



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:49 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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

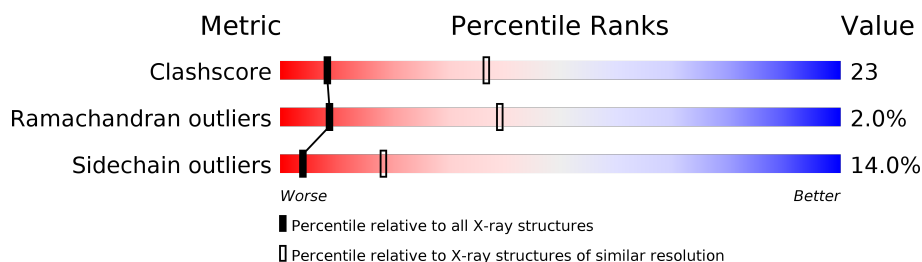
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (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. 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.

Note EDS was not executed.

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	A	1234	-	-	X	-
4	SF4	B	1241	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18894 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 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).

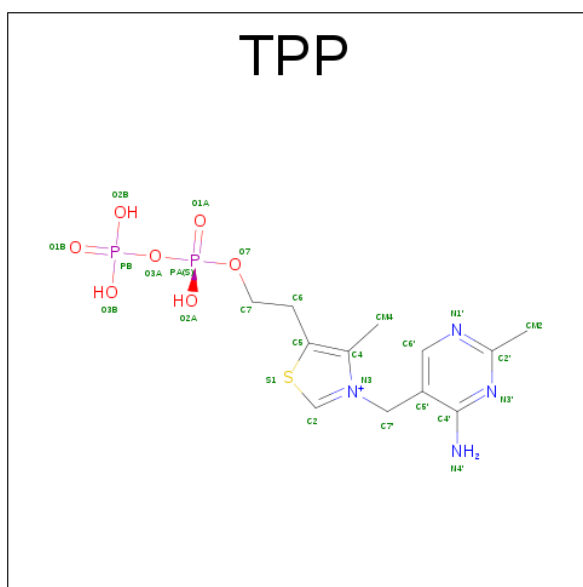
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

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



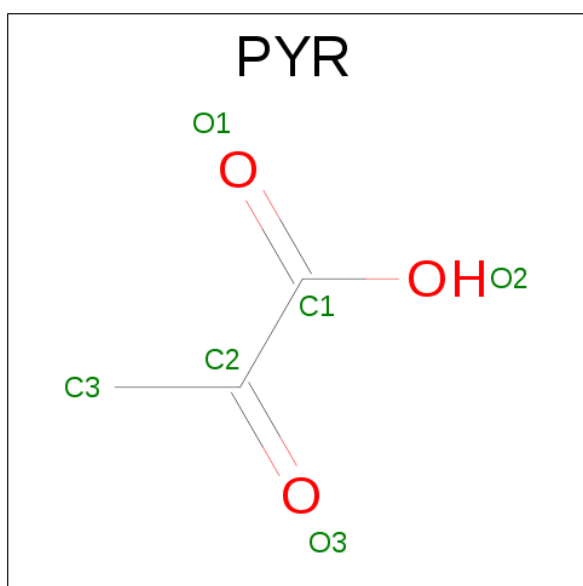
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- 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:  $C_3H_4O_3$ ).



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.

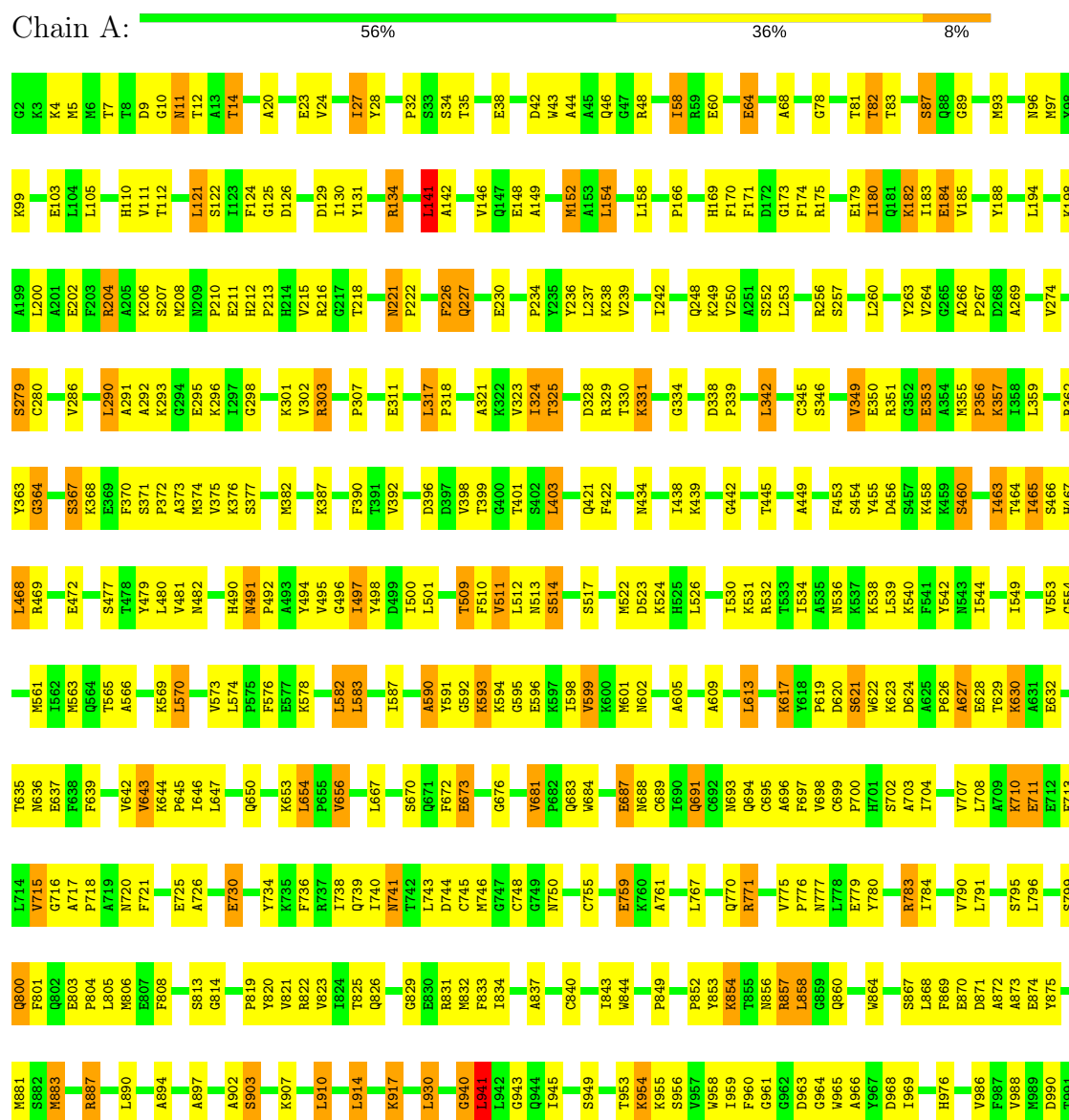
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total 7	O 7	0	0
7	B	7	Total 7	O 7	0	0

### 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.

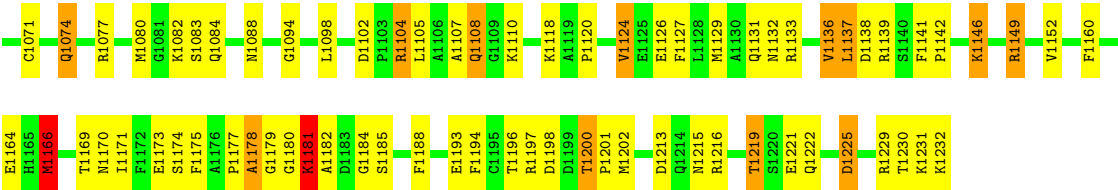
Note EDS was not executed.

#### • Molecule 1: PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE)









## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 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	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

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 23.

All (864) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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	Interatomic distance (Å)	Clash overlap (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:A:9:ASP:OD1	1:A:12:THR:HG23	1.77	0.84
1:B:9:ASP:OD1	1:B: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:GLN:HE22	1:B:777:ASN:HB3	1.50	0.77
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:PYR:O1	1.86	0.76
1:A:1193:GLU:OE1	1:B:1077:ARG:HA	1.86	0.76
1:B:1137:LEU:HD22	1:B:1141:PHE:HB2	1.67	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:PYR:O1	1.86	0.75
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.36	0.74
1:B:639:PHE:CE2	1:B:672:PHE:HB2	2.22	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:A:697:PHE:HD2	1:A:800:GLN:NE2	1.92	0.68
1:B:467:HIS:HB3	1:B:481:VAL:HG23	1.75	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1219:THR:HG21	1:B:1082:LYS:HZ3	1.65	0.62
1:A:142:ALA:HB2	1:A:170:PHE:CZ	2.35	0.62
1:A:325:THR:CG2	1:A:382:MET:SD	2.88	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:A:917:LYS:HB3	1:A:917:LYS:HZ3	1.65	0.61
1:B:325:THR:CG2	1:B:382:MET:SD	2.88	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:1124:VAL:O	1:A:1127:PHE:HB3	2.01	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: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:154:LEU:HD22	1:A:158:LEU:CD1	2.31	0.60
1:A:465:ILE:HD12	1:A:466:SER:N	2.17	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:A:236:TYR:HA	1:A:239:VAL:HG12	1.84	0.59
1:B:465:ILE:HD12	1:B:466:SER:N	2.17	0.59
1:A:1016:ALA:HB1	1:A:1019:ARG:HH21	1.66	0.59
1:A:700:PRO:HG3	1:A:814:GLY:HA2	1.85	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: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:A:730:GLU:H	1:A:730:GLU:CD	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ILE:O	1:B:553:VAL:HG22	2.03	0.59
1:B:639:PHE:CD2	1:B:672:PHE:HB2	2.37	0.59
1:B:894:ALA:CB	1:B:914:LEU:HD21	2.33	0.59
1:A:639:PHE:CD2	1:A:672:PHE:HB2	2.37	0.59
1:A:676:GLY:HA3	1:A:743:LEU:HD22	1.84	0.59
1:A:87:SER:HA	1:A:129:ASP:HB3	1.85	0.59
1:A:917:LYS:HB3	1:A:917:LYS:NZ	2.18	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:A:894:ALA:CB	1:A:914:LEU:HD21	2.33	0.58
1:B:494:TYR:HB3	1:B:500:ILE:HD11	1.84	0.58
1:A:396:ASP:HA	1:A:656:VAL:HG13	1.84	0.58
1:B:356:PRO:O	1:B:357:LYS:HB3	2.02	0.58
1:B:676:GLY:HA3	1:B:743:LEU:HD22	1.84	0.58
1:B:643:VAL:HB	1:B:849:PRO:HB2	1.85	0.58
1:B:87:SER:HA	1:B:129:ASP:HB3	1.85	0.58
1:A:643:VAL:HB	1:A:849:PRO:HB2	1.85	0.58
1:A:9:ASP:HA	1:A:179:GLU:O	2.03	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:A:699:CYS:SG	1:A:703:ALA:HB3	2.44	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: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:A:1160:PHE:O	1:A:1164:GLU:HG3	2.04	0.57
1:B:236:TYR:HA	1:B:239:VAL:HG12	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HB3	1:A:185:VAL:HG23	1.86	0.57
1:B:20:ALA:HB2	1:B:188:TYR:CE1	2.39	0.57
1:B:263:TYR:CZ	1:B:318:PRO:HG2	2.38	0.57
1:A:805:LEU:HA	1:A:854:LYS:HZ1	1.68	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:A:565:THR:HG21	1:A:609:ALA:HB3	1.87	0.57
5:B:1243:TPP:HN42	5:B:1243:TPP:H2	1.70	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:986:VAL:HG22	1:A:1064:LEU:HD23	1.88	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:1215:ASN:ND2	1:B:1080:MET:H	2.03	0.56
1:B:1225:ASP:O	1:B:1229:ARG:HG3	2.06	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:986:VAL:HG22	1:B:1064:LEU:HD23	1.88	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:1004:ALA:O	1:B:1022:LYS:HG3	2.06	0.55
1:B:124:PHE:CB	1:B:367:SER:HB2	2.26	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: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:B:20:ALA:HB2	1:B:188:TYR:CZ	2.40	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:A:681:VAL:HG23	1:A:770:GLN:HG3	1.88	0.55
1:B:1219:THR:HG22	1:B:1222:GLN:H	1.72	0.55
1:A:434:ASN:O	1:A:438:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1193:GLU:H	1:B:1193:GLU:CD	2.11	0.55
1:B:495:VAL:HG13	1:B:496:GLY:N	2.22	0.55
1:A:456:ASP:OD1	1:A:458:LYS:HB2	2.07	0.55
1:B:1077:ARG:HB2	1:B:1077:ARG:NH1	2.22	0.55
1:B:110:HIS:CD2	1:B:169:HIS:CD2	2.88	0.55
1:B:422:PHE:HE1	1:B:468:LEU:HG	1.72	0.54
1:A:422:PHE:HE1	1:A:468:LEU:HG	1.72	0.54
1:A:495:VAL:HG13	1:A:496:GLY:N	2.22	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:1048:GLN:HE21	1:A:1048:GLN:C	2.11	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:1146:LYS:HA	1:A:1149:ARG:HH12	1.72	0.54
1:A:249:LYS:O	1:A:252:SER:HB3	2.07	0.54
1:A:99:LYS:HE3	1:B:867:SER:O	2.06	0.54
1:B:1149:ARG:HH11	1:B:1149:ARG:CG	2.16	0.54
1:B:323:VAL:CG1	1:B:382:MET:HG2	2.38	0.54
1:B:688:ASN:HD21	1:B:759:GLU:HB2	1.73	0.54
1:A:1131:GLN:OE1	1:A:1133:ARG:NE	2.40	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:210:PRO:HB2	1:B:831:ARG:HA	1.89	0.54
1:A:208:MET:HE2	1:B:833:PHE:HD2	1.72	0.54
1:A:497:ILE:HG13	1:A:498:TYR:CD2	2.43	0.53
1:B:536:ASN:HD22	1:B:623:LYS:NZ	2.05	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:A:1194:PHE:CD2	1:A:1213:ASP:HB3	2.44	0.53
1:A:323:VAL:CG1	1:A:382:MET:HG2	2.38	0.53
1:A:688:ASN:HD21	1:A:759:GLU:HB2	1.73	0.53
1:B:495:VAL:HG13	1:B:496:GLY:H	1.73	0.53
1:A:1219:THR:HG21	1:B:1082:LYS:NZ	2.24	0.53
1:A:1080:MET:O	1:A:1083:SER:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LYS:HG3	1:A:331:LYS:O	2.06	0.53
1:A:536:ASN:HD22	1:A:623:LYS:HZ3	1.57	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: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:A:463:ILE:HG13	1:A:464:THR:N	2.24	0.53
1:A:903:SER:O	1:A:907:LYS:HG3	2.08	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:B:867:SER:O	1:B:868:LEU:HD23	2.09	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:1194:PHE:CD2	1:B:1213:ASP:HB3	2.44	0.53
1:B:630:LYS:HD2	1:B:632:GLU:HG2	1.91	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:1059:PHE:HD1	1:A:1104:ARG:HD3	1.75	0.52
1:A:398:VAL:HG13	1:A:656:VAL:HG22	1.91	0.52
1:B:534:ILE:HA	1:B:539:LEU:HG	1.91	0.52
1:B:619:PRO:HG2	1:B:622:TRP:CD1	2.44	0.52
1:A:1230:THR:O	1:A:1232:LYS:N	2.42	0.52
1:A:867:SER:O	1:A:868:LEU:HD23	2.09	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: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:81:THR:HG22	1:A:82:THR:N	2.24	0.52
1:B:434:ASN:HD22	1:B:453:PHE:HE1	1.56	0.52
1:A:964:GLY:O	1:A:968:ASP:HB2	2.10	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:775:VAL:HB	1:B:776:PRO:CD	2.40	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: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:B:463:ILE:HG13	1:B:464:THR:N	2.24	0.52
1:A:534:ILE:HA	1:A:539:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1036:TYR:O	1:B:1063:SER:HA	2.10	0.52
1:A:230:GLU:OE2	1:B:331:LYS:HE3	2.09	0.52
1:A:1035:VAL:O	1:A:1037:VAL:HG23	2.10	0.52
1:A:619:PRO:HG2	1:A:622:TRP:CD1	2.44	0.52
1:A:853:TYR:CE2	1:A:864:TRP:CD1	2.98	0.52
1:B:323:VAL:HA	1:B:356:PRO:O	2.09	0.52
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.39	0.51
1:A:681:VAL:HG22	1:A:767:LEU:HA	1.91	0.51
1:B:81:THR:HG22	1:B:82:THR:N	2.24	0.51
1:A:1025:LEU:O	1:A:1029:VAL:HG13	2.11	0.51
1:A:1036:TYR:O	1:A:1063:SER:HA	2.10	0.51
1:A:269:ALA:HA	1:A:296:LYS:HB3	1.92	0.51
1:A:873:ALA:HA	1:A:959:ILE:HG21	1.92	0.51
1:A:961:GLY:O	1:A:988:VAL:HA	2.11	0.51
1:B:873:ALA:HA	1:B:959:ILE:HG21	1.92	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:349:VAL:CG2	1:B:350:GLU:N	2.73	0.51
1:B:715:VAL:C	1:B:717:ALA:H	2.14	0.51
1:B:853:TYR:CE2	1:B:864:TRP:CD1	2.98	0.51
1:A:1138:ASP:O	1:A:1142:PRO:HG3	2.10	0.51
1:B:1102:ASP:CG	1:B:1104:ARG:HH11	2.14	0.51
1:B:465:ILE:HG13	1:B:467:HIS:CE1	2.46	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:A:349:VAL:CG2	1:A:350:GLU:N	2.73	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:1160:PHE:O	1:A:1160:PHE:CD1	2.64	0.51
1:A:715:VAL:HG12	1:A:716:GLY:N	2.25	0.51
1:B:1138:ASP:O	1:B:1142:PRO:HG3	2.10	0.51
1:B:695:CYS:HB2	1:B:704:ILE:HD13	1.92	0.51
1:B:681:VAL:HG22	1:B:767:LEU:HA	1.91	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:A:130:ILE:HD13	1:A:170:PHE:CZ	2.46	0.50
1:A:910:LEU:HD12	1:A:930:LEU:HD21	1.92	0.50
1:B:110:HIS:HD2	1:B:169:HIS:CD2	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:GLN:HG2	1:B:736:PHE:CD1	2.47	0.50
1:B:883:MET:HE2	1:B:955:LYS:HD2	1.92	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:A:869:PHE:CE2	1:A:969:ILE:HG21	2.47	0.50
1:B:269:ALA:HA	1:B:296:LYS:HB3	1.92	0.50
1:A:1016:ALA:HB1	1:A:1019:ARG:NH2	2.26	0.50
1:A:131:TYR:O	1:A:134:ARG:HB2	2.12	0.50
1:A:684:TRP:CE2	1:A:738:ILE:HB	2.47	0.50
1:A:82:THR:HG22	1:A:83:THR:N	2.27	0.50
1:B:578:LYS:HE3	1:B:582:LEU:HD21	1.94	0.50
1:A:715:VAL:C	1:A:717:ALA:H	2.13	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:B:578:LYS:HG3	1:B:582:LEU:HD22	1.94	0.50
1:B:587:ILE:O	1:B:591:TYR:HB2	2.12	0.50
1:B:869:PHE:CE2	1:B:969:ILE:HG21	2.46	0.50
1:B:963:ASP:HB3	1:B:990:ASP:OD1	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: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: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:A:870:GLU:OE1	5:A:1236:TPP:HM21	2.12	0.49
1:B:130:ILE:HD13	1:B:170:PHE:CZ	2.46	0.49
1:B:200:LEU:HD11	1:B:204:ARG:NH1	2.27	0.49
1:A:200:LEU:HD11	1:A:204:ARG:NH1	2.27	0.49
1:A:553:VAL:O	1:A:601:MET:HG3	2.11	0.49
1:A:587:ILE:O	1:A:591:TYR:HB2	2.12	0.49
1:A:910:LEU:HD13	1:A:930:LEU:HD11	1.93	0.49
1:A:746:MET:O	1:B:1216:ARG:HA	2.12	0.49
1:B:182:LYS:HE2	1:B:442:GLY:O	2.13	0.49
1:A:323:VAL:HG12	1:A:382:MET:HG2	1.94	0.49
1:B:512:LEU:HD12	1:B:513:ASN:N	2.27	0.49
1:B:636:ASN:ND2	1:B:672:PHE:HE2	2.11	0.49
1:A:1188:PHE:HB3	1:B:1010:VAL:O	2.11	0.49
1:A:182:LYS:HE2	1:A:442:GLY:O	2.13	0.49
1:B:870:GLU:OE1	5:B:1243:TPP:HM21	2.12	0.49
1:B:43:TRP:HB3	1:B:48:ARG:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:PHE:HD1	1:B:777:ASN:HD22	1.59	0.49
1:B:965:TRP:CE3	1:B:966:ALA:HB2	2.48	0.49
1:B:126:ASP:HA	1:B:329:ARG:CD	2.42	0.49
1:B:713:GLU:O	1:B:780:TYR:OH	2.31	0.49
1:A:691:GLN:HE22	1:A:726:ALA:HA	1.78	0.49
1:A:264:VAL:HG21	1:A:301:LYS:HE3	1.93	0.49
1:A:883:MET:HE2	1:A:955:LYS:HD2	1.94	0.49
1:B:27:ILE:HG23	1:B:28:TYR:N	2.28	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:512:LEU:HD12	1:A:513:ASN:N	2.28	0.49
1:A:334:GLY:O	1:B:307:PRO:HA	2.13	0.49
1:B:684:TRP:CE2	1:B:738:ILE:HB	2.47	0.49
1:A:965:TRP:CE3	1:A:966:ALA:HB2	2.48	0.49
1:B:323:VAL:HG12	1:B:382:MET:HG2	1.94	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:A:569:LYS:HB3	1:A:570:LEU:HD13	1.95	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:B:693:ASN:HB3	1:B:800:GLN:HB2	1.94	0.48
1:B:992:GLU:O	1:B:993:VAL:HB	2.13	0.48
1:A:27:ILE:HG23	1:A:28:TYR:N	2.28	0.48
1:A:681:VAL:CG2	1:A:767:LEU:HA	2.43	0.48
1:A:963:ASP:HB3	1:A:990:ASP:OD1	2.12	0.48
1:B:703:ALA:HB3	4:B:1241:SF4:S4	2.53	0.48
1:B:23:GLU:OE1	1:B:204:ARG:NH2	2.46	0.48
1:B:691:GLN:HE22	1:B:726:ALA:HA	1.78	0.48
1:A:583:LEU:O	1:A:587:ILE:HG12	2.13	0.48
1:A:940:GLY:O	1:A:943:GLY:N	2.46	0.48
1:A:834:ILE:HD13	1:A:960:PHE:CE2	2.49	0.48
1:B:264:VAL:HG21	1:B:301:LYS:HE3	1.93	0.48
1:B:590:ALA:O	1:B:591:TYR:HB2	2.14	0.48
1:A:60:GLU:O	1:B:976:HIS:HE1	1.96	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:42:ASP:O	1:B:46:GLN:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:TRP:CD2	1:B:738:ILE:HB	2.48	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:42:ASP:O	1:A:46:GLN:HG3	2.14	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:B:617:LYS:NZ	1:B:617:LYS:HB2	2.28	0.48
1:B:994:TYR:CE1	1:B:1002:SER:HB2	2.48	0.48
1:B:721:PHE:CE1	1:B:780:TYR:HD2	2.32	0.48
1:B:867:SER:HB2	1:B:875:TYR:CG	2.49	0.48
1:B:940:GLY:O	1:B:943:GLY:N	2.46	0.48
1:A:566:ALA:HA	1:A:613:LEU:HD21	1.95	0.48
1:A:867:SER:HB2	1:A:875:TYR:CG	2.49	0.48
1:A:590:ALA:O	1:A:591:TYR:HB2	2.14	0.47
1:A:713:GLU:O	1:A:780:TYR:OH	2.31	0.47
1:B:799:SER:OG	1:B:800:GLN:NE2	2.47	0.47
1:A:1175:PHE:CZ	1:A:1177:PRO:HA	2.49	0.47
1:B:1012:LYS:O	1:B:1013:PHE:HB2	2.14	0.47
1:B:569:LYS:HB3	1:B:570:LEU:HD13	1.95	0.47
1:B:681:VAL:CG2	1:B:767:LEU:HA	2.43	0.47
1:B:646:ILE:HG21	1:B:849:PRO:HD3	1.96	0.47
1:A:154:LEU:HD13	1:A:250:VAL:HG22	1.96	0.47
1:B:1040:VAL:HA	1:B:1098:LEU:HD22	1.96	0.47
1:B:351:ARG:HD3	1:B:353:GLU:HB2	1.96	0.47
1:B:566:ALA:HA	1:B:613:LEU:HD21	1.95	0.47
1:B:871:ASP:HB2	1:B:874:GLU:HG2	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:710:LYS:HD2	1:A:734:TYR:HE1	1.80	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:146:VAL:HG12	1:A:183:ILE:HD13	1.96	0.47
1:A:226:PHE:O	1:A:226:PHE:HD1	1.96	0.47
1:A:286:VAL:HG12	1:A:290:LEU:HD22	1.97	0.47
1:B:121:LEU:HG	1:B:122:SER:N	2.29	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:710:LYS:HD2	1:B:734:TYR:HE1	1.80	0.47
1:B:834:ILE:HD13	1:B:960:PHE:CE2	2.49	0.47
1:A:617:LYS:HB2	1:A:617:LYS:NZ	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:VAL:HG23	1:B:574:LEU:HG	1.97	0.47
1:A:1012:LYS:O	1:A:1013:PHE:HB2	2.14	0.47
1:B:1129:MET:HG2	1:B:1149:ARG:HE	1.80	0.47
1:B:1175:PHE:CZ	1:B:1177:PRO:HA	2.49	0.47
1:A:1214:GLN:NE2	1:B:461:GLY:H	2.12	0.47
1:A:121:LEU:HG	1:A:122:SER:N	2.29	0.47
1:A:126:ASP:HA	1:A:329:ARG:CD	2.42	0.47
1:A:351:ARG:HD3	1:A:353:GLU:HB2	1.96	0.47
1:A:867:SER:O	1:B:99:LYS:HE3	2.15	0.47
1:A:871:ASP:HB2	1:A:874:GLU:HG2	1.96	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: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:646:ILE:HG21	1:A:849:PRO:HD3	1.96	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: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:667:LEU:N	1:B:667:LEU:HD12	2.31	0.46
1:B:1232:LYS:HB3	1:B:1232:LYS:HZ2	1.81	0.46
1:B:154:LEU:HD13	1:B:250:VAL:HG22	1.96	0.46
1:A:390:PHE:CE2	1:A:403:LEU:HD22	2.51	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:373:ALA:O	1:A:376:LYS:HB3	2.15	0.46
1:A:710:LYS:HD2	1:A:734:TYR:CE1	2.51	0.46
1:B:1200:THR:HA	1:B:1201:PRO:HD3	1.83	0.46
1:B:390:PHE:CE2	1:B:403:LEU:HD22	2.51	0.46
1:B:693:ASN:HD21	1:B:736:PHE:HZ	1.63	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: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:A:173:GLY:O	1:A:174:PHE:HB2	2.16	0.46
1:A:684:TRP:HZ2	1:A:689:CYS:SG	2.39	0.46
1:A:917:LYS:NZ	1:A:917:LYS:CB	2.78	0.46
1:B:1200:THR:CG2	1:B:1202:MET:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:MET:O	1:B:97:MET:HG3	2.16	0.46
1:A:820:TYR:HD1	1:A:1049:PHE:CZ	2.34	0.46
1:B:820:TYR:HD1	1:B:1049:PHE:CZ	2.34	0.46
1:A:1043:GLY:HA2	1:A:1084:GLN:NE2	2.31	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:491:ASN:HD22	1:A:491:ASN:C	2.19	0.45
1:B:274:VAL:HG23	1:B:324:ILE:HD12	1.98	0.45
1:B:491:ASN:C	1:B:491:ASN:HD22	2.19	0.45
1:A:1010:VAL:O	1:B:1188:PHE:HB3	2.16	0.45
1:A:1071:CYS:HA	4:A:1235:SF4:S3	2.56	0.45
1:A:1162:GLU:HG3	1:B:1171:ILE:HG21	1.98	0.45
1:A:280:CYS:HB3	1:A:301:LYS:HG2	1.99	0.45
1:A:421:GLN:HA	1:A:466:SER:O	2.16	0.45
1:A:644:LYS:N	1:A:645:PRO:CD	2.79	0.45
1:B:1074:GLN:O	1:B:1133:ARG:HG2	2.16	0.45
1:B:780:TYR:HA	1:B:783:ARG:HD2	1.99	0.45
1:A:1141:PHE:N	1:A:1142:PRO:HD3	2.31	0.45
1:A:198:LYS:O	1:A:202:GLU:HG3	2.17	0.45
1:A:325:THR:HG23	1:A:382:MET:CE	2.47	0.45
1:A:64:GLU:HG3	1:A:89:GLY:CA	2.45	0.45
1:B:1141:PHE:N	1:B:1142:PRO:HD3	2.31	0.45
1:B:87:SER:HA	1:B:129:ASP:CB	2.46	0.45
1:B:146:VAL:HG21	1:B:179:GLU:O	2.16	0.45
1:B:421:GLN:HA	1:B:466:SER:O	2.16	0.45
1:B:817:GLU:HB3	1:B:989:MET:HE3	1.98	0.45
1:A:1129:MET:HG2	1:A:1149:ARG:HE	1.80	0.45
1:A:469:ARG:NH2	1:A:479:TYR:O	2.49	0.45
1:A:93:MET:O	1:A:97:MET:HG3	2.16	0.45
1:B:1071:CYS:HA	4:B:1242:SF4:S3	2.56	0.45
1:A:1080:MET:H	1:B:1215:ASN:ND2	2.14	0.45
1:B:286:VAL:HG12	1:B:290:LEU:HD22	1.97	0.45
1:B:280:CYS:HB3	1:B:301:LYS:HG2	1.99	0.45
1:B:390:PHE:CG	1:B:403:LEU:HD13	2.51	0.45
1:B:710:LYS:HD2	1:B:734:TYR:CE1	2.51	0.45
1:B:755:CYS:HA	1:B:756:PRO:HD3	1.64	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:1219:THR:HB	1:B:1222:GLN:OE1	2.16	0.45
1:B:198:LYS:O	1:B:202:GLU:HG3	2.17	0.45
1:B:469:ARG:NH2	1:B:479:TYR:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ILE:HG12	1:A:740:ILE:CD1	2.47	0.45
1:A:790:VAL:HG13	1:A:791:LEU:N	2.31	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:B:684:TRP:HZ2	1:B:689:CYS:SG	2.39	0.45
1:A:124:PHE:CB	1:A:367:SER:HB2	2.26	0.45
1:A:390:PHE:CG	1:A:403:LEU:HD13	2.51	0.45
1:A:87:SER:N	1:A:129:ASP:OD2	2.49	0.45
1:B:704:ILE:HG12	1:B:740:ILE:CD1	2.47	0.45
1:A:791:LEU:HD23	1:A:791:LEU:HA	1.84	0.45
1:B:14:THR:HG21	1:B:171:PHE:CE1	2.51	0.45
1:B:173:GLY:O	1:B:174:PHE:HB2	2.16	0.45
1:B:512:LEU:HG	1:B:514:SER:HB3	1.98	0.45
1:B:790:VAL:HG13	1:B:791:LEU:N	2.31	0.45
1:A:210:PRO:CB	1:B:831:ARG:HA	2.47	0.45
1:A:780:TYR:HA	1:A:783:ARG:HD2	1.99	0.45
1:B:44:ALA:CB	1:B:58:ILE:HD11	2.47	0.45
1:B:87:SER:N	1:B:129:ASP:OD2	2.49	0.45
1:B:887:ARG:NH2	1:B:954:LYS:N	2.65	0.45
1:A:78:GLY:HA2	1:A:207:SER:OG	2.17	0.45
1:A:349:VAL:HA	1:A:355:MET:HE1	1.98	0.45
1:A:593:LYS:HD3	1:A:594:LYS:H	1.82	0.45
1:A:755:CYS:SG	1:A:761:ALA:CB	3.02	0.45
1:B:1005:THR:HA	1:B:1006:PRO:HD3	1.71	0.45
1:B:707:VAL:O	1:B:736:PHE:HA	2.17	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:A:1108:GLN:HG2	1:A:1108:GLN:H	1.57	0.44
1:A:596:GLU:O	1:A:599:VAL:HB	2.18	0.44
1:A:670:SER:HA	1:A:673:GLU:OE1	2.18	0.44
1:A:636:ASN:ND2	1:A:672:PHE:CE2	2.85	0.44
1:B:636:ASN:ND2	1:B:672:PHE:CE2	2.85	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: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:A:561:MET:HE2	1:A:587:ILE:HD11	1.99	0.44
1:B:644:LYS:N	1:B:645:PRO:CD	2.79	0.44
1:B:82:THR:HG22	1:B:83:THR:N	2.26	0.44
1:A:368:LYS:NZ	1:B:227:GLN:NE2	2.65	0.44
1:A:887:ARG:NH2	1:A:954:LYS:N	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1129:MET:HE3	1:B:1149:ARG:CZ	2.48	0.44
1:B:124:PHE:HB3	1:B:367:SER:CB	2.28	0.44
1:B:325:THR:HG23	1:B:382:MET:CE	2.47	0.44
1:B:35:THR:O	1:B:38:GLU:N	2.51	0.44
1:B:64:GLU:OE2	5:B:1243:TPP:N1'	2.51	0.44
1:A:1219:THR:HG21	1:A:1221:GLU:HG2	2.00	0.44
1:A:263:TYR:OH	1:A:298:GLY:HA3	2.18	0.44
1:B:1082:LYS:HD3	1:B:1082:LYS:HA	1.84	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: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: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
1:B:263:TYR:OH	1:B:298:GLY:HA3	2.18	0.44
1:A:1005:THR:HA	1:A:1006:PRO:HD3	1.71	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:B:596:GLU:O	1:B:599:VAL:HB	2.18	0.44
1:B:805:LEU:HD22	1:B:829:GLY:HA3	2.00	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:B:679:ILE:HA	1:B:679:ILE:HD13	1.90	0.43
1:A:24:VAL:HG13	1:B:881:MET:HE1	2.00	0.43
1:A:64:GLU:OE2	5:A:1236:TPP:N1'	2.51	0.43
1:A:650:GLN:NE2	1:A:653:LYS:NZ	2.66	0.43
1:A:821:VAL:O	1:A:825:THR:HG23	2.18	0.43
1:B:1180:GLY:O	1:B:1181:LYS:HD2	2.19	0.43
1:B:78:GLY:HA2	1:B:207:SER:OG	2.17	0.43
1:B:490:HIS:N	1:B:490:HIS:CD2	2.86	0.43
1:B:650:GLN:NE2	1:B:653:LYS:NZ	2.66	0.43
1:B:670:SER:HA	1:B:673:GLU:OE1	2.18	0.43
1:B:996:ASN:HD21	6:B:1246:PYR:H31	1.84	0.43
1:A:290:LEU:O	1:A:293:LYS:HB2	2.19	0.43
1:A:35:THR:O	1:A:38:GLU:N	2.51	0.43
1:A:593:LYS:CG	1:A:594:LYS:H	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:LYS:CB	1:A:854:LYS:HZ3	2.30	0.43
1:B:290:LEU:O	1:B:293:LYS:HB2	2.19	0.43
1:A:1104:ARG:O	1:A:1107:ALA:HB3	2.18	0.43
1:A:1180:GLY:O	1:A:1181:LYS:HD2	2.19	0.43
1:B:561:MET:HE2	1:B:587:ILE:HD11	1.99	0.43
1:A:317:LEU:HD21	1:A:321:ALA:CB	2.49	0.43
1:B:1104:ARG:O	1:B:1107:ALA:HB3	2.18	0.43
1:B:591:TYR:HA	1:B:593:LYS:HG2	2.00	0.43
1:A:11:ASN:HD21	1:A:112:THR:HG21	1.84	0.43
1:A:1217:ALA:HB2	1:B:679:ILE:HB	2.01	0.43
1:A:687:GLU:H	1:A:687:GLU:HG3	1.65	0.43
1:A:996:ASN:HD21	6:A:1239:PYR:H31	1.84	0.43
1:A:831:ARG:HA	1:B:210:PRO:HB2	2.01	0.43
1:B:736:PHE:C	1:B:736:PHE:CD1	2.92	0.43
1:A:698:VAL:O	1:A:700:PRO:HD3	2.19	0.43
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:867:SER:HB2	1:A:875:TYR:CD2	2.53	0.43
1:B:226:PHE:CD1	1:B:226:PHE:O	2.72	0.43
1:B:509:THR:HA	1:B:540:LYS:HB2	2.01	0.43
1:B:593:LYS:HD2	1:B:598:ILE:HG13	2.01	0.43
1:B:642:VAL:C	1:B:645:PRO:HD2	2.39	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:B:698:VAL:O	1:B:700:PRO:HD3	2.19	0.43
1:A:370:PHE:CZ	1:A:375:VAL:HG22	2.54	0.42
1:A:422:PHE:CE1	1:A:468:LEU:HG	2.54	0.42
1:A:795:SER:O	1:A:796:LEU:C	2.58	0.42
1:B:212:HIS:O	1:B:212:HIS:CG	2.72	0.42
1:B:346:SER:O	1:B:350:GLU:HB3	2.19	0.42
1:B:370:PHE:CZ	1:B:375:VAL:HG22	2.54	0.42
1:A:1094:GLY:HA3	1:A:1120:PRO:HG3	2.00	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:B:154:LEU:HD13	1:B:250:VAL:CG2	2.49	0.42
1:B:266:ALA:HA	1:B:267:PRO:HD3	1.91	0.42
1:B:455:TYR:HB3	1:B:456:ASP:H	1.64	0.42
1:B:821:VAL:O	1:B:825:THR:HG23	2.18	0.42
1:A:1205:ARG:HA	1:A:1205:ARG:HD3	1.82	0.42
1:A:154:LEU:HD13	1:A:250:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:THR:HA	1:A:540:LYS:HB2	2.01	0.42
1:A:511:VAL:HA	1:A:542:TYR:O	2.19	0.42
1:A:956:SER:HG	1:A:958:TRP:HE1	1.67	0.42
1:B:390:PHE:HA	1:B:401:THR:O	2.19	0.42
1:B:593:LYS:CG	1:B:594:LYS:H	2.31	0.42
1:B:795:SER:O	1:B:796:LEU:C	2.58	0.42
1:B:897:ALA:HB3	1:B:910:LEU:HD21	2.01	0.42
1:A:266:ALA:HA	1:A:267:PRO:HD3	1.91	0.42
1:A:346:SER:O	1:A:350:GLU:HB3	2.19	0.42
1:A:490:HIS:CD2	1:A:490:HIS:N	2.86	0.42
1:A:854:LYS:C	1:A:854:LYS:HZ3	2.22	0.42
1:B:154:LEU:CD2	1:B:158:LEU:HD11	2.49	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:B:64:GLU:CG	1:B:89:GLY:HA2	2.48	0.42
1:A:1048:GLN:NE2	1:A:1048:GLN:C	2.73	0.42
1:A:307:PRO:HA	1:B:334:GLY:O	2.19	0.42
1:A:591:TYR:HA	1:A:593:LYS:HG2	2.00	0.42
1:A:779:GLU:C	1:A:783:ARG:HH11	2.23	0.42
1:A:897:ALA:HB3	1:A:910:LEU:HD21	2.01	0.42
1:B:536:ASN:ND2	1:B:623:LYS:HG2	2.34	0.42
1:B:599:VAL:O	1:B:602:ASN:HB2	2.20	0.42
1:A:317:LEU:C	1:A:317:LEU:HD22	2.39	0.42
1:A:390:PHE:HA	1:A:401:THR:O	2.19	0.42
1:A:803:GLU:O	1:A:805:LEU:HD13	2.18	0.42
1:B:1094:GLY:HA3	1:B:1120:PRO:HG3	2.00	0.42
1:B:736:PHE:CD2	1:B:801:PHE:HZ	2.37	0.42
1:A:1082:LYS:HA	1:A:1082:LYS:HD3	1.84	0.42
1:A:374:MET:O	1:A:377:SER:HB3	2.18	0.42
1:A:390:PHE:CD2	1:A:403:LEU:HD22	2.54	0.42
1:A:467:HIS:CE1	1:A:480:LEU:HD22	2.55	0.42
1:A:5:MET:HE1	1:A:184:GLU:HB2	2.02	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:325:THR:HG22	1:B:382:MET:SD	2.60	0.42
1:B:390:PHE:CD2	1:B:403:LEU:HD22	2.54	0.42
1:B:840:CYS:O	1:B:844:TRP:CD1	2.72	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:A:513:ASN:HA	1:A:544:ILE:O	2.20	0.42
1:A:736:PHE:CD2	1:A:801:PHE:HZ	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:LEU:HD23	1:A:941:LEU:HA	1.86	0.42
1:B:1149:ARG:HG3	1:B:1149:ARG:NH1	2.15	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:976:HIS:HE1	1:B:60:GLU:O	2.03	0.42
1:B:687:GLU:HG3	1:B:687:GLU:H	1.65	0.42
1:A:154:LEU:CD2	1:A:158:LEU:HD11	2.49	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:A:840:CYS:O	1:A:844:TRP:CD1	2.72	0.42
1:A:64:GLU:CG	1:A:89:GLY:HA2	2.48	0.42
1:B:1132:ASN:ND2	1:B:1139:ARG:HH12	2.11	0.42
1:B:317:LEU:HD21	1:B:321:ALA:HB3	2.02	0.42
1:B:780:TYR:CE2	1:B:784:ILE:HD11	2.55	0.42
1:A:465:ILE:HG13	1:A:467:HIS:HE1	1.84	0.42
1:B:1129:MET:CE	1:B:1149:ARG:NE	2.83	0.42
1:B:32:PRO:HB3	1:B:174:PHE:CE2	2.55	0.42
1:A:368:LYS:HZ3	1:B:227:GLN:HE22	1.66	0.42
1:A:881:MET:HE1	1:B:24:VAL:HG13	2.02	0.42
1:B:513:ASN:HA	1:B:544:ILE:O	2.20	0.42
1:B:536:ASN:HA	1:B:623:LYS:HZ3	1.85	0.42
1:B:779:GLU:C	1:B:783:ARG:HH11	2.23	0.42
1:A:32:PRO:HB3	1:A:174:PHE:CE2	2.55	0.41
1:A:780:TYR:CE2	1:A:784:ILE:HD11	2.55	0.41
1:A:965:TRP:CZ3	1:A:966:ALA:HB2	2.55	0.41
1:B:197:GLN:H	1:B:197:GLN:HG2	1.64	0.41
1:B:317:LEU:HD22	1:B:317:LEU:C	2.39	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:B:748:CYS:SG	1:B:750:ASN:HB2	2.60	0.41
1:B:837:ALA:HB2	1:B:872:ALA:CB	2.50	0.41
1:A:1129:MET:CE	1:A:1149:ARG:NE	2.83	0.41
1:A:1209:GLY:O	1:B:429:GLY:HA2	2.19	0.41
1:A:317:LEU:HD21	1:A:321:ALA:HB3	2.02	0.41
1:A:837:ALA:HB2	1:A:872:ALA:CB	2.50	0.41
1:B:1059:PHE:CD1	1:B:1104:ARG:HD3	2.55	0.41
1:B:227:GLN:NE2	1:B:227:GLN:H	2.18	0.41
1:A:1132:ASN:ND2	1:A:1139:ARG:HH12	2.11	0.41
1:A:748:CYS:SG	1:A:750:ASN:HB2	2.60	0.41
1:B:1149:ARG:NH1	1:B:1149:ARG:CG	2.80	0.41
1:B:371:SER:HB2	1:B:372:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1149:ARG:NH1	1:A:1149:ARG:HG3	2.15	0.41
1:A:238:LYS:O	1:A:242:ILE:HG13	2.20	0.41
1:A:184:GLU:CD	1:A:256:ARG:HH12	2.23	0.41
1:A:536:ASN:HA	1:A:623:LYS:HZ3	1.85	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:B:1001:SER:HB2	1:B:1011:ALA:HB3	2.01	0.41
1:B:491:ASN:HA	1:B:492:PRO:HD2	1.84	0.41
1:B:644:LYS:HB3	1:B:645:PRO:HD3	2.02	0.41
1:A:1200:THR:HA	1:A:1201:PRO:HD3	1.83	0.41
1:A:279:SER:HG	1:A:363:TYR:HH	1.64	0.41
1:A:536:ASN:ND2	1:A:623:LYS:HG2	2.34	0.41
1:A:593:LYS:HD2	1:A:598:ILE:HG13	2.01	0.41
1:A:371:SER:HB2	1:A:372:PRO:CD	2.50	0.41
1:A:599:VAL:O	1:A:602:ASN:HB2	2.20	0.41
1:A:1215:ASN:HD21	1:B:1080:MET:H	1.68	0.41
1:B:696:ALA:O	1:B:822:ARG:NH2	2.53	0.41
1:B:721:PHE:HD1	1:B:777:ASN:ND2	2.18	0.41
1:A:1001:SER:HB2	1:A:1011:ALA:HB3	2.01	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:A:349:VAL:HG12	1:B:349:VAL:HG12	2.03	0.41
1:A:833:PHE:HD2	1:B:208:MET:HE2	1.86	0.41
1:B:184:GLU:CD	1:B:256:ARG:HH12	2.23	0.41
1:B:700:PRO:HB3	1:B:819:PRO:HD3	2.02	0.41
1:A:1137:LEU:HD23	1:A:1137:LEU:HA	1.90	0.41
1:A:477:SER:HB3	1:A:479:TYR:CE1	2.55	0.41
1:A:593:LYS:CD	1:A:594:LYS:H	2.34	0.41
1:A:897:ALA:HA	1:A:941:LEU:HD13	2.03	0.41
1:B:1048:GLN:C	1:B:1048:GLN:NE2	2.73	0.41
5:B:1243:TPP:C2	5:B:1243:TPP:HN42	2.33	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
1:B:617:LYS:HD3	1:B:617:LYS:HA	1.71	0.41
1:B:718:PRO:HB2	1:B:777:ASN:HD21	1.86	0.41
1:A:234:PRO:CA	1:A:237:LEU:HD12	2.44	0.41
1:A:563:MET:HB3	1:A:563:MET:HE2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1243:TPP:N4'	5:B:1243:TPP:H2	2.36	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:1177:PRO:O	1:A:1178:ALA:HB2	2.21	0.41
1:A:605:ALA:O	1:A:609:ALA:HB2	2.21	0.41
1:A:741:ASN:CG	1:A:744:ASP:HB2	2.42	0.41
1:A:821:VAL:HG21	1:A:844:TRP:HH2	1.86	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:1177:PRO:O	1:B:1178:ALA:HB2	2.21	0.41
1:B:346:SER:O	1:B:350:GLU:CB	2.69	0.41
1:B:605:ALA:O	1:B:609:ALA:HB2	2.21	0.41
1:B:619:PRO:HB2	1:B:621:SER:HB3	2.03	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
5:A:1236:TPP:HN42	5:A:1236:TPP:C2	2.33	0.40
1:A:96:ASN:O	1:A:99:LYS:N	2.55	0.40
1:B:238:LYS:O	1:B:242:ILE:HG13	2.20	0.40
1:B:273:ILE:HD13	1:B:273:ILE:HG21	1.63	0.40
1:A:1214:GLN:CD	1:B:461:GLY:H	2.23	0.40
1:B:563:MET:HB3	1:B:563:MET:HE2	1.92	0.40
1:B:755:CYS:HA	4:B:1240:SF4:S1	2.61	0.40
1:B:893:LEU:HA	1:B:893:LEU:HD12	1.88	0.40
1:B:96:ASN:O	1:B:99:LYS:N	2.55	0.40
1:A:1146:LYS:HA	1:A:1149:ARG:NH1	2.37	0.40
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.82	0.40
1:A:619:PRO:HB2	1:A:621:SER:HB3	2.03	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:B:755:CYS:SG	1:B:761:ALA:CB	3.02	0.40
1:A:467:HIS:C	1:A:468:LEU:HD23	2.42	0.40
1:A:5:MET:CE	1:A:184:GLU:HB2	2.52	0.40
1:A:693:ASN:O	1:A:697:PHE:HB2	2.22	0.40
1:A:755:CYS:HA	4:A:1233:SF4:S1	2.61	0.40
1:B:388:ASN:OD1	1:B:389:HIS:N	2.54	0.40
1:B:467:HIS:C	1:B:468:LEU:HD23	2.42	0.40
1:A:1118:LYS:HE3	1:A:1118:LYS:HB2	1.94	0.40
1:A:718:PRO:HB2	1:A:777:ASN:HD21	1.86	0.40
1:A:856:ASN:HD21	1:A:860:GLN:HG3	1.87	0.40
1:A:1082:LYS:NZ	1:B:1219:THR:HG21	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:811:ALA:HB2	1:B:844:TRP:CB	2.52	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	Interatomic distance (Å)	Clash overlap (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 [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	1229/1231 (100%)	1101 (90%)	103 (8%)	25 (2%)	9	39
1	B	1229/1231 (100%)	1102 (90%)	102 (8%)	25 (2%)	9	39
All	All	2458/2462 (100%)	2203 (90%)	205 (8%)	50 (2%)	9	39

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

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Mol	Chain	Res	Type
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
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%)	4	18
1	B	978/978 (100%)	841 (86%)	137 (14%)	4	18
All	All	1956/1956 (100%)	1682 (86%)	274 (14%)	4	18

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 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 ⓘ

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	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	A	1234	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	A	1235	1	0,12,12	0.00	-	0,24,24	0.00	-
5	TPP	A	1236	2	21,27,27	1.36	4 (19%)	25,40,40	1.64	6 (24%)
6	PYR	A	1239	-	2,5,5	3.95	1 (50%)	2,6,6	0.73	0
4	SF4	B	1240	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	1241	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	1242	1	0,12,12	0.00	-	0,24,24	0.00	-
5	TPP	B	1243	2	21,27,27	1.36	4 (19%)	25,40,40	1.64	6 (24%)
6	PYR	B	1246	-	2,5,5	3.94	1 (50%)	2,6,6	0.72	0

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	0/6/5/5
4	SF4	A	1234	1	-	0/0/48/48	0/6/5/5
4	SF4	A	1235	1	-	0/0/48/48	0/6/5/5
5	TPP	A	1236	2	-	0/16/17/17	0/2/2/2
6	PYR	A	1239	-	-	0/0/4/4	0/0/0/0
4	SF4	B	1240	1	-	0/0/48/48	0/6/5/5
4	SF4	B	1241	1	-	0/0/48/48	0/6/5/5
4	SF4	B	1242	1	-	0/0/48/48	0/6/5/5
5	TPP	B	1243	2	-	0/16/17/17	0/2/2/2
6	PYR	B	1246	-	-	0/0/4/4	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1243	TPP	PB-O3B	-2.21	1.45	1.54
5	A	1236	TPP	PB-O3B	-2.20	1.45	1.54
5	B	1243	TPP	C7'-N3	2.66	1.53	1.48
5	A	1236	TPP	C7'-N3	2.66	1.53	1.48
5	B	1243	TPP	C2'-N1'	2.68	1.38	1.34
5	A	1236	TPP	C2'-N1'	2.71	1.38	1.34
5	A	1236	TPP	C4'-N3'	2.77	1.39	1.35
5	B	1243	TPP	C4'-N3'	2.80	1.39	1.35
6	B	1246	PYR	O3-C2	5.50	1.40	1.22
6	A	1239	PYR	O3-C2	5.51	1.41	1.22

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1236	TPP	N1'-C2'-N3'	-2.44	121.37	125.59
5	B	1243	TPP	N1'-C2'-N3'	-2.42	121.40	125.59
5	A	1236	TPP	C5'-C7'-N3	-2.02	109.95	113.33
5	B	1243	TPP	C5'-C7'-N3	-2.00	109.98	113.33
5	B	1243	TPP	PA-O7-C7	2.13	132.75	121.60
5	A	1236	TPP	PA-O7-C7	2.13	132.75	121.60
5	B	1243	TPP	C6-C5-C4	3.12	129.94	127.43
5	A	1236	TPP	C6-C5-C4	3.14	129.96	127.43
5	B	1243	TPP	CM2-C2'-N1'	3.55	121.07	117.06
5	A	1236	TPP	CM2-C2'-N1'	3.56	121.08	117.06
5	A	1236	TPP	O3B-PB-O2B	3.58	122.04	107.61
5	B	1243	TPP	O3B-PB-O2B	3.58	122.06	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1233	SF4	1	0
4	A	1234	SF4	2	0
4	A	1235	SF4	1	0
5	A	1236	TPP	7	0
6	A	1239	PYR	3	0
4	B	1240	SF4	1	0
4	B	1241	SF4	2	0
4	B	1242	SF4	1	0
5	B	1243	TPP	7	0
6	B	1246	PYR	3	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.