD1	1:A:738:LEU:H	2.27	0.41
1:B:790:ASP:OD2	1:B:791:CYS:N	2.44	0.41
1:A:1214:ILE:C	1:A:1214:ILE:HD12	2.41	0.41
1:A:570:ILE:HD11	1:A:605:TYR:HB2	2.03	0.41
1:B:563:MET:HE1	1:B:607:ALA:HB3	2.01	0.41
1:A:1228:GLY:CA	1:A:1281:THR:HG22	2.43	0.41
1:A:662:ASP:O	1:A:666:MET:HE2	2.22	0.40
1:A:643:LEU:HD21	1:A:824:ARG:NH2	2.36	0.40
1:A:1027:LEU:HD12	1:B:1155:ARG:CZ	2.50	0.40
1:B:868:VAL:HB	1:B:869:PRO:HD2	2.02	0.40
1:A:400:GLY:O	1:A:401:ILE:CB	2.69	0.40
1:A:548:PHE:CD1	1:A:587:PHE:HE2	2.39	0.40
1:A:603:THR:HA	1:A:604:PRO:HD2	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:MET:HE2	1:B:607:ALA:HB3	2.00	0.40
1:B:776:LEU:HD23	1:B:776:LEU:HA	1.90	0.40
1:A:1300:PHE:CG	1:A:1301:GLN:N	2.89	0.40
1:A:512:SER:HB2	1:A:584:HIS:HE1	1.87	0.40
1:A:552:MET:HA	1:A:556:HIS:O	2.21	0.40
1:A:489:ILE:O	1:A:650:CYS:HA	2.21	0.40
1:B:1051:HIS:O	1:B:1052:ALA:C	2.60	0.40
1:B:450:TYR:CZ	1:B:452:ASN:HB3	2.55	0.40
1:B:877:GLN:O	1:B:878:SER:HB2	2.21	0.40
1:B:939:GLN:HA	1:B:996:HIS:O	2.21	0.40
1:A:1024:ALA:O	1:A:1025:ARG:C	2.59	0.40
1:A:1234:GLN:NE2	1:A:1236:ASP:O	2.55	0.40
1:A:1318:ALA:HA	1:A:1325:ILE:HG21	2.03	0.40
1:A:475:VAL:O	1:A:476:VAL:CB	2.70	0.40
1:A:728:TYR:CE2	1:A:876:LEU:CD1	2.99	0.40
1:B:1083:ILE:HD12	1:B:1083:ILE:N	2.36	0.40
1:B:317:ARG:HG2	1:B:337:ASN:HA	2.03	0.40
1:A:1106:LEU:HD11	1:A:1115:ASP:HB2	2.04	0.40
1:A:686:PRO:O	1:A:689:SER:CB	2.69	0.40
1:B:362:PHE:C	1:B:364:ASP:H	2.24	0.40
1:B:493:THR:HB	1:B:495:GLU:OE2	2.22	0.40
1:B:742:MET:HB3	1:B:851:PHE:CE2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1004/1254 (80%)	881 (88%)	97 (10%)	26 (3%)	6	28
1	B	1004/1254 (80%)	881 (88%)	96 (10%)	27 (3%)	6	27
All	All	2008/2508 (80%)	1762 (88%)	193 (10%)	53 (3%)	6	28

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	A	401	ILE
1	A	476	VAL
1	A	477	ALA
1	A	506	LYS
1	A	666	MET
1	A	677	PRO
1	A	689	SER
1	A	792	ILE
1	B	327	SER
1	B	401	ILE
1	B	476	VAL
1	B	477	ALA
1	B	506	LYS
1	B	666	MET
1	B	677	PRO
1	B	689	SER
1	B	792	ILE
1	B	1278	ARG
1	A	306	ASP
1	A	475	VAL
1	A	600	THR
1	A	682	GLU
1	A	920	SER
1	A	930	ALA
1	A	1278	ARG
1	B	434	GLY
1	B	475	VAL
1	B	682	GLU
1	B	930	ALA
1	A	399	ASP
1	A	434	GLY
1	B	399	ASP
1	B	485	THR
1	B	600	THR
1	B	664	ARG
1	B	920	SER
1	A	363	ASN
1	A	833	ASP
1	A	1045	SER
1	B	337	ASN
1	B	573	LEU

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Mol	Chain	Res	Type
1	A	337	ASN
1	A	1179	SER
1	A	1209	GLU
1	B	363	ASN
1	B	791	CYS
1	A	1148	PRO
1	B	436	PRO
1	B	1047	PRO
1	B	483	VAL
1	A	483	VAL
1	B	1148	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	839/1068 (79%)	742 (88%)	97 (12%)	6	24
1	B	839/1068 (79%)	747 (89%)	92 (11%)	7	26
All	All	1678/2136 (79%)	1489 (89%)	189 (11%)	7	25

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	ILE
1	A	303	SER
1	A	305	SER
1	A	307	GLU
1	A	308	ILE
1	A	317	ARG
1	A	326	LYS
1	A	329	ASP
1	A	365	ASN
1	A	377	ARG
1	A	402	LEU
1	A	419	ASP

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Mol	Chain	Res	Type
1	A	421	PHE
1	A	432	LEU
1	A	438	SER
1	A	455	VAL
1	A	458	GLU
1	A	482	ASN
1	A	486	LEU
1	A	489	ILE
1	A	495	GLU
1	A	498	ILE
1	A	506	LYS
1	A	511	ILE
1	A	518	THR
1	A	542	MET
1	A	546	ASP
1	A	548	PHE
1	A	561	LEU
1	A	588	GLN
1	A	589	ARG
1	A	592	ARG
1	A	611	SER
1	A	616	LEU
1	A	617	ASP
1	A	620	LEU
1	A	633	VAL
1	A	656	ILE
1	A	662	ASP
1	A	678	SER
1	A	682	GLU
1	A	688	LEU
1	A	697	MET
1	A	717	ARG
1	A	727	SER
1	A	731	SER
1	A	734	MET
1	A	763	MET
1	A	773	THR
1	A	786	THR
1	A	795	ASN
1	A	824	ARG
1	A	831	THR
1	A	847	THR

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Mol	Chain	Res	Type
1	A	853	ASN
1	A	862	ARG
1	A	867	SER
1	A	898	CYS
1	A	899	GLU
1	A	907	ARG
1	A	914	VAL
1	A	931	TYR
1	A	932	THR
1	A	941	LYS
1	A	944	SER
1	A	952	ASN
1	A	969	LEU
1	A	971	TYR
1	A	985	SER
1	A	989	PRO
1	A	1026	ASN
1	A	1049	LEU
1	A	1054	GLU
1	A	1068	ARG
1	A	1074	SER
1	A	1079	CYS
1	A	1082	GLN
1	A	1085	ARG
1	A	1088	GLU
1	A	1091	SER
1	A	1150	ASP
1	A	1153	SER
1	A	1155	ARG
1	A	1159	LEU
1	A	1173	VAL
1	A	1176	ASP
1	A	1181	LEU
1	A	1183	ASP
1	A	1185	LEU
1	A	1221	VAL
1	A	1234	GLN
1	A	1235	VAL
1	A	1278	ARG
1	A	1281	THR
1	A	1283	PHE
1	A	1295	GLU

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Mol	Chain	Res	Type
1	A	1336	GLU
1	B	283	ILE
1	B	303	SER
1	B	305	SER
1	B	307	GLU
1	B	308	ILE
1	B	317	ARG
1	B	326	LYS
1	B	365	ASN
1	B	377	ARG
1	B	402	LEU
1	B	419	ASP
1	B	421	PHE
1	B	432	LEU
1	B	438	SER
1	B	455	VAL
1	B	458	GLU
1	B	482	ASN
1	B	485	THR
1	B	486	LEU
1	B	489	ILE
1	B	498	ILE
1	B	499	SER
1	B	506	LYS
1	B	511	ILE
1	B	518	THR
1	B	542	MET
1	B	546	ASP
1	B	548	PHE
1	B	561	LEU
1	B	587	PHE
1	B	588	GLN
1	B	589	ARG
1	B	592	ARG
1	B	611	SER
1	B	616	LEU
1	B	617	ASP
1	B	620	LEU
1	B	633	VAL
1	B	648	VAL
1	B	656	ILE
1	B	662	ASP

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Mol	Chain	Res	Type
1	B	665	GLN
1	B	678	SER
1	B	682	GLU
1	B	688	LEU
1	B	717	ARG
1	B	727	SER
1	B	731	SER
1	B	734	MET
1	B	763	MET
1	B	773	THR
1	B	786	THR
1	B	795	ASN
1	B	831	THR
1	B	847	THR
1	B	853	ASN
1	B	862	ARG
1	B	863	ARG
1	B	867	SER
1	B	899	GLU
1	B	907	ARG
1	B	914	VAL
1	B	931	TYR
1	B	932	THR
1	B	941	LYS
1	B	944	SER
1	B	952	ASN
1	B	971	TYR
1	B	1026	ASN
1	B	1049	LEU
1	B	1054	GLU
1	B	1074	SER
1	B	1079	CYS
1	B	1082	GLN
1	B	1085	ARG
1	B	1088	GLU
1	B	1153	SER
1	B	1155	ARG
1	B	1159	LEU
1	B	1173	VAL
1	B	1181	LEU
1	B	1183	ASP
1	B	1185	LEU

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Mol	Chain	Res	Type
1	B	1186	GLU
1	B	1221	VAL
1	B	1234	GLN
1	B	1278	ARG
1	B	1281	THR
1	B	1283	PHE
1	B	1294	LYS
1	B	1295	GLU
1	B	1336	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	365	ASN
1	A	452	ASN
1	A	788	ASN
1	A	952	ASN
1	A	994	GLN
1	A	1301	GLN
1	A	1321	ASN
1	B	365	ASN
1	B	378	GLN
1	B	440	ASN
1	B	452	ASN
1	B	588	GLN
1	B	743	HIS
1	B	788	ASN
1	B	952	ASN
1	B	1008	HIS
1	B	1141	GLN
1	B	1301	GLN
1	B	1321	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

4 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
2	NAG	A	2000	1,2	14,14,15	0.86	0	15,19,21	2.91	10 (66%)
2	NAG	A	2001	2	14,14,15	0.61	0	15,19,21	1.41	2 (13%)
2	NAG	B	2000	1,2	14,14,15	0.82	0	15,19,21	3.01	8 (53%)
2	NAG	B	2001	2	14,14,15	0.82	1 (7%)	15,19,21	1.23	3 (20%)

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	NAG	A	2000	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2001	2	-	0/6/23/26	0/1/1/1
2	NAG	B	2000	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2001	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	NAG	C1-C2	2.16	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2000	NAG	O7-C7-C8	-4.32	114.19	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2000	NAG	O7-C7-C8	-3.64	115.43	122.06
2	B	2000	NAG	O4-C4-C3	-3.21	103.38	110.36
2	A	2000	NAG	O4-C4-C3	-3.09	103.63	110.36
2	A	2001	NAG	C1-O5-C5	-2.69	108.45	112.17
2	A	2001	NAG	C2-N2-C7	-2.35	119.51	122.94
2	B	2001	NAG	C1-O5-C5	-2.30	108.99	112.17
2	B	2001	NAG	C2-N2-C7	-2.02	119.99	122.94
2	A	2000	NAG	O3-C3-C4	2.03	114.78	110.36
2	B	2000	NAG	C6-C5-C4	2.12	117.96	113.00
2	A	2000	NAG	O6-C6-C5	2.31	119.12	111.34
2	B	2001	NAG	C4-C3-C2	2.35	114.46	111.02
2	A	2000	NAG	C6-C5-C4	2.61	119.12	113.00
2	B	2000	NAG	O6-C6-C5	2.64	120.21	111.34
2	A	2000	NAG	O7-C7-N2	2.71	127.14	121.92
2	A	2000	NAG	C4-C3-C2	2.88	115.24	111.02
2	B	2000	NAG	O7-C7-N2	3.07	127.83	121.92
2	A	2000	NAG	C2-N2-C7	3.28	127.73	122.94
2	A	2000	NAG	C1-C2-N2	3.93	117.21	110.49
2	B	2000	NAG	C2-N2-C7	3.99	128.76	122.94
2	B	2000	NAG	C1-C2-N2	4.08	117.45	110.49
2	A	2000	NAG	C1-O5-C5	5.97	120.39	112.17
2	B	2000	NAG	C1-O5-C5	6.90	121.67	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2000	NAG	4	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	1008/1254 (80%)	0.19	76 (7%) 15 8	35, 91, 151, 196	0
1	B	1008/1254 (80%)	0.20	68 (6%) 19 10	34, 92, 152, 201	0
All	All	2016/2508 (80%)	0.20	144 (7%) 17 9	34, 91, 152, 201	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	472	ILE	5.9
1	A	359	ASN	5.7
1	B	358	VAL	5.7
1	A	480	CYS	5.5
1	B	284	ALA	5.5
1	B	445	LEU	5.4
1	A	358	VAL	5.2
1	B	794	ILE	5.2
1	A	294	TYR	5.1
1	A	445	LEU	5.0
1	A	300	PRO	4.9
1	A	1337	VAL	4.8
1	A	481	GLU	4.7
1	A	284	ALA	4.6
1	A	296	LEU	4.6
1	B	359	ASN	4.6
1	A	478	PHE	4.6
1	A	293	CYS	4.3
1	A	425	GLY	4.1
1	A	444	CYS	4.0
1	B	481	GLU	3.9
1	B	614	LEU	3.9
1	A	295	ASP	3.8
1	B	476	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	1335	GLY	3.7
1	B	312	PHE	3.7
1	A	312	PHE	3.7
1	B	301	ILE	3.7
1	B	615	ASP	3.7
1	A	357	PRO	3.7
1	B	478	PHE	3.6
1	A	301	ILE	3.6
1	B	795	ASN	3.6
1	A	417	SER	3.5
1	A	283	ILE	3.5
1	A	311	SER	3.4
1	B	311	SER	3.4
1	A	362	PHE	3.4
1	A	367	TRP	3.4
1	A	462	LEU	3.3
1	B	470	MET	3.3
1	B	293	CYS	3.3
1	B	294	TYR	3.3
1	B	283	ILE	3.3
1	A	356	GLU	3.2
1	A	472	ILE	3.1
1	A	795	ASN	3.1
1	B	1337	VAL	3.1
1	A	422	TYR	3.1
1	A	470	MET	3.1
1	A	297	SER	3.1
1	A	538	LYS	3.1
1	A	794	ILE	3.1
1	A	320	LEU	3.1
1	A	423	VAL	3.0
1	B	367	TRP	3.0
1	B	413	THR	3.0
1	B	357	PRO	3.0
1	B	444	CYS	3.0
1	B	538	LYS	3.0
1	A	488	PRO	2.9
1	A	615	ASP	2.9
1	B	286	PHE	2.9
1	B	1303	GLN	2.8
1	B	308	ILE	2.8
1	A	285	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1025	ARG	2.8
1	B	616	LEU	2.8
1	B	480	CYS	2.7
1	B	1319	ALA	2.7
1	B	362	PHE	2.7
1	B	613	ILE	2.7
1	B	462	LEU	2.7
1	A	424	GLY	2.7
1	A	310	LEU	2.6
1	B	1336	GLU	2.6
1	A	286	PHE	2.6
1	B	417	SER	2.6
1	A	471	LYS	2.6
1	A	298	GLN	2.6
1	A	468	PRO	2.6
1	A	614	LEU	2.6
1	B	1133	TYR	2.6
1	B	356	GLU	2.5
1	A	482	ASN	2.5
1	A	651	ILE	2.5
1	A	475	VAL	2.5
1	B	407	TYR	2.5
1	A	1200	VAL	2.5
1	A	420	PHE	2.4
1	A	476	VAL	2.4
1	A	465	GLN	2.4
1	A	792	ILE	2.4
1	B	1100	SER	2.4
1	A	616	LEU	2.4
1	A	407	TYR	2.4
1	B	421	PHE	2.4
1	A	299	ASN	2.4
1	B	792	ILE	2.4
1	B	504	ASN	2.4
1	A	292	PHE	2.3
1	A	669	VAL	2.3
1	A	368	HIS	2.3
1	A	453	ASN	2.3
1	B	793	ARG	2.3
1	A	1336	GLU	2.3
1	B	791	CYS	2.3
1	B	422	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	801	GLY	2.3
1	B	1332	ARG	2.3
1	B	320	LEU	2.3
1	B	465	GLN	2.3
1	B	534	GLN	2.3
1	A	414	MET	2.3
1	B	475	VAL	2.2
1	A	421	PHE	2.2
1	B	1132	THR	2.2
1	B	298	GLN	2.2
1	A	793	ARG	2.2
1	A	720	GLU	2.2
1	B	468	PRO	2.2
1	B	454	ASP	2.2
1	B	285	THR	2.2
1	A	427	PRO	2.2
1	B	503	TRP	2.1
1	B	617	ASP	2.1
1	B	471	LYS	2.1
1	A	533	HIS	2.1
1	B	300	PRO	2.1
1	A	413	THR	2.1
1	A	473	HIS	2.1
1	B	303	SER	2.1
1	B	355	VAL	2.1
1	B	297	SER	2.1
1	A	640	THR	2.1
1	B	401	ILE	2.1
1	B	1327	ILE	2.1
1	A	282	TYR	2.0
1	B	296	LEU	2.0
1	A	608	PRO	2.0
1	B	368	HIS	2.0
1	A	1213	ILE	2.0
1	A	370	VAL	2.0
1	A	446	LYS	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 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	NAG	B	2000	14/15	0.85	0.18	-0.15	87,101,111,114	0
2	NAG	A	2000	14/15	0.86	0.16	-0.35	89,102,110,114	0
2	NAG	A	2001	14/15	0.84	0.23	-	110,124,129,133	0
2	NAG	B	2001	14/15	0.82	0.33	-	113,126,132,134	0

6.5 Other polymers [i](#)

There are no such residues in this entry.