



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:01 AM GMT

PDB ID : 2PDA  
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN PYRUVATE-FERREDOXIN OXIDOREDUCTASE FROM DESULFOVIBRIO AFRICANUS AND PYRUVATE.  
Authors : Chabriere, E.; Charon, M.H.  
Deposited on : 1998-11-10  
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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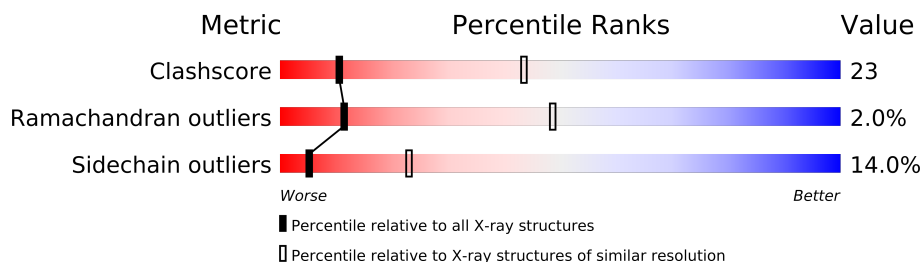
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1231	
1	B	1231	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18894 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1231	Total	C	N	O	S	25	0	0
			9382	5941	1599	1783	59			
1	B	1231	Total	C	N	O	S	25	0	0
			9382	5941	1599	1783	59			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

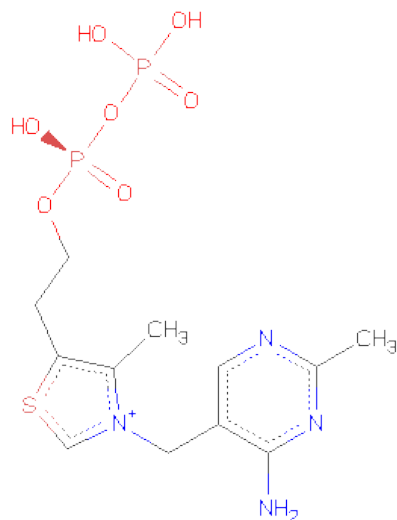
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



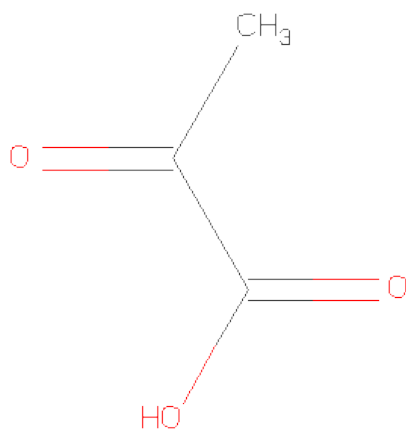
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
5	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 6 is PYRUVIC ACID (three-letter code: PYR) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>).

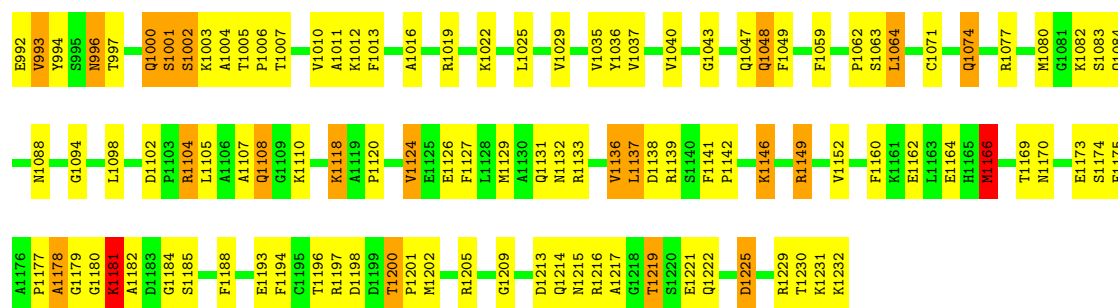


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

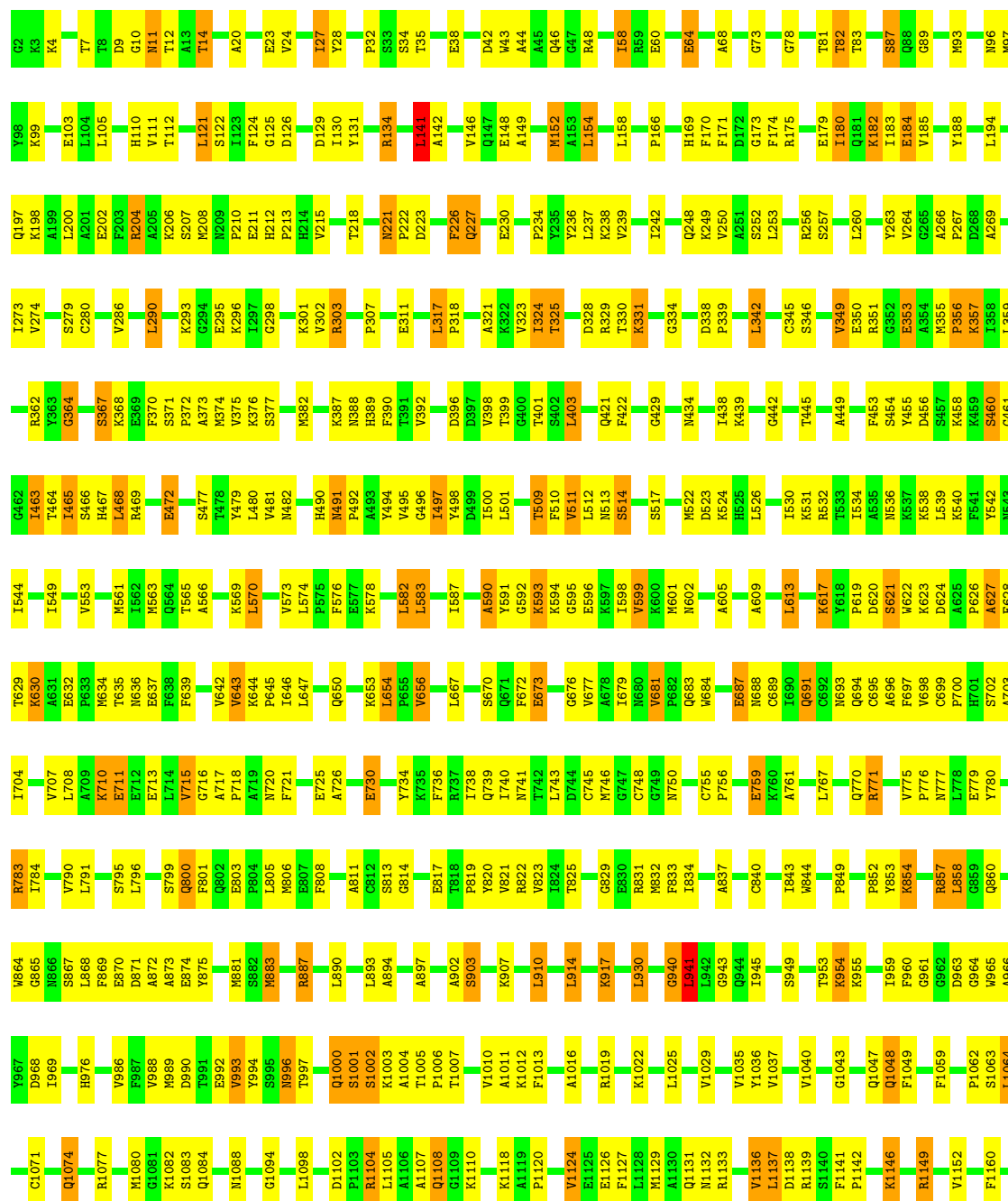
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total 7	O 7	0	0
7	B	7	Total 7	O 7	0	0





• Molecule 1: PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE)

Chain B:





E1164	H1165	M1166	T1169	N1170	I1171	F1172	E1173	S1174	F1175	A1176	P1177	A1178	G1179	G1180	K1181	A1182	D1183	G1184	S1185	F1188	E1193	F1194	G1195	T1196	R1197	D1198	D1199	T1200	P1201	M1202	D1213	Q1214	N1215	R1216	T1219	S1220	E1221	Q1222	D1225	R1229	T1230	K1231	K1232
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.00Å 146.30Å 211.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	94.2 (10.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	X-PLOR 3.854	Depositor
R, $R_{free}$	0.234 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18894	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, PYR, CA, TPP

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	0.66	0/9584	0.89	13/12954 (0.1%)
1	B	0.66	0/9584	0.89	13/12954 (0.1%)
All	All	0.66	0/19168	0.89	26/25908 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1166	MET	N-CA-C	-6.13	94.45	111.00
1	B	1166	MET	N-CA-C	-6.13	94.45	111.00
1	A	364	GLY	N-CA-C	5.78	127.55	113.10
1	B	364	GLY	N-CA-C	5.78	127.54	113.10
1	A	141	LEU	CA-CB-CG	5.72	128.46	115.30
1	B	141	LEU	CA-CB-CG	5.71	128.44	115.30
1	B	592	GLY	N-CA-C	-5.62	99.05	113.10
1	A	592	GLY	N-CA-C	-5.60	99.09	113.10
1	A	654	LEU	CA-CB-CG	5.49	127.92	115.30
1	B	654	LEU	CA-CB-CG	5.48	127.91	115.30
1	B	627	ALA	N-CA-C	5.47	125.77	111.00
1	A	627	ALA	N-CA-C	5.45	125.72	111.00
1	A	711	GLU	N-CA-C	5.35	125.45	111.00
1	B	497	ILE	N-CA-C	5.35	125.44	111.00
1	A	497	ILE	N-CA-C	5.35	125.44	111.00
1	B	711	GLU	N-CA-C	5.34	125.41	111.00
1	B	759	GLU	N-CA-C	-5.23	96.87	111.00
1	A	253	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	759	GLU	N-CA-C	-5.23	96.88	111.00
1	B	253	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	708	LEU	N-CA-C	-5.10	97.22	111.00
1	A	708	LEU	N-CA-C	-5.10	97.22	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	GLY	N-CA-C	5.06	125.74	113.10
1	B	125	GLY	N-CA-C	5.06	125.74	113.10
1	B	590	ALA	N-CA-C	-5.03	97.43	111.00
1	A	590	ALA	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9382	0	9263	458	4
1	B	9382	0	9263	454	4
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	24	0	0	4	0
4	B	24	0	0	4	0
5	A	26	0	16	7	0
5	B	26	0	16	7	0
6	A	6	0	3	3	0
6	B	6	0	3	3	0
7	A	7	0	0	0	0
7	B	7	0	0	0	0
All	All	18894	0	18564	864	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (864) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1184:GLY:HA3	1:B:1141:PHE:HZ	1.17	1.08
1:B:805:LEU:HA	1:B:854:LYS:HZ2	1.17	1.06

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.37	1.04
1:B:124:PHE:HB3	1:B:367:SER:HB2	1.37	1.02
1:A:68:ALA:HB2	1:A:93:MET:HG2	1.46	0.97
1:B:68:ALA:HB2	1:B:93:MET:HG2	1.46	0.97
1:A:1141:PHE:HZ	1:B:1184:GLY:HA3	1.31	0.95
1:A:1184:GLY:HA3	1:B:1141:PHE:CZ	2.02	0.94
1:A:805:LEU:HA	1:A:854:LYS:NZ	1.83	0.92
1:B:805:LEU:HA	1:B:854:LYS:NZ	1.83	0.92
1:B:1149:ARG:HG3	1:B:1149:ARG:HH11	1.36	0.91
1:A:1149:ARG:HH11	1:A:1149:ARG:HG3	1.36	0.90
1:A:805:LEU:HA	1:A:854:LYS:HZ2	1.38	0.88
1:A:1132:ASN:O	1:A:1136:VAL:HG22	1.75	0.86
1:B:1132:ASN:O	1:B:1136:VAL:HG22	1.75	0.86
1:B:639:PHE:HA	1:B:643:VAL:HG13	1.58	0.85
1:B:9:ASP:OD1	1:B:12:THR:HG23	1.77	0.84
1:A:9:ASP:OD1	1:A:12:THR:HG23	1.77	0.84
1:A:492:PRO:O	1:A:495:VAL:HG12	1.78	0.84
1:A:1000:GLN:HA	1:A:1012:LYS:HB2	1.60	0.83
1:A:639:PHE:HA	1:A:643:VAL:HG13	1.58	0.83
1:B:1000:GLN:HA	1:B:1012:LYS:HB2	1.60	0.82
1:B:110:HIS:CD2	1:B:169:HIS:HD2	1.97	0.82
1:B:99:LYS:O	1:B:103:GLU:HG3	1.79	0.82
1:B:492:PRO:O	1:B:495:VAL:HG12	1.78	0.82
1:A:110:HIS:CD2	1:A:169:HIS:HD2	1.97	0.81
1:A:99:LYS:O	1:A:103:GLU:HG3	1.79	0.81
1:A:130:ILE:HG13	1:A:131:TYR:N	1.95	0.80
1:A:688:ASN:ND2	1:A:759:GLU:HB2	1.97	0.80
1:B:831:ARG:HD2	1:B:954:LYS:O	1.82	0.80
1:A:1184:GLY:CA	1:B:1141:PHE:HZ	1.95	0.80
1:B:544:ILE:HD12	1:B:613:LEU:HD13	1.63	0.80
1:A:455:TYR:HB2	1:B:1201:PRO:HG3	1.63	0.80
1:B:130:ILE:HG13	1:B:131:TYR:N	1.95	0.79
1:A:831:ARG:HD2	1:A:954:LYS:O	1.82	0.79
1:A:544:ILE:HD12	1:A:613:LEU:HD13	1.63	0.79
1:B:688:ASN:ND2	1:B:759:GLU:HB2	1.97	0.78
1:A:755:CYS:SG	1:A:761:ALA:HB3	2.23	0.78
1:B:1132:ASN:HD21	1:B:1139:ARG:HH12	1.32	0.77
1:B:755:CYS:SG	1:B:761:ALA:HB3	2.23	0.77
1:A:1141:PHE:CZ	1:B:1184:GLY:HA3	2.18	0.77
1:A:330:THR:O	1:A:362:ARG:HD3	1.84	0.77
1:A:1132:ASN:HD21	1:A:1139:ARG:HH12	1.32	0.77
1:B:739:GLN:HE22	1:B:777:ASN:HB3	1.50	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:330:THR:O	1:B:362:ARG:HD3	1.84	0.77
1:A:739:GLN:HE22	1:A:777:ASN:HB3	1.49	0.76
5:B:1243:TPP:H7'2	6:B:1246:PYP:O1	1.86	0.76
1:B:1137:LEU:HD22	1:B:1141:PHE:HB2	1.67	0.76
1:A:1193:GLU:OE1	1:B:1077:ARG:HA	1.86	0.76
1:A:639:PHE:CE2	1:A:672:PHE:HB2	2.22	0.75
1:A:1137:LEU:HD22	1:A:1141:PHE:HB2	1.67	0.75
5:A:1236:TPP:H7'2	6:A:1239:PYP:O1	1.86	0.75
1:B:639:PHE:CE2	1:B:672:PHE:HB2	2.22	0.74
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.36	0.74
1:A:857:ARG:HG3	1:A:858:LEU:HD13	1.69	0.74
1:A:523:ASP:HA	1:A:531:LYS:HZ3	1.52	0.74
1:B:857:ARG:HG3	1:B:858:LEU:HD13	1.69	0.74
1:A:110:HIS:HD2	1:A:169:HIS:HD2	1.36	0.74
1:A:1201:PRO:HG3	1:B:455:TYR:HB2	1.69	0.73
1:A:234:PRO:HA	1:A:237:LEU:HD12	1.71	0.73
1:B:234:PRO:HA	1:B:237:LEU:HD12	1.71	0.72
1:B:523:ASP:HA	1:B:531:LYS:NZ	2.05	0.72
1:B:14:THR:HG22	1:B:149:ALA:HB1	1.72	0.72
1:A:14:THR:HG22	1:A:149:ALA:HB1	1.72	0.72
1:A:523:ASP:HA	1:A:531:LYS:NZ	2.05	0.72
1:B:126:ASP:HA	1:B:329:ARG:HD3	1.71	0.71
1:A:126:ASP:HA	1:A:329:ARG:HD3	1.71	0.71
1:B:180:ILE:HD11	1:B:438:ILE:HG21	1.72	0.70
1:A:561:MET:HE1	1:A:583:LEU:HD21	1.74	0.70
1:A:130:ILE:HG13	1:A:131:TYR:H	1.56	0.70
1:B:82:THR:HG22	1:B:83:THR:H	1.57	0.69
1:A:180:ILE:HD11	1:A:438:ILE:HG21	1.72	0.69
1:B:561:MET:HE1	1:B:583:LEU:HD21	1.74	0.69
1:A:467:HIS:HB3	1:A:481:VAL:HG23	1.75	0.69
1:A:873:ALA:HA	1:A:959:ILE:HD13	1.75	0.68
1:B:130:ILE:HG13	1:B:131:TYR:H	1.56	0.68
1:B:467:HIS:HB3	1:B:481:VAL:HG23	1.75	0.68
1:A:697:PHE:HD2	1:A:800:GLN:NE2	1.92	0.68
1:B:643:VAL:O	1:B:647:LEU:HG	1.94	0.68
1:A:82:THR:HG22	1:A:83:THR:H	1.57	0.67
1:A:643:VAL:O	1:A:647:LEU:HG	1.94	0.67
1:B:883:MET:O	1:B:887:ARG:HB2	1.95	0.67
1:A:883:MET:O	1:A:887:ARG:HB2	1.95	0.67
1:B:873:ALA:HA	1:B:959:ILE:HD13	1.75	0.67
1:B:697:PHE:HD2	1:B:800:GLN:NE2	1.92	0.66
1:A:1181:LYS:H	1:B:1019:ARG:HH12	1.43	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1166:MET:O	1:A:1169:THR:HG22	1.96	0.66
1:B:1077:ARG:HH11	1:B:1077:ARG:HB2	1.61	0.66
1:A:141:LEU:HD13	1:A:152:MET:HG3	1.77	0.66
1:B:771:ARG:O	1:B:775:VAL:HG23	1.96	0.66
1:B:1035:VAL:HG22	1:B:1062:PRO:HB2	1.79	0.65
1:B:1166:MET:O	1:B:1169:THR:HG22	1.96	0.65
1:A:771:ARG:O	1:A:775:VAL:HG23	1.96	0.65
1:A:456:ASP:HB2	1:A:463:ILE:O	1.96	0.65
1:B:917:LYS:HZ3	1:B:917:LYS:HB3	1.60	0.65
1:B:460:SER:HB3	1:B:746:MET:HE2	1.79	0.65
1:B:141:LEU:HD13	1:B:152:MET:HG3	1.77	0.65
1:A:1077:ARG:HH11	1:A:1077:ARG:HB2	1.61	0.64
1:A:460:SER:HB3	1:A:746:MET:HE2	1.79	0.64
1:B:456:ASP:HB2	1:B:463:ILE:O	1.96	0.64
1:A:154:LEU:HD22	1:A:158:LEU:HD11	1.79	0.64
1:B:154:LEU:HD22	1:B:158:LEU:HD11	1.80	0.64
1:A:667:LEU:HB3	1:A:853:TYR:O	1.97	0.64
1:A:1035:VAL:HG22	1:A:1062:PRO:HB2	1.79	0.64
1:B:667:LEU:HB3	1:B:853:TYR:O	1.97	0.64
1:A:1216:ARG:HA	1:B:746:MET:O	1.97	0.64
1:A:368:LYS:NZ	1:B:227:GLN:HE22	1.95	0.64
1:B:968:ASP:OD1	1:B:1003:LYS:HB2	1.99	0.63
1:A:1232:LYS:NZ	1:A:1232:LYS:HB3	2.14	0.63
1:A:779:GLU:HB3	1:A:783:ARG:NH1	2.13	0.63
1:B:64:GLU:HG3	1:B:89:GLY:HA2	1.81	0.63
1:B:779:GLU:HB3	1:B:783:ARG:NH1	2.13	0.63
1:B:523:ASP:HA	1:B:531:LYS:HZ3	1.63	0.63
1:A:832:MET:HE1	1:A:834:ILE:HD11	1.81	0.63
1:A:64:GLU:HG3	1:A:89:GLY:HA2	1.81	0.63
1:B:445:THR:HG21	1:B:574:LEU:HD21	1.80	0.63
1:A:34:SER:O	1:A:38:GLU:HG3	1.98	0.63
1:B:34:SER:O	1:B:38:GLU:HG3	1.97	0.63
1:B:438:ILE:HG23	1:B:449:ALA:HB1	1.80	0.62
1:B:890:LEU:HD11	1:B:945:ILE:HG23	1.81	0.62
1:A:445:THR:HG21	1:A:574:LEU:HD21	1.80	0.62
1:B:1198:ASP:OD1	1:B:1200:THR:HB	2.00	0.62
1:A:890:LEU:HD11	1:A:945:ILE:HG23	1.81	0.62
1:A:968:ASP:OD1	1:A:1003:LYS:HB2	1.99	0.62
1:A:1141:PHE:HZ	1:B:1184:GLY:CA	2.10	0.62
1:A:438:ILE:HG23	1:A:449:ALA:HB1	1.80	0.62
1:B:1232:LYS:HB3	1:B:1232:LYS:NZ	2.14	0.62
1:A:142:ALA:HB2	1:A:170:PHE:CZ	2.35	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:325:THR:CG2	1:A:382:MET:SD	2.88	0.62
1:A:1219:THR:HG21	1:B:1082:LYS:HZ3	1.65	0.62
1:B:522:MET:SD	1:B:526:LEU:HD13	2.40	0.62
1:B:142:ALA:HB2	1:B:170:PHE:CZ	2.35	0.62
1:A:1198:ASP:OD1	1:A:1200:THR:HB	1.99	0.62
1:B:467:HIS:CD2	1:B:481:VAL:H	2.18	0.61
1:A:325:THR:HG23	1:A:382:MET:SD	2.40	0.61
1:B:325:THR:CG2	1:B:382:MET:SD	2.88	0.61
1:A:917:LYS:HB3	1:A:917:LYS:HZ3	1.65	0.61
1:A:467:HIS:CD2	1:A:481:VAL:H	2.18	0.61
1:B:148:GLU:O	1:B:152:MET:HB2	2.00	0.61
1:A:148:GLU:O	1:A:152:MET:HB2	2.00	0.61
1:B:325:THR:HG23	1:B:382:MET:SD	2.41	0.61
1:B:1124:VAL:O	1:B:1127:PHE:HB3	2.01	0.61
1:A:398:VAL:HG13	1:A:656:VAL:CG2	2.31	0.61
1:A:180:ILE:HD11	1:A:438:ILE:CG2	2.30	0.61
1:A:522:MET:SD	1:A:526:LEU:HD13	2.40	0.61
1:A:1124:VAL:O	1:A:1127:PHE:HB3	2.01	0.61
1:B:180:ILE:HD11	1:B:438:ILE:CG2	2.30	0.60
1:B:398:VAL:HG13	1:B:656:VAL:CG2	2.31	0.60
1:A:993:VAL:HG22	1:A:1000:GLN:O	2.01	0.60
1:A:465:ILE:HD12	1:A:466:SER:N	2.17	0.60
1:A:154:LEU:HD22	1:A:158:LEU:CD1	2.31	0.60
1:B:993:VAL:HG22	1:B:1000:GLN:O	2.01	0.60
1:B:779:GLU:HB3	1:B:783:ARG:HH12	1.68	0.59
1:A:976:HIS:CD2	1:B:1003:LYS:HD3	2.38	0.59
1:A:460:SER:HB3	1:A:746:MET:CE	2.33	0.59
1:B:154:LEU:HD22	1:B:158:LEU:CD1	2.31	0.59
1:B:465:ILE:HD12	1:B:466:SER:N	2.17	0.59
1:A:236:TYR:HA	1:A:239:VAL:HG12	1.84	0.59
1:A:700:PRO:HG3	1:A:814:GLY:HA2	1.85	0.59
1:A:1016:ALA:HB1	1:A:1019:ARG:HH21	1.66	0.59
1:A:549:ILE:O	1:A:553:VAL:HG22	2.03	0.59
1:B:700:PRO:HG3	1:B:814:GLY:HA2	1.85	0.59
1:B:832:MET:HE1	1:B:834:ILE:HD11	1.82	0.59
1:B:639:PHE:CD2	1:B:672:PHE:HB2	2.37	0.59
1:A:1181:LYS:H	1:B:1019:ARG:NH1	2.01	0.59
1:A:356:PRO:O	1:A:357:LYS:HB3	2.02	0.59
1:B:894:ALA:CB	1:B:914:LEU:HD21	2.33	0.59
1:B:549:ILE:O	1:B:553:VAL:HG22	2.03	0.59
1:A:730:GLU:H	1:A:730:GLU:CD	2.05	0.59
1:A:639:PHE:CD2	1:A:672:PHE:HB2	2.37	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:917:LYS:HB3	1:A:917:LYS:NZ	2.18	0.59
1:A:87:SER:HA	1:A:129:ASP:HB3	1.85	0.59
1:A:676:GLY:HA3	1:A:743:LEU:HD22	1.84	0.59
1:A:494:TYR:HB3	1:A:500:ILE:HD11	1.84	0.59
1:B:730:GLU:CD	1:B:730:GLU:H	2.05	0.59
1:A:1077:ARG:HA	1:B:1193:GLU:OE1	2.02	0.58
1:B:494:TYR:HB3	1:B:500:ILE:HD11	1.84	0.58
1:A:894:ALA:CB	1:A:914:LEU:HD21	2.33	0.58
1:B:643:VAL:HB	1:B:849:PRO:HB2	1.85	0.58
1:B:356:PRO:O	1:B:357:LYS:HB3	2.02	0.58
1:A:396:ASP:HA	1:A:656:VAL:HG13	1.84	0.58
1:B:676:GLY:HA3	1:B:743:LEU:HD22	1.84	0.58
1:B:87:SER:HA	1:B:129:ASP:HB3	1.85	0.58
1:A:9:ASP:HA	1:A:179:GLU:O	2.03	0.58
1:A:643:VAL:HB	1:A:849:PRO:HB2	1.85	0.58
1:B:1193:GLU:N	1:B:1193:GLU:CD	2.57	0.58
1:B:1016:ALA:HB1	1:B:1019:ARG:HH21	1.66	0.58
1:B:894:ALA:HB3	1:B:914:LEU:HD21	1.86	0.58
1:A:263:TYR:CZ	1:A:318:PRO:HG2	2.38	0.58
1:B:396:ASP:HA	1:B:656:VAL:HG13	1.84	0.58
1:B:806:MET:SD	1:B:852:PRO:HB2	2.44	0.58
1:A:699:CYS:SG	1:A:703:ALA:HB3	2.44	0.58
1:A:779:GLU:HB3	1:A:783:ARG:HH12	1.68	0.58
1:A:894:ALA:HB3	1:A:914:LEU:HD21	1.86	0.58
1:B:699:CYS:SG	1:B:703:ALA:HB3	2.44	0.58
1:B:10:GLY:O	1:B:14:THR:HG23	2.04	0.58
1:A:806:MET:SD	1:A:852:PRO:HB2	2.44	0.58
1:A:1193:GLU:N	1:A:1193:GLU:CD	2.57	0.58
1:B:917:LYS:NZ	1:B:917:LYS:HB3	2.18	0.58
1:B:236:TYR:HA	1:B:239:VAL:HG12	1.84	0.57
1:A:1160:PHE:O	1:A:1164:GLU:HG3	2.04	0.57
1:B:4:LYS:HB3	1:B:185:VAL:HG23	1.86	0.57
1:A:10:GLY:O	1:A:14:THR:HG23	2.04	0.57
1:B:460:SER:HB3	1:B:746:MET:CE	2.33	0.57
1:B:9:ASP:HA	1:B:179:GLU:O	2.03	0.57
1:B:349:VAL:HA	1:B:355:MET:HE1	1.85	0.57
1:B:1160:PHE:O	1:B:1164:GLU:HG3	2.04	0.57
1:B:263:TYR:CZ	1:B:318:PRO:HG2	2.38	0.57
1:B:20:ALA:HB2	1:B:188:TYR:CE1	2.39	0.57
1:A:4:LYS:HB3	1:A:185:VAL:HG23	1.86	0.57
1:A:805:LEU:HA	1:A:854:LYS:HZ1	1.68	0.57
1:A:565:THR:HG21	1:A:609:ALA:HB3	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:1243:TPP:HN42	5:B:1243:TPP:H2	1.70	0.57
1:A:1219:THR:CG2	1:A:1221:GLU:HG2	2.35	0.57
1:A:20:ALA:HB2	1:A:188:TYR:CE1	2.39	0.57
1:B:495:VAL:HG23	1:B:530:ILE:HD12	1.87	0.57
1:A:697:PHE:CD2	1:A:800:GLN:NE2	2.73	0.56
1:B:1219:THR:CG2	1:B:1221:GLU:HG2	2.35	0.56
1:A:110:HIS:HD2	1:A:169:HIS:CD2	2.22	0.56
1:B:345:CYS:O	1:B:349:VAL:HG13	2.06	0.56
1:A:986:VAL:HG22	1:A:1064:LEU:HD23	1.88	0.56
1:B:467:HIS:HD2	1:B:481:VAL:H	1.53	0.56
1:B:697:PHE:CD2	1:B:800:GLN:NE2	2.73	0.56
1:B:1225:ASP:O	1:B:1229:ARG:HG3	2.06	0.56
1:B:986:VAL:HG22	1:B:1064:LEU:HD23	1.88	0.56
1:A:1215:ASN:ND2	1:B:1080:MET:H	2.03	0.56
1:B:434:ASN:O	1:B:438:ILE:HG13	2.06	0.56
1:B:565:THR:HG21	1:B:609:ALA:HB3	1.87	0.56
1:A:20:ALA:HB2	1:A:188:TYR:CZ	2.40	0.56
1:B:124:PHE:CB	1:B:367:SER:HB2	2.26	0.55
1:B:1004:ALA:O	1:B:1022:LYS:HG3	2.06	0.55
5:A:1236:TPP:H2	5:A:1236:TPP:HN42	1.70	0.55
1:B:290:LEU:HG	1:B:295:GLU:OE1	2.07	0.55
1:B:20:ALA:HB2	1:B:188:TYR:CZ	2.40	0.55
1:A:1004:ALA:O	1:A:1022:LYS:HG3	2.06	0.55
1:A:1225:ASP:O	1:A:1229:ARG:HG3	2.06	0.55
1:A:345:CYS:O	1:A:349:VAL:HG13	2.06	0.55
1:B:681:VAL:HG23	1:B:770:GLN:HG3	1.88	0.55
1:A:1082:LYS:HZ3	1:B:1219:THR:HG21	1.72	0.55
1:A:495:VAL:HG23	1:A:530:ILE:HD12	1.87	0.55
5:B:1243:TPP:H7'2	6:B:1246:PYR:C1	2.36	0.55
1:B:260:LEU:O	1:B:303:ARG:HB2	2.07	0.55
5:A:1236:TPP:H7'2	6:A:1239:PYR:C1	2.36	0.55
1:A:536:ASN:HD22	1:A:623:LYS:NZ	2.05	0.55
1:B:331:LYS:O	1:B:331:LYS:HG3	2.06	0.55
1:B:1219:THR:HG22	1:B:1222:GLN:H	1.72	0.55
1:A:681:VAL:HG23	1:A:770:GLN:HG3	1.88	0.55
1:B:495:VAL:HG13	1:B:496:GLY:N	2.22	0.55
1:A:434:ASN:O	1:A:438:ILE:HG13	2.06	0.55
1:B:1193:GLU:H	1:B:1193:GLU:CD	2.11	0.55
1:B:110:HIS:CD2	1:B:169:HIS:CD2	2.88	0.55
1:B:1077:ARG:HB2	1:B:1077:ARG:NH1	2.22	0.55
1:A:456:ASP:OD1	1:A:458:LYS:HB2	2.07	0.55
1:B:422:PHE:HE1	1:B:468:LEU:HG	1.72	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:495:VAL:HG13	1:A:496:GLY:N	2.22	0.54
1:A:422:PHE:HE1	1:A:468:LEU:HG	1.72	0.54
1:A:1219:THR:HG22	1:A:1222:GLN:H	1.72	0.54
1:B:1146:LYS:HA	1:B:1149:ARG:HH12	1.72	0.54
1:B:456:ASP:OD1	1:B:458:LYS:HB2	2.07	0.54
1:B:58:ILE:HD12	1:B:58:ILE:H	1.72	0.54
1:A:495:VAL:HG13	1:A:496:GLY:H	1.73	0.54
1:A:260:LEU:O	1:A:303:ARG:HB2	2.07	0.54
1:A:1193:GLU:CD	1:A:1193:GLU:H	2.11	0.54
1:A:434:ASN:HD22	1:A:453:PHE:HE1	1.56	0.54
1:A:467:HIS:HD2	1:A:481:VAL:H	1.54	0.54
1:A:1048:GLN:HE21	1:A:1048:GLN:C	2.11	0.54
1:B:1149:ARG:HH11	1:B:1149:ARG:CG	2.16	0.54
1:A:1146:LYS:HA	1:A:1149:ARG:HH12	1.72	0.54
1:A:99:LYS:HE3	1:B:867:SER:O	2.06	0.54
1:B:688:ASN:HD21	1:B:759:GLU:HB2	1.73	0.54
1:B:323:VAL:CG1	1:B:382:MET:HG2	2.38	0.54
1:A:249:LYS:O	1:A:252:SER:HB3	2.07	0.54
1:A:210:PRO:HB2	1:B:831:ARG:HA	1.89	0.54
1:A:290:LEU:HG	1:A:295:GLU:OE1	2.07	0.54
1:B:1048:GLN:C	1:B:1048:GLN:HE21	2.11	0.54
1:A:1131:GLN:OE1	1:A:1133:ARG:NE	2.40	0.54
1:A:208:MET:HE2	1:B:833:PHE:HD2	1.72	0.54
1:B:536:ASN:HD22	1:B:623:LYS:NZ	2.05	0.53
1:A:497:ILE:HG13	1:A:498:TYR:CD2	2.43	0.53
1:A:609:ALA:O	1:A:613:LEU:HB2	2.08	0.53
1:B:1230:THR:O	1:B:1232:LYS:N	2.42	0.53
1:B:249:LYS:O	1:B:252:SER:HB3	2.07	0.53
1:A:227:GLN:HE22	1:B:368:LYS:NZ	2.07	0.53
1:B:495:VAL:HG13	1:B:496:GLY:H	1.73	0.53
1:A:688:ASN:HD21	1:A:759:GLU:HB2	1.73	0.53
1:A:323:VAL:CG1	1:A:382:MET:HG2	2.38	0.53
1:A:1194:PHE:CD2	1:A:1213:ASP:HB3	2.44	0.53
1:A:1219:THR:HG21	1:B:1082:LYS:NZ	2.24	0.53
1:A:699:CYS:HA	4:A:1234:SF4:S2	2.48	0.53
1:B:1080:MET:O	1:B:1083:SER:HB2	2.08	0.53
1:A:536:ASN:HD22	1:A:623:LYS:HZ3	1.57	0.53
1:A:331:LYS:HG3	1:A:331:LYS:O	2.06	0.53
1:A:1080:MET:O	1:A:1083:SER:HB2	2.08	0.53
1:A:110:HIS:CD2	1:A:169:HIS:CD2	2.88	0.53
1:B:609:ALA:O	1:B:613:LEU:HB2	2.08	0.53
1:B:867:SER:O	1:B:868:LEU:HD23	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:463:ILE:HG13	1:A:464:THR:N	2.24	0.53
1:B:1131:GLN:OE1	1:B:1133:ARG:NE	2.40	0.53
1:B:221:ASN:HB3	1:B:222:PRO:CD	2.39	0.53
1:A:903:SER:O	1:A:907:LYS:HG3	2.08	0.53
1:B:903:SER:O	1:B:907:LYS:HG3	2.08	0.53
1:A:1077:ARG:NH1	1:A:1077:ARG:HB2	2.22	0.53
1:B:630:LYS:HD2	1:B:632:GLU:HG2	1.91	0.53
1:B:1194:PHE:CD2	1:B:1213:ASP:HB3	2.44	0.53
1:A:630:LYS:HD2	1:A:632:GLU:HG2	1.91	0.53
1:A:1149:ARG:CG	1:A:1149:ARG:HH11	2.16	0.53
1:A:398:VAL:HG13	1:A:656:VAL:HG22	1.91	0.52
1:B:619:PRO:HG2	1:B:622:TRP:CD1	2.44	0.52
1:B:534:ILE:HA	1:B:539:LEU:HG	1.91	0.52
1:A:1059:PHE:HD1	1:A:1104:ARG:HD3	1.75	0.52
1:A:867:SER:O	1:A:868:LEU:HD23	2.09	0.52
1:A:1230:THR:O	1:A:1232:LYS:N	2.42	0.52
1:B:699:CYS:HA	4:B:1241:SF4:S2	2.48	0.52
1:B:497:ILE:HG13	1:B:498:TYR:CD2	2.43	0.52
1:B:434:ASN:HD22	1:B:453:PHE:HE1	1.56	0.52
1:A:81:THR:HG22	1:A:82:THR:N	2.24	0.52
1:A:1019:ARG:HH12	1:B:1181:LYS:H	1.57	0.52
1:A:387:LYS:HD3	1:A:390:PHE:HB3	1.91	0.52
1:A:964:GLY:O	1:A:968:ASP:HB2	2.10	0.52
1:B:775:VAL:HB	1:B:776:PRO:CD	2.40	0.52
1:A:323:VAL:HA	1:A:356:PRO:O	2.09	0.52
1:B:387:LYS:HD3	1:B:390:PHE:HB3	1.91	0.52
1:B:964:GLY:O	1:B:968:ASP:HB2	2.10	0.52
1:A:775:VAL:HB	1:A:776:PRO:CD	2.40	0.52
1:B:398:VAL:HG13	1:B:656:VAL:HG22	1.91	0.52
1:B:463:ILE:HG13	1:B:464:THR:N	2.24	0.52
1:A:1102:ASP:CG	1:A:1104:ARG:HH11	2.14	0.52
1:A:58:ILE:H	1:A:58:ILE:HD12	1.72	0.52
1:B:1059:PHE:HD1	1:B:1104:ARG:HD3	1.75	0.52
1:A:230:GLU:OE2	1:B:331:LYS:HE3	2.09	0.52
1:A:534:ILE:HA	1:A:539:LEU:HG	1.91	0.52
1:B:1036:TYR:O	1:B:1063:SER:HA	2.10	0.52
1:A:853:TYR:CE2	1:A:864:TRP:CD1	2.98	0.52
1:A:1035:VAL:O	1:A:1037:VAL:HG23	2.10	0.52
1:B:323:VAL:HA	1:B:356:PRO:O	2.09	0.52
1:A:619:PRO:HG2	1:A:622:TRP:CD1	2.44	0.52
1:A:681:VAL:HG22	1:A:767:LEU:HA	1.91	0.51
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.39	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:81:THR:HG22	1:B:82:THR:N	2.24	0.51
1:A:873:ALA:HA	1:A:959:ILE:HG21	1.92	0.51
1:A:1036:TYR:O	1:A:1063:SER:HA	2.10	0.51
1:A:961:GLY:O	1:A:988:VAL:HA	2.11	0.51
1:A:269:ALA:HA	1:A:296:LYS:HB3	1.92	0.51
1:A:1025:LEU:O	1:A:1029:VAL:HG13	2.11	0.51
1:B:873:ALA:HA	1:B:959:ILE:HG21	1.92	0.51
1:B:349:VAL:CG2	1:B:350:GLU:N	2.73	0.51
1:A:105:LEU:O	1:A:166:PRO:HG3	2.11	0.51
1:A:695:CYS:HB2	1:A:704:ILE:HD13	1.92	0.51
1:B:853:TYR:CE2	1:B:864:TRP:CD1	2.98	0.51
1:B:715:VAL:C	1:B:717:ALA:H	2.14	0.51
1:A:1138:ASP:O	1:A:1142:PRO:HG3	2.10	0.51
1:B:465:ILE:HG13	1:B:467:HIS:CE1	2.46	0.51
1:B:1102:ASP:CG	1:B:1104:ARG:HH11	2.14	0.51
1:A:465:ILE:HG13	1:A:467:HIS:CE1	2.46	0.51
1:B:105:LEU:O	1:B:166:PRO:HG3	2.11	0.51
1:B:1016:ALA:HB1	1:B:1019:ARG:NH2	2.26	0.51
1:B:1035:VAL:O	1:B:1037:VAL:HG23	2.10	0.51
1:A:349:VAL:CG2	1:A:350:GLU:N	2.73	0.51
1:B:1138:ASP:O	1:B:1142:PRO:HG3	2.10	0.51
1:A:1160:PHE:O	1:A:1160:PHE:CD1	2.64	0.51
1:B:681:VAL:HG22	1:B:767:LEU:HA	1.91	0.51
1:A:715:VAL:HG12	1:A:716:GLY:N	2.25	0.51
1:B:695:CYS:HB2	1:B:704:ILE:HD13	1.92	0.51
1:B:1160:PHE:CD1	1:B:1160:PHE:O	2.64	0.50
1:B:715:VAL:HG12	1:B:716:GLY:N	2.25	0.50
1:B:1025:LEU:O	1:B:1029:VAL:HG13	2.11	0.50
1:B:110:HIS:HD2	1:B:169:HIS:CD2	2.22	0.50
1:A:130:ILE:HD13	1:A:170:PHE:CZ	2.46	0.50
1:B:131:TYR:O	1:B:134:ARG:HB2	2.12	0.50
1:B:902:ALA:O	1:B:907:LYS:HE3	2.11	0.50
1:A:910:LEU:HD12	1:A:930:LEU:HD21	1.92	0.50
1:B:883:MET:HE2	1:B:955:LYS:HD2	1.92	0.50
1:B:691:GLN:HG2	1:B:736:PHE:CD1	2.47	0.50
1:B:910:LEU:HD12	1:B:930:LEU:HD21	1.93	0.50
1:B:910:LEU:HD13	1:B:930:LEU:HD11	1.93	0.50
1:B:269:ALA:HA	1:B:296:LYS:HB3	1.92	0.50
1:A:869:PHE:CE2	1:A:969:ILE:HG21	2.47	0.50
1:A:131:TYR:O	1:A:134:ARG:HB2	2.12	0.50
1:A:82:THR:HG22	1:A:83:THR:N	2.27	0.50
1:A:1016:ALA:HB1	1:A:1019:ARG:NH2	2.26	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:684:TRP:CE2	1:A:738:ILE:HB	2.47	0.50
1:B:578:LYS:HE3	1:B:582:LEU:HD21	1.94	0.50
1:B:587:ILE:O	1:B:591:TYR:HB2	2.12	0.50
1:A:691:GLN:HG2	1:A:736:PHE:CD1	2.47	0.50
1:B:536:ASN:HD22	1:B:623:LYS:HZ3	1.58	0.50
1:A:715:VAL:C	1:A:717:ALA:H	2.13	0.50
1:B:578:LYS:HG3	1:B:582:LEU:HD22	1.94	0.50
1:B:963:ASP:HB3	1:B:990:ASP:OD1	2.12	0.50
1:B:869:PHE:CE2	1:B:969:ILE:HG21	2.46	0.50
1:A:721:PHE:HD1	1:A:777:ASN:HD22	1.59	0.50
1:A:902:ALA:O	1:A:907:LYS:HE3	2.11	0.50
1:A:216:ARG:O	1:B:865:GLY:HA2	2.12	0.50
1:A:43:TRP:HB3	1:A:48:ARG:HD3	1.94	0.50
1:A:578:LYS:HE3	1:A:582:LEU:HD21	1.94	0.50
1:A:693:ASN:HB3	1:A:800:GLN:HB2	1.94	0.50
1:B:961:GLY:O	1:B:988:VAL:HA	2.11	0.50
1:B:130:ILE:HD13	1:B:170:PHE:CZ	2.46	0.49
1:A:870:GLU:OE1	5:A:1236:TPP:HM21	2.12	0.49
1:B:200:LEU:HD11	1:B:204:ARG:NH1	2.27	0.49
1:A:587:ILE:O	1:A:591:TYR:HB2	2.12	0.49
1:A:746:MET:O	1:B:1216:ARG:HA	2.12	0.49
1:A:553:VAL:O	1:A:601:MET:HG3	2.11	0.49
1:A:910:LEU:HD13	1:A:930:LEU:HD11	1.93	0.49
1:B:182:LYS:HE2	1:B:442:GLY:O	2.13	0.49
1:A:200:LEU:HD11	1:A:204:ARG:NH1	2.27	0.49
1:B:636:ASN:ND2	1:B:672:PHE:HE2	2.11	0.49
1:B:512:LEU:HD12	1:B:513:ASN:N	2.27	0.49
1:A:323:VAL:HG12	1:A:382:MET:HG2	1.94	0.49
1:B:721:PHE:HD1	1:B:777:ASN:HD22	1.59	0.49
1:B:870:GLU:OE1	5:B:1243:TPP:HM21	2.12	0.49
1:B:965:TRP:CE3	1:B:966:ALA:HB2	2.48	0.49
1:A:182:LYS:HE2	1:A:442:GLY:O	2.13	0.49
1:A:1188:PHE:HB3	1:B:1010:VAL:O	2.11	0.49
1:B:43:TRP:HB3	1:B:48:ARG:HD3	1.94	0.49
1:B:713:GLU:O	1:B:780:TYR:OH	2.31	0.49
1:B:126:ASP:HA	1:B:329:ARG:CD	2.42	0.49
1:A:691:GLN:HE22	1:A:726:ALA:HA	1.78	0.49
1:A:883:MET:HE2	1:A:955:LYS:HD2	1.94	0.49
1:B:561:MET:HE1	1:B:583:LEU:CD2	2.42	0.49
1:B:553:VAL:O	1:B:601:MET:HG3	2.11	0.49
1:A:264:VAL:HG21	1:A:301:LYS:HE3	1.93	0.49
1:B:27:ILE:HG23	1:B:28:TYR:N	2.28	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:512:LEU:HD12	1:A:513:ASN:N	2.28	0.49
1:B:684:TRP:CE2	1:B:738:ILE:HB	2.47	0.49
1:A:334:GLY:O	1:B:307:PRO:HA	2.13	0.49
1:B:323:VAL:HG12	1:B:382:MET:HG2	1.94	0.49
1:A:965:TRP:CE3	1:A:966:ALA:HB2	2.48	0.49
1:A:992:GLU:O	1:A:993:VAL:HB	2.13	0.49
1:B:349:VAL:HA	1:B:355:MET:CE	2.43	0.49
1:A:578:LYS:HG3	1:A:582:LEU:HD22	1.94	0.48
1:B:992:GLU:O	1:B:993:VAL:HB	2.13	0.48
1:B:693:ASN:HB3	1:B:800:GLN:HB2	1.94	0.48
1:A:703:ALA:HB3	4:A:1234:SF4:S4	2.53	0.48
1:A:994:TYR:CE1	1:A:1002:SER:HB2	2.48	0.48
1:A:569:LYS:HB3	1:A:570:LEU:HD13	1.95	0.48
1:B:691:GLN:HE22	1:B:726:ALA:HA	1.78	0.48
1:B:703:ALA:HB3	4:B:1241:SF4:S4	2.53	0.48
1:A:681:VAL:CG2	1:A:767:LEU:HA	2.43	0.48
1:B:23:GLU:OE1	1:B:204:ARG:NH2	2.46	0.48
1:A:27:ILE:HG23	1:A:28:TYR:N	2.28	0.48
1:A:963:ASP:HB3	1:A:990:ASP:OD1	2.12	0.48
1:A:583:LEU:O	1:A:587:ILE:HG12	2.13	0.48
1:B:590:ALA:O	1:B:591:TYR:HB2	2.14	0.48
1:A:834:ILE:HD13	1:A:960:PHE:CE2	2.49	0.48
1:A:60:GLU:O	1:B:976:HIS:HE1	1.96	0.48
1:A:940:GLY:O	1:A:943:GLY:N	2.46	0.48
1:B:264:VAL:HG21	1:B:301:LYS:HE3	1.93	0.48
1:A:1019:ARG:NH1	1:B:1181:LYS:H	2.12	0.48
1:A:23:GLU:OE1	1:A:204:ARG:NH2	2.46	0.48
1:A:274:VAL:HG23	1:A:324:ILE:CD1	2.44	0.48
1:B:226:PHE:HD1	1:B:226:PHE:O	1.96	0.48
1:A:349:VAL:HA	1:A:355:MET:CE	2.43	0.48
1:B:684:TRP:CD2	1:B:738:ILE:HB	2.48	0.48
1:B:42:ASP:O	1:B:46:GLN:HG3	2.14	0.48
1:A:561:MET:HE1	1:A:583:LEU:CD2	2.42	0.48
1:A:684:TRP:CD2	1:A:738:ILE:HB	2.48	0.48
1:A:338:ASP:OD2	1:A:362:ARG:NH1	2.47	0.48
1:A:681:VAL:HG12	1:A:745:CYS:SG	2.53	0.48
1:B:274:VAL:HG23	1:B:324:ILE:CD1	2.44	0.48
1:A:42:ASP:O	1:A:46:GLN:HG3	2.14	0.48
1:B:617:LYS:NZ	1:B:617:LYS:HB2	2.28	0.48
1:B:867:SER:HB2	1:B:875:TYR:CG	2.49	0.48
1:B:721:PHE:CE1	1:B:780:TYR:HD2	2.32	0.48
1:B:994:TYR:CE1	1:B:1002:SER:HB2	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:940:GLY:O	1:B:943:GLY:N	2.46	0.48
1:A:867:SER:HB2	1:A:875:TYR:CG	2.49	0.48
1:A:566:ALA:HA	1:A:613:LEU:HD21	1.95	0.48
1:A:713:GLU:O	1:A:780:TYR:OH	2.31	0.47
1:A:590:ALA:O	1:A:591:TYR:HB2	2.14	0.47
1:B:799:SER:OG	1:B:800:GLN:NE2	2.47	0.47
1:B:646:ILE:HG21	1:B:849:PRO:HD3	1.96	0.47
1:B:1012:LYS:O	1:B:1013:PHE:HB2	2.14	0.47
1:B:681:VAL:CG2	1:B:767:LEU:HA	2.43	0.47
1:A:1175:PHE:CZ	1:A:1177:PRO:HA	2.49	0.47
1:B:569:LYS:HB3	1:B:570:LEU:HD13	1.95	0.47
1:B:566:ALA:HA	1:B:613:LEU:HD21	1.95	0.47
1:A:154:LEU:HD13	1:A:250:VAL:HG22	1.96	0.47
1:B:871:ASP:HB2	1:B:874:GLU:HG2	1.96	0.47
1:B:351:ARG:HD3	1:B:353:GLU:HB2	1.96	0.47
1:B:1040:VAL:HA	1:B:1098:LEU:HD22	1.96	0.47
1:B:146:VAL:HG12	1:B:183:ILE:HD13	1.96	0.47
1:A:636:ASN:ND2	1:A:672:PHE:HE2	2.11	0.47
1:A:799:SER:OG	1:A:800:GLN:NE2	2.47	0.47
1:B:681:VAL:HG12	1:B:745:CYS:SG	2.53	0.47
1:A:710:LYS:HD2	1:A:734:TYR:HE1	1.80	0.47
1:A:146:VAL:HG12	1:A:183:ILE:HD13	1.96	0.47
1:B:338:ASP:OD2	1:B:362:ARG:NH1	2.47	0.47
1:B:583:LEU:O	1:B:587:ILE:HG12	2.13	0.47
1:B:834:ILE:HD13	1:B:960:PHE:CE2	2.49	0.47
1:A:286:VAL:HG12	1:A:290:LEU:HD22	1.97	0.47
1:B:710:LYS:HD2	1:B:734:TYR:HE1	1.80	0.47
1:A:226:PHE:O	1:A:226:PHE:HD1	1.96	0.47
1:B:121:LEU:HG	1:B:122:SER:N	2.29	0.47
1:B:1129:MET:HG2	1:B:1149:ARG:HE	1.80	0.47
1:A:1012:LYS:O	1:A:1013:PHE:HB2	2.14	0.47
1:B:573:VAL:HG23	1:B:574:LEU:HG	1.97	0.47
1:A:617:LYS:HB2	1:A:617:LYS:NZ	2.28	0.47
1:A:1214:GLN:NE2	1:B:461:GLY:H	2.12	0.47
1:B:1175:PHE:CZ	1:B:1177:PRO:HA	2.49	0.47
1:A:126:ASP:HA	1:A:329:ARG:CD	2.42	0.47
1:A:121:LEU:HG	1:A:122:SER:N	2.29	0.47
1:A:867:SER:O	1:B:99:LYS:HE3	2.15	0.47
1:B:64:GLU:HG3	1:B:89:GLY:CA	2.45	0.47
1:B:917:LYS:NZ	1:B:917:LYS:CB	2.78	0.47
1:B:890:LEU:CD1	1:B:945:ILE:HG23	2.45	0.47
1:A:351:ARG:HD3	1:A:353:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:871:ASP:HB2	1:A:874:GLU:HG2	1.96	0.47
1:A:646:ILE:HG21	1:A:849:PRO:HD3	1.96	0.47
1:A:14:THR:HG21	1:A:171:PHE:CE1	2.50	0.47
1:A:573:VAL:HG23	1:A:574:LEU:HG	1.97	0.47
1:A:1003:LYS:HD3	1:B:976:HIS:CD2	2.50	0.47
1:A:721:PHE:CE1	1:A:780:TYR:HD2	2.32	0.46
1:B:1007:THR:HB	1:B:1152:VAL:HG22	1.96	0.46
1:A:1216:ARG:HE	1:B:677:VAL:HG23	1.79	0.46
1:B:667:LEU:N	1:B:667:LEU:HD12	2.31	0.46
1:A:1232:LYS:HZ2	1:A:1232:LYS:HB3	1.79	0.46
1:B:373:ALA:O	1:B:376:LYS:HB3	2.15	0.46
1:B:154:LEU:HD13	1:B:250:VAL:HG22	1.96	0.46
1:B:1232:LYS:HB3	1:B:1232:LYS:HZ2	1.81	0.46
1:A:667:LEU:N	1:A:667:LEU:HD12	2.31	0.46
1:B:694:GLN:O	1:B:698:VAL:HB	2.16	0.46
1:A:390:PHE:CE2	1:A:403:LEU:HD22	2.51	0.46
1:B:1200:THR:HA	1:B:1201:PRO:HD3	1.83	0.46
1:B:693:ASN:HD21	1:B:736:PHE:HZ	1.63	0.46
1:B:390:PHE:CE2	1:B:403:LEU:HD22	2.51	0.46
1:A:710:LYS:HD2	1:A:734:TYR:CE1	2.51	0.46
1:A:373:ALA:O	1:A:376:LYS:HB3	2.15	0.46
1:A:1200:THR:CG2	1:A:1202:MET:H	2.28	0.46
1:A:274:VAL:HG23	1:A:324:ILE:HD12	1.98	0.46
1:B:93:MET:O	1:B:97:MET:HG3	2.16	0.46
1:B:1200:THR:CG2	1:B:1202:MET:H	2.28	0.46
1:A:917:LYS:NZ	1:A:917:LYS:CB	2.78	0.46
1:A:684:TRP:HZ2	1:A:689:CYS:SG	2.39	0.46
1:A:173:GLY:O	1:A:174:PHE:HB2	2.16	0.46
1:A:1040:VAL:HA	1:A:1098:LEU:HD22	1.96	0.46
1:A:1007:THR:HB	1:A:1152:VAL:HG22	1.96	0.46
1:B:820:TYR:HD1	1:B:1049:PHE:CZ	2.34	0.46
1:A:820:TYR:HD1	1:A:1049:PHE:CZ	2.34	0.46
1:A:1219:THR:HB	1:A:1222:GLN:OE1	2.16	0.46
1:A:694:GLN:O	1:A:698:VAL:HB	2.16	0.46
1:A:1043:GLY:HA2	1:A:1084:GLN:NE2	2.31	0.46
1:B:491:ASN:C	1:B:491:ASN:HD22	2.19	0.45
1:B:274:VAL:HG23	1:B:324:ILE:HD12	1.98	0.45
1:A:491:ASN:HD22	1:A:491:ASN:C	2.19	0.45
1:B:780:TYR:HA	1:B:783:ARG:HD2	1.99	0.45
1:A:421:GLN:HA	1:A:466:SER:O	2.16	0.45
1:B:1074:GLN:O	1:B:1133:ARG:HG2	2.16	0.45
1:A:280:CYS:HB3	1:A:301:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1162:GLU:HG3	1:B:1171:ILE:HG21	1.98	0.45
1:A:1071:CYS:HA	4:A:1235:SF4:S3	2.56	0.45
1:A:644:LYS:N	1:A:645:PRO:CD	2.79	0.45
1:A:1010:VAL:O	1:B:1188:PHE:HB3	2.16	0.45
1:B:1141:PHE:N	1:B:1142:PRO:HD3	2.31	0.45
1:A:1141:PHE:N	1:A:1142:PRO:HD3	2.31	0.45
1:B:146:VAL:HG21	1:B:179:GLU:O	2.16	0.45
1:A:64:GLU:HG3	1:A:89:GLY:CA	2.45	0.45
1:B:421:GLN:HA	1:B:466:SER:O	2.16	0.45
1:A:325:THR:HG23	1:A:382:MET:CE	2.47	0.45
1:B:87:SER:HA	1:B:129:ASP:CB	2.46	0.45
1:B:817:GLU:HB3	1:B:989:MET:HE3	1.98	0.45
1:A:198:LYS:O	1:A:202:GLU:HG3	2.17	0.45
1:A:93:MET:O	1:A:97:MET:HG3	2.16	0.45
1:A:1129:MET:HG2	1:A:1149:ARG:HE	1.80	0.45
1:B:755:CYS:HA	1:B:756:PRO:HD3	1.64	0.45
1:B:286:VAL:HG12	1:B:290:LEU:HD22	1.97	0.45
1:A:1080:MET:H	1:B:1215:ASN:ND2	2.14	0.45
1:B:390:PHE:CG	1:B:403:LEU:HD13	2.51	0.45
1:B:280:CYS:HB3	1:B:301:LYS:HG2	1.99	0.45
1:B:710:LYS:HD2	1:B:734:TYR:CE1	2.51	0.45
1:B:1071:CYS:HA	4:B:1242:SF4:S3	2.56	0.45
1:A:469:ARG:NH2	1:A:479:TYR:O	2.49	0.45
1:B:1219:THR:HB	1:B:1222:GLN:OE1	2.16	0.45
1:A:1074:GLN:O	1:A:1133:ARG:HG2	2.16	0.45
1:A:617:LYS:HA	1:A:617:LYS:HD3	1.71	0.45
1:B:469:ARG:NH2	1:B:479:TYR:O	2.49	0.45
1:B:198:LYS:O	1:B:202:GLU:HG3	2.17	0.45
1:A:87:SER:HA	1:A:129:ASP:CB	2.47	0.45
1:B:1059:PHE:HD1	1:B:1104:ARG:CD	2.30	0.45
1:A:704:ILE:HG12	1:A:740:ILE:CD1	2.47	0.45
1:B:684:TRP:HZ2	1:B:689:CYS:SG	2.39	0.45
1:A:790:VAL:HG13	1:A:791:LEU:N	2.31	0.45
1:A:124:PHE:CB	1:A:367:SER:HB2	2.26	0.45
1:A:87:SER:N	1:A:129:ASP:OD2	2.49	0.45
1:A:390:PHE:CG	1:A:403:LEU:HD13	2.51	0.45
1:B:704:ILE:HG12	1:B:740:ILE:CD1	2.47	0.45
1:A:210:PRO:CB	1:B:831:ARG:HA	2.47	0.45
1:B:512:LEU:HG	1:B:514:SER:HB3	1.98	0.45
1:B:14:THR:HG21	1:B:171:PHE:CE1	2.51	0.45
1:A:791:LEU:HD23	1:A:791:LEU:HA	1.84	0.45
1:B:790:VAL:HG13	1:B:791:LEU:N	2.31	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:173:GLY:O	1:B:174:PHE:HB2	2.16	0.45
1:B:887:ARG:NH2	1:B:954:LYS:N	2.65	0.45
1:A:780:TYR:HA	1:A:783:ARG:HD2	1.99	0.45
1:B:87:SER:N	1:B:129:ASP:OD2	2.49	0.45
1:B:44:ALA:CB	1:B:58:ILE:HD11	2.47	0.45
1:A:755:CYS:SG	1:A:761:ALA:CB	3.02	0.45
1:A:593:LYS:HD3	1:A:594:LYS:H	1.82	0.45
1:B:707:VAL:O	1:B:736:PHE:HA	2.17	0.45
1:A:349:VAL:HA	1:A:355:MET:HE1	1.98	0.45
1:A:78:GLY:HA2	1:A:207:SER:OG	2.17	0.45
1:B:1005:THR:HA	1:B:1006:PRO:HD3	1.71	0.45
1:A:707:VAL:O	1:A:736:PHE:HA	2.17	0.44
1:B:1043:GLY:HA2	1:B:1084:GLN:NE2	2.31	0.44
1:B:636:ASN:ND2	1:B:672:PHE:CE2	2.85	0.44
1:A:636:ASN:ND2	1:A:672:PHE:CE2	2.85	0.44
1:A:670:SER:HA	1:A:673:GLU:OE1	2.18	0.44
1:A:596:GLU:O	1:A:599:VAL:HB	2.18	0.44
1:A:1108:GLN:HG2	1:A:1108:GLN:H	1.57	0.44
1:A:1059:PHE:HD1	1:A:1104:ARG:CD	2.30	0.44
1:A:146:VAL:HG21	1:A:179:GLU:O	2.16	0.44
1:A:561:MET:HE2	1:A:587:ILE:HD11	1.99	0.44
1:B:82:THR:HG22	1:B:83:THR:N	2.26	0.44
1:A:325:THR:HA	1:A:359:LEU:O	2.18	0.44
1:A:44:ALA:CB	1:A:58:ILE:HD11	2.47	0.44
1:B:644:LYS:N	1:B:645:PRO:CD	2.79	0.44
1:B:124:PHE:HB3	1:B:367:SER:CB	2.28	0.44
1:B:1129:MET:HE3	1:B:1149:ARG:CZ	2.48	0.44
1:A:887:ARG:NH2	1:A:954:LYS:N	2.65	0.44
1:A:368:LYS:NZ	1:B:227:GLN:NE2	2.65	0.44
1:B:325:THR:HG23	1:B:382:MET:CE	2.47	0.44
1:B:64:GLU:OE2	5:B:1243:TPP:N1'	2.51	0.44
1:B:35:THR:O	1:B:38:GLU:N	2.51	0.44
1:B:523:ASP:HA	1:B:531:LYS:HZ1	1.78	0.44
1:B:593:LYS:HD3	1:B:594:LYS:H	1.82	0.44
1:B:746:MET:HB3	1:B:813:SER:OG	2.18	0.44
1:A:1219:THR:HG21	1:A:1221:GLU:HG2	2.00	0.44
1:B:1082:LYS:HD3	1:B:1082:LYS:HA	1.84	0.44
1:A:263:TYR:OH	1:A:298:GLY:HA3	2.18	0.44
1:B:1219:THR:HG21	1:B:1221:GLU:HG2	2.00	0.44
1:A:331:LYS:HE3	1:B:230:GLU:OE2	2.17	0.44
1:A:512:LEU:HG	1:A:514:SER:HB3	1.98	0.44
1:A:890:LEU:CD1	1:A:945:ILE:HG23	2.45	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:263:TYR:OH	1:B:298:GLY:HA3	2.18	0.44
1:B:805:LEU:HD22	1:B:829:GLY:HA3	2.00	0.44
1:A:805:LEU:HD22	1:A:829:GLY:HA3	2.00	0.44
1:A:843:ILE:HG13	1:A:996:ASN:OD1	2.18	0.44
1:A:1005:THR:HA	1:A:1006:PRO:HD3	1.71	0.44
1:B:596:GLU:O	1:B:599:VAL:HB	2.18	0.44
1:B:803:GLU:O	1:B:805:LEU:HD13	2.18	0.43
1:B:867:SER:HB2	1:B:875:TYR:CD2	2.53	0.43
1:B:1000:GLN:HE21	1:B:1000:GLN:HB2	1.67	0.43
1:B:843:ILE:HG13	1:B:996:ASN:OD1	2.18	0.43
1:A:746:MET:HB3	1:A:813:SER:OG	2.18	0.43
1:B:325:THR:HA	1:B:359:LEU:O	2.18	0.43
1:A:24:VAL:HG13	1:B:881:MET:HE1	2.00	0.43
1:B:679:ILE:HA	1:B:679:ILE:HD13	1.90	0.43
1:B:996:ASN:HD21	6:B:1246:PYR:H31	1.84	0.43
1:A:64:GLU:OE2	5:A:1236:TPP:N1'	2.51	0.43
1:B:1180:GLY:O	1:B:1181:LYS:HD2	2.19	0.43
1:A:821:VAL:O	1:A:825:THR:HG23	2.18	0.43
1:A:650:GLN:NE2	1:A:653:LYS:NZ	2.66	0.43
1:B:650:GLN:NE2	1:B:653:LYS:NZ	2.66	0.43
1:B:490:HIS:N	1:B:490:HIS:CD2	2.86	0.43
1:B:78:GLY:HA2	1:B:207:SER:OG	2.17	0.43
1:B:670:SER:HA	1:B:673:GLU:OE1	2.18	0.43
1:A:854:LYS:CB	1:A:854:LYS:HZ3	2.30	0.43
1:A:593:LYS:CG	1:A:594:LYS:H	2.31	0.43
1:A:35:THR:O	1:A:38:GLU:N	2.51	0.43
1:B:290:LEU:O	1:B:293:LYS:HB2	2.19	0.43
1:A:290:LEU:O	1:A:293:LYS:HB2	2.19	0.43
1:B:561:MET:HE2	1:B:587:ILE:HD11	1.99	0.43
1:A:1180:GLY:O	1:A:1181:LYS:HD2	2.19	0.43
1:A:1104:ARG:O	1:A:1107:ALA:HB3	2.18	0.43
1:B:591:TYR:HA	1:B:593:LYS:HG2	2.00	0.43
1:B:1104:ARG:O	1:B:1107:ALA:HB3	2.18	0.43
1:A:317:LEU:HD21	1:A:321:ALA:CB	2.49	0.43
1:A:831:ARG:HA	1:B:210:PRO:HB2	2.01	0.43
1:A:996:ASN:HD21	6:A:1239:PYR:H31	1.84	0.43
1:B:736:PHE:C	1:B:736:PHE:CD1	2.92	0.43
1:A:1217:ALA:HB2	1:B:679:ILE:HB	2.01	0.43
1:A:11:ASN:HD21	1:A:112:THR:HG21	1.84	0.43
1:A:687:GLU:H	1:A:687:GLU:HG3	1.65	0.43
1:A:867:SER:HB2	1:A:875:TYR:CD2	2.53	0.43
1:B:593:LYS:HD2	1:B:598:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:736:PHE:CD1	1:A:736:PHE:C	2.92	0.43
1:A:693:ASN:HD21	1:A:736:PHE:HZ	1.63	0.43
1:A:698:VAL:O	1:A:700:PRO:HD3	2.19	0.43
1:B:226:PHE:CD1	1:B:226:PHE:O	2.72	0.43
1:B:642:VAL:C	1:B:645:PRO:HD2	2.39	0.43
1:B:509:THR:HA	1:B:540:LYS:HB2	2.01	0.43
1:B:698:VAL:O	1:B:700:PRO:HD3	2.19	0.43
1:B:317:LEU:HD21	1:B:321:ALA:CB	2.49	0.43
1:B:374:MET:O	1:B:377:SER:HB3	2.18	0.43
1:A:422:PHE:CE1	1:A:468:LEU:HG	2.54	0.42
1:B:346:SER:O	1:B:350:GLU:HB3	2.19	0.42
1:A:370:PHE:CZ	1:A:375:VAL:HG22	2.54	0.42
1:B:370:PHE:CZ	1:B:375:VAL:HG22	2.54	0.42
1:B:212:HIS:O	1:B:212:HIS:CG	2.72	0.42
1:A:795:SER:O	1:A:796:LEU:C	2.58	0.42
1:B:455:TYR:HB3	1:B:456:ASP:H	1.64	0.42
1:B:154:LEU:HD13	1:B:250:VAL:CG2	2.49	0.42
1:A:554:GLY:HA3	1:A:601:MET:HE2	2.01	0.42
1:A:630:LYS:H	1:A:630:LYS:HG3	1.57	0.42
1:A:642:VAL:C	1:A:645:PRO:HD2	2.39	0.42
1:A:1094:GLY:HA3	1:A:1120:PRO:HG3	2.00	0.42
1:B:266:ALA:HA	1:B:267:PRO:HD3	1.91	0.42
1:B:821:VAL:O	1:B:825:THR:HG23	2.18	0.42
1:B:593:LYS:CG	1:B:594:LYS:H	2.31	0.42
1:A:154:LEU:HD13	1:A:250:VAL:CG2	2.49	0.42
1:B:390:PHE:HA	1:B:401:THR:O	2.19	0.42
1:B:897:ALA:HB3	1:B:910:LEU:HD21	2.01	0.42
1:A:511:VAL:HA	1:A:542:TYR:O	2.19	0.42
1:B:795:SER:O	1:B:796:LEU:C	2.58	0.42
1:A:956:SER:HG	1:A:958:TRP:HE1	1.67	0.42
1:A:1205:ARG:HA	1:A:1205:ARG:HD3	1.82	0.42
1:A:509:THR:HA	1:A:540:LYS:HB2	2.01	0.42
1:A:854:LYS:C	1:A:854:LYS:HZ3	2.22	0.42
1:B:64:GLU:CG	1:B:89:GLY:HA2	2.48	0.42
1:B:154:LEU:CD2	1:B:158:LEU:HD11	2.49	0.42
1:A:346:SER:O	1:A:350:GLU:HB3	2.19	0.42
1:A:266:ALA:HA	1:A:267:PRO:HD3	1.91	0.42
1:B:342:LEU:HA	1:B:342:LEU:HD12	1.82	0.42
1:B:472:GLU:HG2	1:B:472:GLU:H	1.55	0.42
1:A:490:HIS:CD2	1:A:490:HIS:N	2.86	0.42
1:A:779:GLU:C	1:A:783:ARG:HH11	2.23	0.42
1:A:591:TYR:HA	1:A:593:LYS:HG2	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1048:GLN:NE2	1:A:1048:GLN:C	2.73	0.42
1:B:536:ASN:ND2	1:B:623:LYS:HG2	2.34	0.42
1:A:897:ALA:HB3	1:A:910:LEU:HD21	2.01	0.42
1:B:599:VAL:O	1:B:602:ASN:HB2	2.20	0.42
1:A:307:PRO:HA	1:B:334:GLY:O	2.19	0.42
1:A:803:GLU:O	1:A:805:LEU:HD13	2.18	0.42
1:B:736:PHE:CD2	1:B:801:PHE:HZ	2.37	0.42
1:A:390:PHE:HA	1:A:401:THR:O	2.19	0.42
1:A:317:LEU:C	1:A:317:LEU:HD22	2.39	0.42
1:B:1094:GLY:HA3	1:B:1120:PRO:HG3	2.00	0.42
1:A:467:HIS:CE1	1:A:480:LEU:HD22	2.55	0.42
1:B:325:THR:HG22	1:B:382:MET:SD	2.60	0.42
1:A:1082:LYS:HA	1:A:1082:LYS:HD3	1.84	0.42
1:A:390:PHE:CD2	1:A:403:LEU:HD22	2.54	0.42
1:B:390:PHE:CD2	1:B:403:LEU:HD22	2.54	0.42
1:A:5:MET:HE1	1:A:184:GLU:HB2	2.02	0.42
1:A:374:MET:O	1:A:377:SER:HB3	2.18	0.42
1:B:1108:GLN:H	1:B:1108:GLN:HG2	1.57	0.42
1:B:11:ASN:HD21	1:B:112:THR:HG21	1.84	0.42
1:B:840:CYS:O	1:B:844:TRP:CD1	2.72	0.42
1:B:1149:ARG:HG3	1:B:1149:ARG:NH1	2.15	0.42
1:A:513:ASN:HA	1:A:544:ILE:O	2.20	0.42
1:B:338:ASP:HB3	1:B:339:PRO:CD	2.50	0.42
1:B:465:ILE:HG13	1:B:467:HIS:HE1	1.84	0.42
1:A:736:PHE:CD2	1:A:801:PHE:HZ	2.37	0.42
1:A:976:HIS:HE1	1:B:60:GLU:O	2.03	0.42
1:A:941:LEU:HD23	1:A:941:LEU:HA	1.86	0.42
1:A:226:PHE:O	1:A:226:PHE:CD1	2.72	0.42
1:A:24:VAL:HG13	1:B:881:MET:CE	2.50	0.42
1:B:687:GLU:HG3	1:B:687:GLU:H	1.65	0.42
1:B:1132:ASN:ND2	1:B:1139:ARG:HH12	2.11	0.42
1:B:780:TYR:CE2	1:B:784:ILE:HD11	2.55	0.42
1:A:64:GLU:CG	1:A:89:GLY:HA2	2.48	0.42
1:A:154:LEU:CD2	1:A:158:LEU:HD11	2.49	0.42
1:A:840:CYS:O	1:A:844:TRP:CD1	2.72	0.42
1:B:317:LEU:HD21	1:B:321:ALA:HB3	2.02	0.42
1:A:212:HIS:CG	1:A:212:HIS:O	2.72	0.42
1:A:696:ALA:O	1:A:822:ARG:NH2	2.53	0.42
1:B:1129:MET:CE	1:B:1149:ARG:NE	2.83	0.42
1:B:513:ASN:HA	1:B:544:ILE:O	2.20	0.42
1:B:779:GLU:C	1:B:783:ARG:HH11	2.23	0.42
1:A:465:ILE:HG13	1:A:467:HIS:HE1	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:368:LYS:HZ3	1:B:227:GLN:HE22	1.66	0.42
1:B:536:ASN:HA	1:B:623:LYS:HZ3	1.85	0.42
1:B:32:PRO:HB3	1:B:174:PHE:CE2	2.55	0.42
1:A:881:MET:HE1	1:B:24:VAL:HG13	2.02	0.42
1:A:780:TYR:CE2	1:A:784:ILE:HD11	2.55	0.41
1:B:467:HIS:CE1	1:B:480:LEU:HD22	2.55	0.41
1:B:630:LYS:H	1:B:630:LYS:HG3	1.57	0.41
1:A:965:TRP:CZ3	1:A:966:ALA:HB2	2.55	0.41
1:A:32:PRO:HB3	1:A:174:PHE:CE2	2.55	0.41
1:B:317:LEU:HD22	1:B:317:LEU:C	2.39	0.41
1:B:837:ALA:HB2	1:B:872:ALA:CB	2.50	0.41
1:B:197:GLN:H	1:B:197:GLN:HG2	1.64	0.41
1:B:748:CYS:SG	1:B:750:ASN:HB2	2.60	0.41
1:A:1129:MET:CE	1:A:1149:ARG:NE	2.83	0.41
1:B:227:GLN:NE2	1:B:227:GLN:H	2.18	0.41
1:B:1059:PHE:CD1	1:B:1104:ARG:HD3	2.55	0.41
1:A:317:LEU:HD21	1:A:321:ALA:HB3	2.02	0.41
1:A:1209:GLY:O	1:B:429:GLY:HA2	2.19	0.41
1:A:837:ALA:HB2	1:A:872:ALA:CB	2.50	0.41
1:B:1149:ARG:NH1	1:B:1149:ARG:CG	2.80	0.41
1:A:1132:ASN:ND2	1:A:1139:ARG:HH12	2.11	0.41
1:B:897:ALA:HA	1:B:941:LEU:HD13	2.03	0.41
1:B:965:TRP:CZ3	1:B:966:ALA:HB2	2.55	0.41
1:B:371:SER:HB2	1:B:372:PRO:CD	2.51	0.41
1:A:748:CYS:SG	1:A:750:ASN:HB2	2.60	0.41
1:A:1149:ARG:NH1	1:A:1149:ARG:HG3	2.15	0.41
1:B:491:ASN:HA	1:B:492:PRO:HD2	1.84	0.41
1:A:700:PRO:HB3	1:A:819:PRO:HD3	2.02	0.41
1:A:743:LEU:HA	1:A:743:LEU:HD23	1.73	0.41
1:A:536:ASN:HA	1:A:623:LYS:HZ3	1.85	0.41
1:B:644:LYS:HB3	1:B:645:PRO:HD3	2.02	0.41
1:A:184:GLU:CD	1:A:256:ARG:HH12	2.23	0.41
1:B:1001:SER:HB2	1:B:1011:ALA:HB3	2.01	0.41
1:A:238:LYS:O	1:A:242:ILE:HG13	2.20	0.41
1:A:1200:THR:HA	1:A:1201:PRO:HD3	1.83	0.41
1:A:593:LYS:HD2	1:A:598:ILE:HG13	2.01	0.41
1:A:536:ASN:ND2	1:A:623:LYS:HG2	2.34	0.41
1:A:279:SER:HG	1:A:363:TYR:HH	1.64	0.41
1:B:721:PHE:HD1	1:B:777:ASN:ND2	2.18	0.41
1:A:1215:ASN:HD21	1:B:1080:MET:H	1.68	0.41
1:A:599:VAL:O	1:A:602:ASN:HB2	2.20	0.41
1:B:696:ALA:O	1:B:822:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:371:SER:HB2	1:A:372:PRO:CD	2.50	0.41
1:A:210:PRO:O	1:B:860:GLN:HB2	2.19	0.41
1:A:338:ASP:HB3	1:A:339:PRO:CD	2.50	0.41
1:B:700:PRO:HB3	1:B:819:PRO:HD3	2.02	0.41
1:A:349:VAL:HG12	1:B:349:VAL:HG12	2.03	0.41
1:B:184:GLU:CD	1:B:256:ARG:HH12	2.23	0.41
1:A:1001:SER:HB2	1:A:1011:ALA:HB3	2.01	0.41
1:A:833:PHE:HD2	1:B:208:MET:HE2	1.86	0.41
1:A:1137:LEU:HD23	1:A:1137:LEU:HA	1.90	0.41
1:B:718:PRO:HB2	1:B:777:ASN:HD21	1.86	0.41
5:B:1243:TPP:C2	5:B:1243:TPP:HN42	2.33	0.41
1:A:593:LYS:CD	1:A:594:LYS:H	2.34	0.41
1:B:1048:GLN:C	1:B:1048:GLN:NE2	2.73	0.41
1:A:897:ALA:HA	1:A:941:LEU:HD13	2.03	0.41
1:B:617:LYS:HD3	1:B:617:LYS:HA	1.71	0.41
1:A:477:SER:HB3	1:A:479:TYR:CE1	2.55	0.41
1:B:477:SER:HB3	1:B:479:TYR:CE1	2.55	0.41
1:B:511:VAL:HA	1:B:542:TYR:O	2.19	0.41
5:B:1243:TPP:N4'	5:B:1243:TPP:H2	2.36	0.41
1:A:234:PRO:CA	1:A:237:LEU:HD12	2.44	0.41
1:B:593:LYS:CD	1:B:594:LYS:H	2.34	0.41
1:A:368:LYS:NZ	1:B:223:ASP:O	2.54	0.41
1:A:644:LYS:HB3	1:A:645:PRO:HD3	2.02	0.41
1:A:804:PRO:HG3	1:A:826:GLN:HE21	1.86	0.41
1:A:563:MET:HB3	1:A:563:MET:HE2	1.87	0.41
1:A:805:LEU:HD12	1:A:854:LYS:HZ1	1.85	0.41
1:A:875:TYR:CE1	1:B:73:GLY:HA2	2.56	0.41
1:B:605:ALA:O	1:B:609:ALA:HB2	2.21	0.41
1:A:605:ALA:O	1:A:609:ALA:HB2	2.21	0.41
1:B:346:SER:O	1:B:350:GLU:CB	2.69	0.41
1:B:619:PRO:HB2	1:B:621:SER:HB3	2.03	0.41
1:A:1177:PRO:O	1:A:1178:ALA:HB2	2.21	0.41
1:B:1177:PRO:O	1:B:1178:ALA:HB2	2.21	0.41
1:A:821:VAL:HG21	1:A:844:TRP:HH2	1.86	0.41
1:A:741:ASN:CG	1:A:744:ASP:HB2	2.42	0.41
5:A:1236:TPP:H2	5:A:1236:TPP:N4'	2.36	0.40
1:A:697:PHE:HD2	1:A:800:GLN:HE21	1.67	0.40
1:B:853:TYR:CE2	1:B:864:TRP:NE1	2.89	0.40
1:B:96:ASN:O	1:B:99:LYS:N	2.55	0.40
1:A:96:ASN:O	1:A:99:LYS:N	2.55	0.40
1:B:755:CYS:HA	4:B:1240:SF4:S1	2.61	0.40
5:A:1236:TPP:HN42	5:A:1236:TPP:C2	2.33	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1214:GLN:CD	1:B:461:GLY:H	2.23	0.40
1:B:238:LYS:O	1:B:242:ILE:HG13	2.20	0.40
1:B:893:LEU:HA	1:B:893:LEU:HD12	1.88	0.40
1:B:273:ILE:HD13	1:B:273:ILE:HG21	1.63	0.40
1:B:563:MET:HB3	1:B:563:MET:HE2	1.92	0.40
1:A:1146:LYS:HA	1:A:1149:ARG:NH1	2.37	0.40
1:B:755:CYS:SG	1:B:761:ALA:CB	3.02	0.40
1:A:721:PHE:HD1	1:A:777:ASN:ND2	2.18	0.40
1:A:853:TYR:CE2	1:A:864:TRP:NE1	2.89	0.40
1:A:619:PRO:HB2	1:A:621:SER:HB3	2.03	0.40
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.82	0.40
1:A:755:CYS:HA	4:A:1233:SF4:S1	2.61	0.40
1:A:467:HIS:C	1:A:468:LEU:HD23	2.42	0.40
1:B:467:HIS:C	1:B:468:LEU:HD23	2.42	0.40
1:A:693:ASN:O	1:A:697:PHE:HB2	2.22	0.40
1:A:5:MET:CE	1:A:184:GLU:HB2	2.52	0.40
1:B:388:ASN:OD1	1:B:389:HIS:N	2.54	0.40
1:A:718:PRO:HB2	1:A:777:ASN:HD21	1.86	0.40
1:A:1082:LYS:NZ	1:B:1219:THR:HG21	2.34	0.40
1:B:811:ALA:HB2	1:B:844:TRP:CB	2.52	0.40
1:A:856:ASN:HD21	1:A:860:GLN:HG3	1.87	0.40
1:A:1118:LYS:HE3	1:A:1118:LYS:HB2	1.94	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:292:ALA:N	1:B:634:MET:CE[3_445]	2.01	0.19
1:A:292:ALA:CA	1:B:634:MET:CE[3_445]	2.05	0.15
1:A:291:ALA:C	1:B:634:MET:CE[3_445]	2.12	0.08
1:A:291:ALA:O	1:B:634:MET:CE[3_445]	2.18	0.02

## 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	1229/1231 (100%)	1101 (90%)	103 (8%)	25 (2%)	11	48
1	B	1229/1231 (100%)	1102 (90%)	102 (8%)	25 (2%)	11	48
All	All	2458/2462 (100%)	2203 (90%)	205 (8%)	50 (2%)	11	48

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	218	THR
1	A	595	GLY
1	A	626	PRO
1	A	627	ALA
1	A	1124	VAL
1	A	1178	ALA
1	A	1231	LYS
1	B	87	SER
1	B	218	THR
1	B	595	GLY
1	B	626	PRO
1	B	627	ALA
1	B	1124	VAL
1	B	1178	ALA
1	B	1231	LYS
1	A	711	GLU
1	A	940	GLY
1	A	941	LEU
1	A	993	VAL
1	A	996	ASN
1	A	1181	LYS
1	B	711	GLU
1	B	940	GLY
1	B	941	LEU
1	B	993	VAL
1	B	996	ASN
1	B	1181	LYS
1	A	356	PRO
1	A	903	SER
1	A	1174	SER
1	B	356	PRO
1	B	903	SER
1	B	1174	SER
1	A	221	ASN

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Mol	Chain	Res	Type
1	A	353	GLU
1	A	364	GLY
1	A	691	GLN
1	A	1182	ALA
1	B	221	ASN
1	B	353	GLU
1	B	364	GLY
1	B	691	GLN
1	B	1182	ALA
1	A	576	PHE
1	A	599	VAL
1	B	576	PHE
1	B	599	VAL
1	A	1179	GLY
1	B	1179	GLY

### 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	978/978 (100%)	841 (86%)	137 (14%)	5	23
1	B	978/978 (100%)	841 (86%)	137 (14%)	5	23
All	All	1956/1956 (100%)	1682 (86%)	274 (14%)	5	23

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	11	ASN
1	A	14	THR
1	A	27	ILE
1	A	58	ILE
1	A	64	GLU
1	A	82	THR
1	A	111	VAL
1	A	121	LEU
1	A	134	ARG

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Mol	Chain	Res	Type
1	A	141	LEU
1	A	152	MET
1	A	154	LEU
1	A	175	ARG
1	A	180	ILE
1	A	182	LYS
1	A	184	GLU
1	A	194	LEU
1	A	204	ARG
1	A	206	LYS
1	A	211	GLU
1	A	213	PRO
1	A	215	VAL
1	A	226	PHE
1	A	227	GLN
1	A	248	GLN
1	A	257	SER
1	A	279	SER
1	A	290	LEU
1	A	302	VAL
1	A	303	ARG
1	A	311	GLU
1	A	317	LEU
1	A	324	ILE
1	A	325	THR
1	A	328	ASP
1	A	331	LYS
1	A	342	LEU
1	A	349	VAL
1	A	357	LYS
1	A	367	SER
1	A	392	VAL
1	A	399	THR
1	A	403	LEU
1	A	439	LYS
1	A	454	SER
1	A	460	SER
1	A	463	ILE
1	A	465	ILE
1	A	468	LEU
1	A	472	GLU
1	A	482	ASN

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Mol	Chain	Res	Type
1	A	491	ASN
1	A	501	LEU
1	A	509	THR
1	A	510	PHE
1	A	511	VAL
1	A	514	SER
1	A	517	SER
1	A	524	LYS
1	A	532	ARG
1	A	538	LYS
1	A	570	LEU
1	A	582	LEU
1	A	583	LEU
1	A	593	LYS
1	A	613	LEU
1	A	617	LYS
1	A	620	ASP
1	A	621	SER
1	A	624	ASP
1	A	628	GLU
1	A	629	THR
1	A	630	LYS
1	A	635	THR
1	A	637	GLU
1	A	643	VAL
1	A	654	LEU
1	A	656	VAL
1	A	673	GLU
1	A	681	VAL
1	A	683	GLN
1	A	687	GLU
1	A	702	SER
1	A	710	LYS
1	A	715	VAL
1	A	720	ASN
1	A	725	GLU
1	A	730	GLU
1	A	741	ASN
1	A	771	ARG
1	A	783	ARG
1	A	800	GLN
1	A	808	PHE

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Mol	Chain	Res	Type
1	A	823	VAL
1	A	854	LYS
1	A	857	ARG
1	A	858	LEU
1	A	883	MET
1	A	887	ARG
1	A	910	LEU
1	A	914	LEU
1	A	917	LYS
1	A	930	LEU
1	A	941	LEU
1	A	949	SER
1	A	953	THR
1	A	954	LYS
1	A	997	THR
1	A	1000	GLN
1	A	1001	SER
1	A	1002	SER
1	A	1047	GLN
1	A	1048	GLN
1	A	1064	LEU
1	A	1074	GLN
1	A	1088	ASN
1	A	1104	ARG
1	A	1105	LEU
1	A	1108	GLN
1	A	1110	LYS
1	A	1118	LYS
1	A	1126	GLU
1	A	1136	VAL
1	A	1137	LEU
1	A	1146	LYS
1	A	1149	ARG
1	A	1166	MET
1	A	1170	ASN
1	A	1173	GLU
1	A	1181	LYS
1	A	1185	SER
1	A	1196	THR
1	A	1197	ARG
1	A	1200	THR
1	A	1219	THR

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Mol	Chain	Res	Type
1	A	1225	ASP
1	B	7	THR
1	B	11	ASN
1	B	14	THR
1	B	27	ILE
1	B	58	ILE
1	B	64	GLU
1	B	82	THR
1	B	111	VAL
1	B	121	LEU
1	B	134	ARG
1	B	141	LEU
1	B	152	MET
1	B	154	LEU
1	B	175	ARG
1	B	180	ILE
1	B	182	LYS
1	B	184	GLU
1	B	194	LEU
1	B	204	ARG
1	B	206	LYS
1	B	211	GLU
1	B	213	PRO
1	B	215	VAL
1	B	226	PHE
1	B	227	GLN
1	B	248	GLN
1	B	257	SER
1	B	279	SER
1	B	290	LEU
1	B	302	VAL
1	B	303	ARG
1	B	311	GLU
1	B	317	LEU
1	B	324	ILE
1	B	325	THR
1	B	328	ASP
1	B	331	LYS
1	B	342	LEU
1	B	349	VAL
1	B	357	LYS
1	B	367	SER

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Mol	Chain	Res	Type
1	B	392	VAL
1	B	399	THR
1	B	403	LEU
1	B	439	LYS
1	B	454	SER
1	B	460	SER
1	B	463	ILE
1	B	465	ILE
1	B	468	LEU
1	B	472	GLU
1	B	482	ASN
1	B	491	ASN
1	B	501	LEU
1	B	509	THR
1	B	510	PHE
1	B	511	VAL
1	B	514	SER
1	B	517	SER
1	B	524	LYS
1	B	532	ARG
1	B	538	LYS
1	B	570	LEU
1	B	582	LEU
1	B	583	LEU
1	B	593	LYS
1	B	613	LEU
1	B	617	LYS
1	B	620	ASP
1	B	621	SER
1	B	624	ASP
1	B	628	GLU
1	B	629	THR
1	B	630	LYS
1	B	635	THR
1	B	637	GLU
1	B	643	VAL
1	B	654	LEU
1	B	656	VAL
1	B	673	GLU
1	B	681	VAL
1	B	683	GLN
1	B	687	GLU

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Mol	Chain	Res	Type
1	B	702	SER
1	B	710	LYS
1	B	715	VAL
1	B	720	ASN
1	B	725	GLU
1	B	730	GLU
1	B	741	ASN
1	B	771	ARG
1	B	783	ARG
1	B	800	GLN
1	B	808	PHE
1	B	823	VAL
1	B	854	LYS
1	B	857	ARG
1	B	858	LEU
1	B	883	MET
1	B	887	ARG
1	B	910	LEU
1	B	914	LEU
1	B	917	LYS
1	B	930	LEU
1	B	941	LEU
1	B	949	SER
1	B	953	THR
1	B	954	LYS
1	B	997	THR
1	B	1000	GLN
1	B	1001	SER
1	B	1002	SER
1	B	1047	GLN
1	B	1048	GLN
1	B	1064	LEU
1	B	1074	GLN
1	B	1088	ASN
1	B	1104	ARG
1	B	1105	LEU
1	B	1108	GLN
1	B	1110	LYS
1	B	1118	LYS
1	B	1126	GLU
1	B	1136	VAL
1	B	1137	LEU

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Mol	Chain	Res	Type
1	B	1146	LYS
1	B	1149	ARG
1	B	1166	MET
1	B	1170	ASN
1	B	1173	GLU
1	B	1181	LYS
1	B	1185	SER
1	B	1196	THR
1	B	1197	ARG
1	B	1200	THR
1	B	1219	THR
1	B	1225	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	16	HIS
1	A	46	GLN
1	A	110	HIS
1	A	147	GLN
1	A	169	HIS
1	A	212	HIS
1	A	220	GLN
1	A	227	GLN
1	A	233	ASN
1	A	288	ASN
1	A	389	HIS
1	A	421	GLN
1	A	434	ASN
1	A	467	HIS
1	A	491	ASN
1	A	513	ASN
1	A	536	ASN
1	A	543	ASN
1	A	560	ASN
1	A	636	ASN
1	A	650	GLN
1	A	671	GLN
1	A	683	GLN
1	A	688	ASN
1	A	691	GLN

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Mol	Chain	Res	Type
1	A	693	ASN
1	A	720	ASN
1	A	739	GLN
1	A	741	ASN
1	A	750	ASN
1	A	777	ASN
1	A	800	GLN
1	A	866	ASN
1	A	918	ASN
1	A	976	HIS
1	A	1000	GLN
1	A	1048	GLN
1	A	1088	ASN
1	A	1132	ASN
1	A	1215	ASN
1	A	1223	GLN
1	B	11	ASN
1	B	16	HIS
1	B	46	GLN
1	B	110	HIS
1	B	147	GLN
1	B	169	HIS
1	B	212	HIS
1	B	220	GLN
1	B	221	ASN
1	B	227	GLN
1	B	233	ASN
1	B	288	ASN
1	B	389	HIS
1	B	421	GLN
1	B	434	ASN
1	B	467	HIS
1	B	491	ASN
1	B	513	ASN
1	B	536	ASN
1	B	543	ASN
1	B	560	ASN
1	B	636	ASN
1	B	650	GLN
1	B	671	GLN
1	B	683	GLN
1	B	688	ASN

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Mol	Chain	Res	Type
1	B	691	GLN
1	B	693	ASN
1	B	720	ASN
1	B	739	GLN
1	B	741	ASN
1	B	750	ASN
1	B	777	ASN
1	B	800	GLN
1	B	866	ASN
1	B	918	ASN
1	B	976	HIS
1	B	1000	GLN
1	B	1048	GLN
1	B	1088	ASN
1	B	1132	ASN
1	B	1215	ASN
1	B	1223	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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
4	SF4	A	1233	1	12,12,12	5.95	9 (75%)	0,24,24	0.00	-
4	SF4	A	1234	1	12,12,12	10.88	11 (91%)	0,24,24	0.00	-
4	SF4	A	1235	1	12,12,12	7.90	11 (91%)	0,24,24	0.00	-
5	TPP	A	1236	2	27,27,27	1.38	5 (18%)	40,40,40	1.95	8 (20%)
6	PYR	A	1239	-	5,5,5	4.34	3 (60%)	6,6,6	2.29	3 (50%)
4	SF4	B	1240	1	12,12,12	5.93	9 (75%)	0,24,24	0.00	-
4	SF4	B	1241	1	12,12,12	10.89	11 (91%)	0,24,24	0.00	-
4	SF4	B	1242	1	12,12,12	7.93	11 (91%)	0,24,24	0.00	-
5	TPP	B	1243	2	27,27,27	1.38	5 (18%)	40,40,40	1.95	8 (20%)
6	PYR	B	1246	-	5,5,5	4.33	3 (60%)	6,6,6	2.30	2 (33%)

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
4	SF4	A	1233	1	-	0/0/48/48	0/0/5/5
4	SF4	A	1234	1	-	0/0/48/48	0/0/5/5
4	SF4	A	1235	1	-	0/0/48/48	0/0/5/5
5	TPP	A	1236	2	-	0/17/17/17	0/2/2/2
6	PYR	A	1239	-	-	0/4/4/4	0/0/0/0
4	SF4	B	1240	1	-	0/0/48/48	0/0/5/5
4	SF4	B	1241	1	-	0/0/48/48	0/0/5/5
4	SF4	B	1242	1	-	0/0/48/48	0/0/5/5
5	TPP	B	1243	2	-	0/17/17/17	0/2/2/2
6	PYR	B	1246	-	-	0/4/4/4	0/0/0/0

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1241	SF4	S2-FE3	-20.52	2.19	2.33
4	A	1234	SF4	S2-FE3	-20.49	2.19	2.33
4	B	1241	SF4	S4-FE3	-14.79	2.23	2.33
4	A	1234	SF4	S4-FE3	-14.79	2.23	2.33
4	B	1242	SF4	S4-FE1	-12.95	2.24	2.33
4	A	1235	SF4	S4-FE1	-12.89	2.24	2.33
4	A	1234	SF4	S1-FE4	-12.43	2.24	2.33
4	B	1241	SF4	S1-FE4	-12.39	2.24	2.33
4	A	1234	SF4	S4-FE1	-12.10	2.25	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1241	SF4	S4-FE1	-12.09	2.25	2.33
4	A	1233	SF4	S1-FE4	-11.38	2.25	2.33
4	B	1242	SF4	S1-FE3	-11.35	2.25	2.33
4	B	1240	SF4	S1-FE4	-11.32	2.25	2.33
4	A	1235	SF4	S1-FE3	-11.28	2.25	2.33
4	B	1241	SF4	S2-FE1	-10.61	2.26	2.33
4	A	1234	SF4	S2-FE1	-10.56	2.26	2.33
4	B	1242	SF4	S2-FE4	-9.90	2.26	2.33
4	A	1235	SF4	S2-FE4	-9.81	2.26	2.33
4	B	1242	SF4	S1-FE2	-9.50	2.26	2.33
4	A	1235	SF4	S1-FE2	-9.47	2.26	2.33
4	B	1242	SF4	S4-FE2	-9.35	2.27	2.33
4	B	1241	SF4	S2-FE4	-9.33	2.27	2.33
4	A	1235	SF4	S4-FE2	-9.33	2.27	2.33
4	A	1234	SF4	S2-FE4	-9.29	2.27	2.33
4	A	1234	SF4	S3-FE2	-9.07	2.27	2.33
4	B	1241	SF4	S3-FE2	-8.98	2.27	2.33
4	A	1234	SF4	S4-FE2	-8.64	2.27	2.33
4	B	1241	SF4	S4-FE2	-8.63	2.27	2.33
6	A	1239	PYR	O3-C2	8.05	1.41	1.23
6	B	1246	PYR	O3-C2	8.03	1.40	1.23
4	A	1233	SF4	S3-FE1	-7.92	2.27	2.33
4	B	1240	SF4	S3-FE1	-7.86	2.28	2.33
4	A	1235	SF4	S4-FE3	-7.32	2.28	2.33
4	A	1235	SF4	S1-FE4	-7.31	2.28	2.33
4	B	1242	SF4	S4-FE3	-7.30	2.28	2.33
4	B	1242	SF4	S1-FE4	-7.29	2.28	2.33
4	B	1240	SF4	S4-FE2	-7.19	2.28	2.33
4	A	1233	SF4	S4-FE2	-7.11	2.28	2.33
4	B	1241	SF4	S3-FE4	-6.96	2.28	2.33
4	A	1234	SF4	S3-FE1	-6.91	2.28	2.33
4	A	1234	SF4	S3-FE4	-6.89	2.28	2.33
4	B	1241	SF4	S3-FE1	-6.87	2.28	2.33
4	A	1233	SF4	S2-FE1	-6.81	2.28	2.33
4	B	1240	SF4	S2-FE1	-6.78	2.28	2.33
4	A	1233	SF4	S1-FE3	-6.77	2.28	2.33
4	B	1240	SF4	S1-FE3	-6.76	2.28	2.33
4	A	1233	SF4	S2-FE3	-5.73	2.29	2.33
4	A	1234	SF4	S1-FE2	-5.67	2.29	2.33
4	B	1240	SF4	S2-FE3	-5.66	2.29	2.33
4	B	1241	SF4	S1-FE2	-5.61	2.29	2.33
4	A	1235	SF4	S3-FE2	-5.59	2.29	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1242	SF4	S3-FE2	-5.57	2.29	2.33
4	A	1233	SF4	S3-FE2	-4.77	2.30	2.33
4	B	1240	SF4	S3-FE2	-4.64	2.30	2.33
4	A	1233	SF4	S3-FE4	-4.63	2.30	2.33
4	B	1240	SF4	S3-FE4	-4.62	2.30	2.33
6	A	1239	PYR	C2-C1	-4.59	1.42	1.53
6	B	1246	PYR	C2-C1	-4.57	1.42	1.53
4	B	1242	SF4	S3-FE4	-4.32	2.30	2.33
4	A	1235	SF4	S3-FE4	-4.22	2.30	2.33
4	A	1235	SF4	S3-FE1	-3.54	2.30	2.33
4	B	1242	SF4	S3-FE1	-3.52	2.30	2.33
4	A	1235	SF4	S2-FE1	-3.45	2.30	2.33
4	B	1242	SF4	S2-FE1	-3.38	2.31	2.33
5	A	1236	TPP	C6-C5	-2.83	1.47	1.51
5	B	1243	TPP	C6-C5	-2.83	1.47	1.51
6	B	1246	PYR	O1-C1	2.74	1.30	1.22
6	A	1239	PYR	O1-C1	2.74	1.30	1.22
4	B	1240	SF4	S2-FE4	2.68	2.35	2.33
4	A	1233	SF4	S2-FE4	2.62	2.35	2.33
5	B	1243	TPP	C4'-N3'	2.61	1.39	1.35
5	A	1236	TPP	C4'-N3'	2.58	1.39	1.35
5	A	1236	TPP	C7'-N3	2.55	1.53	1.48
5	B	1243	TPP	C7'-N3	2.55	1.53	1.48
5	A	1236	TPP	C2'-N1'	2.54	1.38	1.34
5	B	1243	TPP	C2'-N1'	2.52	1.38	1.34
5	B	1243	TPP	PB-O3B	-2.45	1.45	1.54
5	A	1236	TPP	PB-O3B	-2.45	1.45	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1236	TPP	C7'-N3-C2	5.28	136.25	125.05
5	B	1243	TPP	C7'-N3-C2	5.28	136.24	125.05
5	A	1236	TPP	C7'-N3-C4	-5.04	114.01	124.34
5	B	1243	TPP	C7'-N3-C4	-5.03	114.02	124.34
6	B	1246	PYR	O2-C1-C2	4.00	123.19	114.37
6	A	1239	PYR	O2-C1-C2	3.99	123.16	114.37
5	B	1243	TPP	O3B-PB-O2B	3.71	122.06	107.61
5	A	1236	TPP	O3B-PB-O2B	3.71	122.04	107.61
5	A	1236	TPP	C6-C5-C4	3.46	129.96	127.44
5	B	1243	TPP	C6-C5-C4	3.43	129.94	127.44
5	A	1236	TPP	CM2-C2'-N1'	3.41	121.08	117.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1243	TPP	CM2-C2'-N1'	3.40	121.07	117.02
5	A	1236	TPP	C6-C5-S1	-3.39	117.55	122.28
5	B	1243	TPP	C6-C5-S1	-3.36	117.58	122.28
6	B	1246	PYR	O2-C1-O1	-3.33	115.74	123.62
6	A	1239	PYR	O2-C1-O1	-3.32	115.75	123.62
5	A	1236	TPP	C2-S1-C5	-2.80	89.75	91.63
5	B	1243	TPP	C2-S1-C5	-2.79	89.75	91.63
5	A	1236	TPP	N1'-C2'-N3'	-2.37	121.37	125.65
5	B	1243	TPP	N1'-C2'-N3'	-2.36	121.40	125.65
6	A	1239	PYR	C3-C2-C1	2.00	122.13	117.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.