



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:58 PM GMT

PDB ID : 4B3N  
Title : Crystal structure of rhesus TRIM5alpha PRY/SPRY domain  
Authors : Yang, H.; Ji, X.; Zhao, Q.; Xiong, Y.  
Deposited on : 2012-07-25  
Resolution : 3.30 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

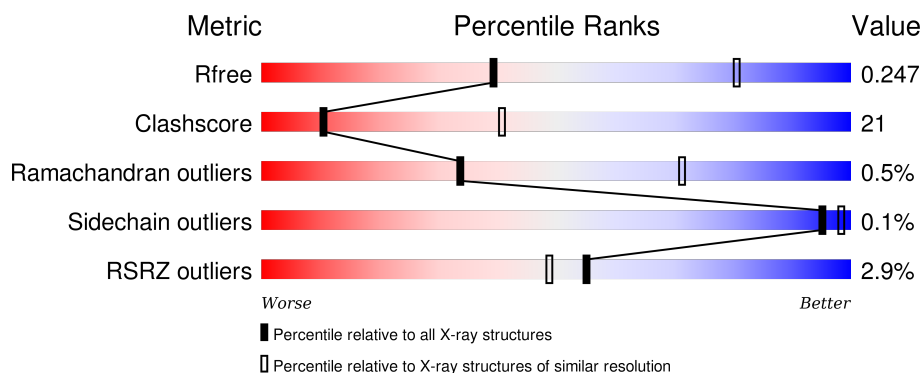
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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.

Mol	Chain	Length	Quality of chain
1	A	602	
1	B	602	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MES	A	600	-	-	X	X
3	MES	B	600	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8860 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 MALTOSE-BINDING PERIPLASMIC PROTEIN, TRIPARTITE MOTIF-CONTAINING PROTEIN 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4380	2822	721	821	16			
1	B	556	Total	C	N	O	S	0	0	0
			4366	2811	720	819	16			

There are 32 discrepancies between the modelled and reference sequences:

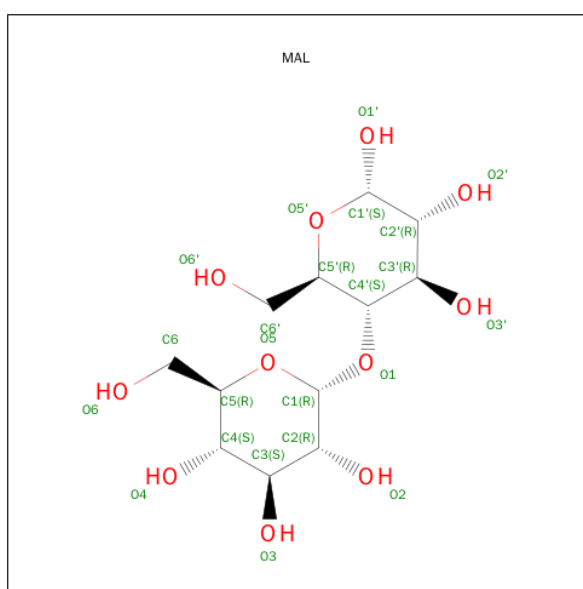
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP P0AEX9
A	-12	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	-11	THR	-	EXPRESSION TAG	UNP P0AEX9
A	-10	ILE	-	EXPRESSION TAG	UNP P0AEX9
A	-9	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-8	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-7	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-6	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-5	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-4	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-3	ASN	-	EXPRESSION TAG	UNP P0AEX9
A	-2	THR	-	EXPRESSION TAG	UNP P0AEX9
A	-1	SER	-	EXPRESSION TAG	UNP P0AEX9
A	0	MET	-	EXPRESSION TAG	UNP P0AEX9
A	1307	THR	PRO	CONFLICT	UNP Q0PF16
A	267	ASP	ASN	CONFLICT	UNP P0AEX9
B	-13	MET	-	EXPRESSION TAG	UNP P0AEX9
B	-12	ASN	-	EXPRESSION TAG	UNP P0AEX9
B	-11	THR	-	EXPRESSION TAG	UNP P0AEX9
B	-10	ILE	-	EXPRESSION TAG	UNP P0AEX9
B	-9	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-8	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-7	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-6	HIS	-	EXPRESSION TAG	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-4	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-3	ASN	-	EXPRESSION TAG	UNP P0AEX9
B	-2	THR	-	EXPRESSION TAG	UNP P0AEX9
B	-1	SER	-	EXPRESSION TAG	UNP P0AEX9
B	0	MET	-	EXPRESSION TAG	UNP P0AEX9
B	267	ASP	ASN	CONFLICT	UNP P0AEX9
B	1307	THR	PRO	CONFLICT	UNP Q0PF16

- Molecule 2 is SUGAR (MALTOSE) (three-letter code: MAL) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

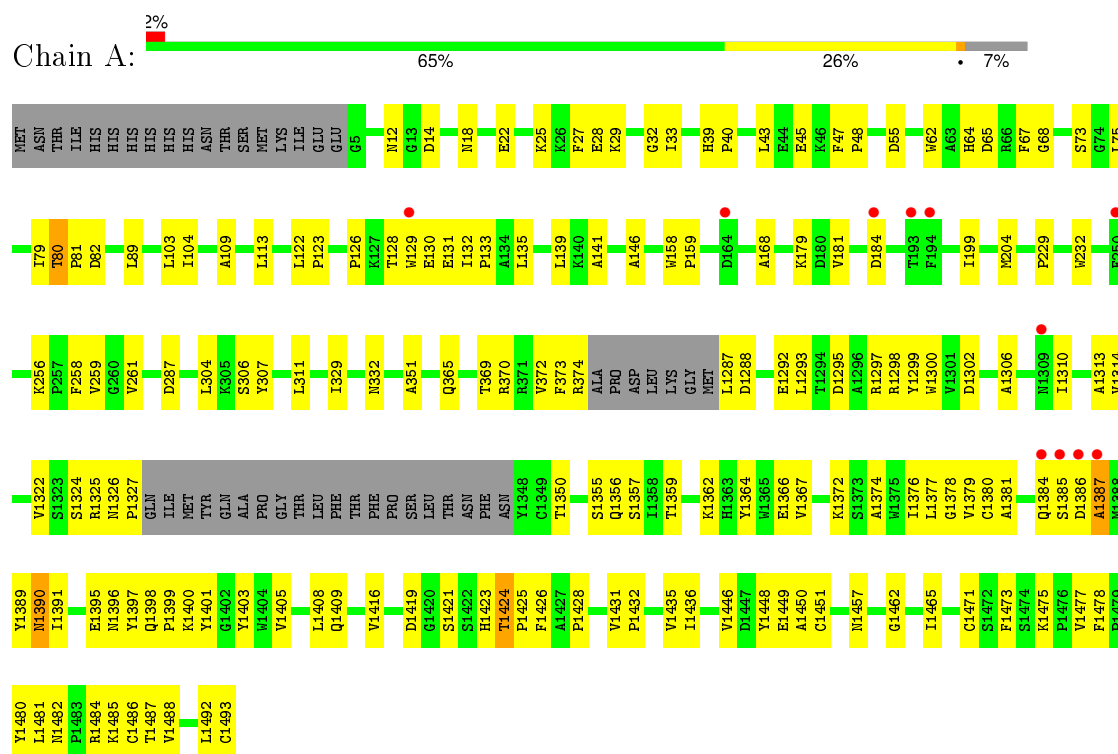
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	22	Total	O	0	0
			22	22		

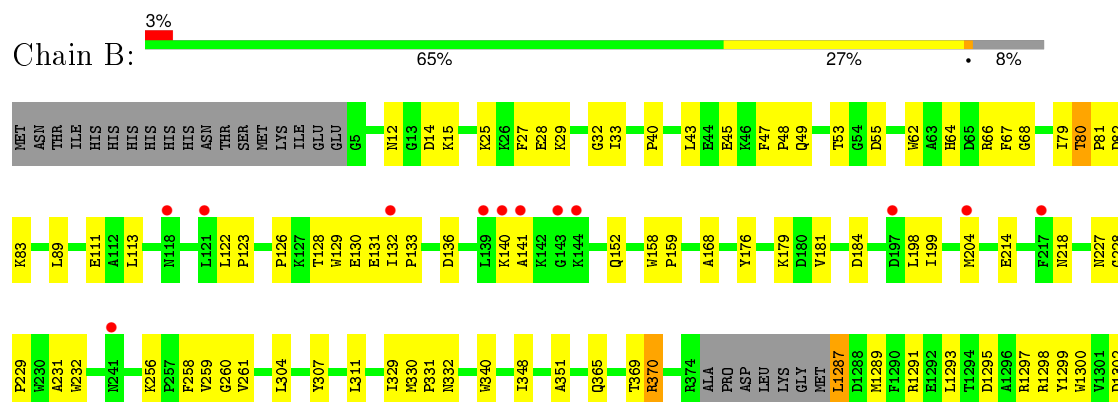
### 3 Residue-property plots

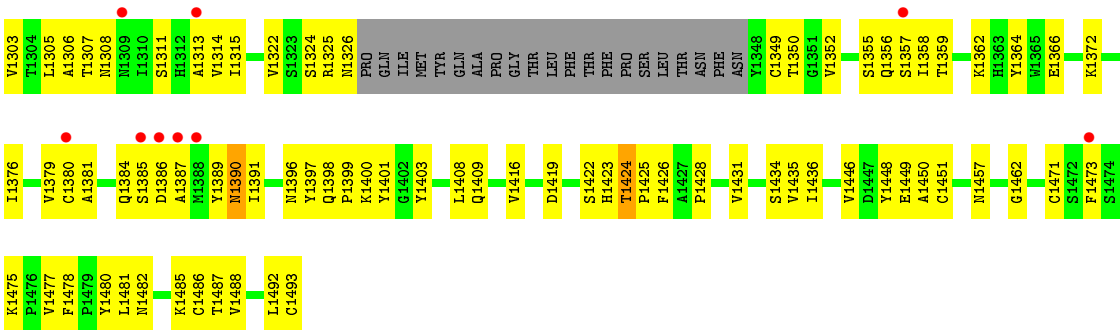
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, TRIPARTITE MOTIF-CONTAINING PROTEIN 5



#### • Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, TRIPARTITE MOTIF-CONTAINING PROTEIN 5







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.84 Å   98.73 Å   110.33 Å 90.00°   122.99°   90.00°	Depositor
Resolution (Å)	49.42 – 3.30 49.37 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (49.42-3.30) 96.0 (49.37-3.30)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 3.33 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.208 , 0.248 0.209 , 0.247	Depositor DCC
$R_{free}$ test set	1135 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.2	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 73.3	EDS
Estimated twinning fraction	0.022 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.025 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 22383 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.51	0/4493	0.71	1/6101 (0.0%)
1	B	0.52	0/4477	0.72	2/6078 (0.0%)
All	All	0.51	0/8970	0.71	3/12179 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1390	ASN	N-CA-C	6.40	128.29	111.00
1	B	1390	ASN	N-CA-C	5.90	126.92	111.00
1	B	370	ARG	NE-CZ-NH1	5.31	122.95	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1310	ILE	Peptide
1	A	1387	ALA	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4380	0	4305	188	1
1	B	4366	0	4292	186	1
2	A	23	0	22	0	0
2	B	23	0	22	2	0
3	A	12	0	13	10	0
3	B	12	0	13	15	0
4	A	22	0	0	1	0
4	B	22	0	0	1	0
All	All	8860	0	8667	374	1

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 21.

All (374) 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:1389:TYR:CE2	1:A:1390:ASN:ND2	1.77	1.51
1:B:1389:TYR:CE1	1:B:1390:ASN:ND2	1.88	1.41
1:B:1486:CYS:O	1:B:1487:THR:HG22	1.25	1.27
1:A:1423:HIS:C	1:A:1425:PRO:HD3	1.61	1.21
1:A:1423:HIS:O	1:A:1425:PRO:CD	1.94	1.15
1:A:1423:HIS:O	1:A:1425:PRO:HD3	1.48	1.13
1:A:1486:CYS:O	1:A:1487:THR:HG22	1.49	1.12
1:B:1389:TYR:CZ	1:B:1390:ASN:ND2	2.17	1.11
1:B:184:ASP:HB3	1:B:365:GLN:OE1	1.52	1.10
1:A:184:ASP:HB3	1:A:365:GLN:OE1	1.53	1.09
1:B:1350:THR:O	1:B:1482:ASN:ND2	1.86	1.08
1:A:1350:THR:O	1:A:1482:ASN:ND2	1.89	1.05
1:A:1287:LEU:HG	1:A:1288:ASP:OD1	1.58	1.03
1:B:1389:TYR:CE1	1:B:1390:ASN:CG	2.32	1.02
1:B:1486:CYS:O	1:B:1487:THR:CG2	2.08	1.01
1:A:1374:ALA:HB1	1:A:1484:ARG:CD	1.90	1.00
1:B:1295:ASP:O	1:B:1298:ARG:HG2	1.62	0.99
1:A:1374:ALA:CB	1:A:1484:ARG:HD2	1.91	0.99
1:A:27:PHE:HE2	1:A:33:ILE:HD11	1.27	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1389:TYR:CZ	1:A:1390:ASN:ND2	2.31	0.98
1:A:1380:CYS:HB2	1:A:1480:TYR:HB2	1.46	0.97
1:A:1389:TYR:CE2	1:A:1390:ASN:CG	2.38	0.97
1:A:1374:ALA:HB1	1:A:1484:ARG:HD2	0.99	0.97
1:B:1423:HIS:O	1:B:1425:PRO:HD2	1.66	0.96
1:A:126:PRO:CA	1:A:131:GLU:OE2	2.15	0.95
1:B:1303:VAL:HB	1:B:1492:LEU:HD21	1.50	0.93
1:A:126:PRO:HA	1:A:131:GLU:OE2	1.69	0.93
1:A:1423:HIS:O	1:A:1425:PRO:HD2	1.66	0.92
1:B:27:PHE:HE2	1:B:33:ILE:HD11	1.34	0.92
1:A:1389:TYR:HE2	1:A:1390:ASN:ND2	1.56	0.91
1:B:227:ASN:OD1	1:B:228:GLY:N	2.03	0.91
1:B:1380:CYS:HB2	1:B:1480:TYR:HB2	1.49	0.91
1:A:372:VAL:CG1	1:A:374:ARG:HG3	2.01	0.90
1:B:128:THR:OG1	1:B:130:GLU:OE1	1.89	0.89
1:B:1457:ASN:ND2	3:B:600:MES:O1	2.06	0.88
1:B:184:ASP:CB	1:B:365:GLN:OE1	2.22	0.87
1:A:126:PRO:HB3	1:A:131:GLU:OE2	1.73	0.87
1:B:89:LEU:HD23	1:B:304:LEU:HA	1.54	0.87
1:B:1423:HIS:C	1:B:1425:PRO:CD	2.43	0.87
1:B:1457:ASN:HD22	3:B:600:MES:C2	1.87	0.86
1:A:89:LEU:HD23	1:A:304:LEU:HA	1.54	0.86
1:A:184:ASP:CB	1:A:365:GLN:OE1	2.23	0.86
1:A:126:PRO:CB	1:A:131:GLU:OE2	2.25	0.85
1:A:1287:LEU:HG	1:A:1288:ASP:H	1.42	0.84
1:A:1380:CYS:CB	1:A:1480:TYR:HB2	2.06	0.83
1:B:1380:CYS:CB	1:B:1480:TYR:HB2	2.07	0.83
1:A:1436:ILE:HD12	3:A:600:MES:H72	1.60	0.83
1:A:1457:ASN:HB2	3:A:600:MES:H21	1.59	0.82
1:A:372:VAL:HG12	1:A:374:ARG:H	1.43	0.82
1:B:1380:CYS:SG	1:B:1403:TYR:CE1	2.73	0.82
1:B:129:TRP:O	1:B:132:ILE:HG13	1.80	0.82
1:B:1396:ASN:OD1	1:B:1396:ASN:O	1.98	0.81
1:B:128:THR:HG22	1:B:131:GLU:HG3	1.61	0.81
1:B:214:GLU:O	1:B:218:ASN:OD1	1.99	0.81
1:A:1396:ASN:O	1:A:1396:ASN:OD1	1.98	0.80
1:A:55:ASP:OD1	1:A:55:ASP:O	1.99	0.80
1:B:1303:VAL:HB	1:B:1492:LEU:CD2	2.10	0.80
1:B:1424:THR:N	1:B:1425:PRO:CD	2.45	0.80
1:A:1380:CYS:SG	1:A:1403:TYR:CE1	2.76	0.79
1:A:372:VAL:HG12	1:A:374:ARG:HG3	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1307:THR:HG22	1:B:1315:ILE:HD12	1.64	0.79
1:A:1486:CYS:O	1:A:1487:THR:CG2	2.30	0.78
1:B:1311:SER:O	1:B:1350:THR:HA	1.82	0.78
1:B:1303:VAL:O	1:B:1492:LEU:HD23	1.83	0.78
1:B:1423:HIS:C	1:B:1425:PRO:HD3	2.04	0.78
1:B:1389:TYR:HE1	1:B:1390:ASN:ND2	1.80	0.77
1:A:259:VAL:O	1:A:329:ILE:HD12	1.85	0.76
1:A:1306:ALA:HB2	1:A:1355:SER:HA	1.68	0.75
1:A:1423:HIS:CD2	1:A:1424:THR:HG23	2.22	0.75
1:B:1306:ALA:HB2	1:B:1355:SER:HA	1.67	0.75
1:B:1435:VAL:HB	3:B:600:MES:H61	1.68	0.75
1:B:1423:HIS:C	1:B:1425:PRO:HD2	2.03	0.75
1:A:122:LEU:HD12	1:A:123:PRO:HD2	1.70	0.73
1:A:1457:ASN:HB2	3:A:600:MES:C2	2.18	0.73
1:B:259:VAL:O	1:B:329:ILE:HD12	1.88	0.73
1:A:1389:TYR:HE2	1:A:1390:ASN:HD21	1.14	0.72
1:B:1400:LYS:HE3	1:B:1419:ASP:HB2	1.72	0.72
1:A:1400:LYS:HE3	1:A:1419:ASP:HB2	1.72	0.72
1:B:1313:ALA:HB2	1:B:1350:THR:HB	1.71	0.71
1:A:1396:ASN:ND2	1:A:1426:PHE:O	2.23	0.71
1:B:62:TRP:CD1	1:B:66:ARG:HG3	2.26	0.71
1:B:122:LEU:HD12	1:B:123:PRO:HD2	1.71	0.71
1:A:1295:ASP:OD1	1:A:1298:ARG:NH1	2.25	0.70
1:A:1372:LYS:HZ1	1:A:1486:CYS:HB3	1.57	0.69
1:A:1313:ALA:HB2	1:A:1350:THR:HB	1.73	0.69
1:B:27:PHE:CE2	1:B:33:ILE:HD11	2.25	0.69
1:B:227:ASN:ND2	1:B:231:ALA:HB2	2.08	0.69
1:A:372:VAL:HG11	1:A:374:ARG:HG3	1.74	0.68
1:A:1326:ASN:N	1:A:1327:PRO:HD2	2.08	0.68
1:A:18:ASN:O	1:A:22:GLU:HG2	1.93	0.68
1:A:1423:HIS:C	1:A:1425:PRO:CD	2.46	0.67
1:B:1396:ASN:ND2	1:B:1426:PHE:O	2.25	0.67
1:A:370:ARG:NH2	1:A:1357:SER:O	2.27	0.67
1:B:1385:SER:O	1:B:1386:ASP:CG	2.33	0.67
1:A:1385:SER:O	1:A:1386:ASP:CG	2.34	0.66
1:B:49:GLN:O	1:B:53:THR:HG23	1.93	0.66
1:A:65:ASP:HA	1:A:332:ASN:HA	1.76	0.66
1:A:373:PHE:O	1:A:374:ARG:C	2.33	0.66
1:B:370:ARG:NH2	1:B:1357:SER:O	2.28	0.66
1:B:1435:VAL:CB	3:B:600:MES:H61	2.26	0.65
1:B:1287:LEU:HD23	1:B:1289:MET:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1372:LYS:NZ	1:A:1486:CYS:HB3	2.11	0.65
1:B:1435:VAL:HA	3:B:600:MES:C6	2.26	0.65
1:B:1307:THR:O	1:B:1308:ASN:ND2	2.30	0.65
1:B:1424:THR:N	1:B:1425:PRO:HD3	2.11	0.64
1:B:1303:VAL:CB	1:B:1492:LEU:HD21	2.24	0.64
1:A:1386:ASP:OD1	1:A:1386:ASP:C	2.35	0.64
1:A:27:PHE:CE2	1:A:33:ILE:HD11	2.20	0.64
1:A:1435:VAL:HA	3:A:600:MES:H32	1.80	0.64
1:A:1465:ILE:HG12	3:A:600:MES:H22	1.79	0.63
1:B:1380:CYS:HB2	1:B:1480:TYR:CB	2.27	0.63
1:B:1457:ASN:ND2	3:B:600:MES:C2	2.59	0.63
1:A:79:ILE:HD11	1:A:103:LEU:HB3	1.81	0.63
1:B:1435:VAL:HB	3:B:600:MES:C6	2.29	0.62
1:A:1380:CYS:HB2	1:A:1480:TYR:CB	2.26	0.62
1:B:1386:ASP:C	1:B:1386:ASP:OD1	2.35	0.62
1:A:1391:ILE:O	1:A:1391:ILE:HG22	1.99	0.61
1:B:130:GLU:O	1:B:133:PRO:HG2	2.00	0.61
1:B:258:PHE:CD1	1:B:330:MET:HG2	2.35	0.61
1:B:1391:ILE:O	1:B:1391:ILE:HG22	1.99	0.61
1:B:1384:GLN:O	1:B:1387:ALA:HB3	2.01	0.61
1:B:1424:THR:HG23	1:B:1424:THR:O	1.99	0.60
1:A:1457:ASN:CB	3:A:600:MES:H21	2.31	0.60
1:A:1436:ILE:CD1	3:A:600:MES:H72	2.30	0.60
1:A:1389:TYR:CD2	1:A:1390:ASN:CG	2.75	0.60
1:A:1324:SER:CB	1:A:1485:LYS:HA	2.32	0.59
1:A:1376:ILE:CG1	1:A:1484:ARG:NH2	2.65	0.59
1:A:40:PRO:HG2	1:A:43:LEU:HB3	1.84	0.59
1:B:369:THR:HG22	1:B:370:ARG:HG3	1.85	0.59
1:A:372:VAL:CG1	1:A:374:ARG:CG	2.79	0.59
1:B:1485:LYS:HG2	1:B:1485:LYS:O	2.02	0.59
1:B:128:THR:HG23	1:B:131:GLU:H	1.68	0.59
1:A:1384:GLN:O	1:A:1387:ALA:HB3	2.03	0.59
1:B:89:LEU:CD2	1:B:304:LEU:HA	2.30	0.58
1:A:1408:LEU:HD12	1:A:1409:GLN:H	1.68	0.58
1:A:369:THR:HG22	1:A:370:ARG:HG3	1.85	0.58
1:B:1389:TYR:CE1	1:B:1390:ASN:OD1	2.57	0.58
1:A:1376:ILE:HD13	1:A:1397:TYR:CE2	2.39	0.58
1:A:1398:GLN:NE2	1:A:1428:PRO:HA	2.19	0.58
1:A:1416:VAL:CG1	1:A:1431:VAL:HB	2.33	0.58
1:B:1416:VAL:CG1	1:B:1431:VAL:HB	2.33	0.58
1:B:1389:TYR:HE1	1:B:1390:ASN:CG	1.98	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1305:LEU:HD22	1:B:1352:VAL:CG2	2.32	0.58
1:A:25:LYS:O	1:A:29:LYS:HG2	2.04	0.58
1:A:1325:ARG:HB3	1:A:1327:PRO:HD2	1.86	0.58
1:B:1398:GLN:NE2	1:B:1428:PRO:HA	2.18	0.57
1:B:1486:CYS:O	1:B:1487:THR:CB	2.52	0.57
1:A:1484:ARG:O	1:A:1484:ARG:HG2	2.04	0.57
1:B:1372:LYS:HZ1	1:B:1486:CYS:HB3	1.69	0.57
1:A:73:SER:HB2	1:A:75:LEU:HD23	1.86	0.57
1:B:12:ASN:OD1	1:B:14:ASP:N	2.38	0.57
1:A:1381:ALA:HA	1:A:1477:VAL:HA	1.87	0.57
1:A:1287:LEU:CG	1:A:1288:ASP:OD1	2.45	0.57
1:A:1287:LEU:HG	1:A:1288:ASP:N	2.18	0.57
1:B:82:ASP:OD1	1:B:83:LYS:N	2.38	0.57
1:A:89:LEU:CD2	1:A:304:LEU:HA	2.31	0.56
1:B:1293:LEU:HD13	1:B:1293:LEU:C	2.25	0.56
1:B:1435:VAL:HA	3:B:600:MES:H51	1.87	0.56
1:A:1457:ASN:CB	3:A:600:MES:C2	2.82	0.56
1:A:1293:LEU:C	1:A:1293:LEU:HD13	2.26	0.56
1:B:27:PHE:HE2	1:B:33:ILE:CD1	2.12	0.56
1:A:1359:THR:O	1:A:1448:TYR:CE2	2.59	0.56
1:B:1436:ILE:HD12	3:B:600:MES:H82	1.86	0.56
1:B:128:THR:CG2	1:B:131:GLU:HG3	2.33	0.56
1:A:158:TRP:NE1	1:A:258:PHE:CE2	2.74	0.55
1:B:25:LYS:O	1:B:29:LYS:HG2	2.07	0.55
1:B:1436:ILE:CD1	3:B:600:MES:H82	2.35	0.55
1:B:1389:TYR:HE1	1:B:1390:ASN:OD1	1.89	0.55
1:B:1372:LYS:NZ	1:B:1486:CYS:HB3	2.21	0.55
1:B:1384:GLN:O	1:B:1387:ALA:CB	2.55	0.55
1:A:1367:VAL:HG21	1:A:1377:LEU:HD11	1.89	0.55
1:A:1384:GLN:O	1:A:1387:ALA:CB	2.55	0.55
1:B:1389:TYR:CD1	1:B:1390:ASN:CG	2.79	0.54
1:A:1326:ASN:O	1:A:1327:PRO:C	2.46	0.54
1:A:12:ASN:OD1	1:A:14:ASP:N	2.39	0.54
1:A:181:VAL:O	1:A:365:GLN:NE2	2.41	0.54
1:A:372:VAL:HG12	1:A:374:ARG:CG	2.36	0.54
1:A:372:VAL:HG11	1:A:374:ARG:CG	2.37	0.54
1:B:152:GLN:HA	1:B:348:ILE:HD11	1.89	0.54
1:B:1297:ARG:HG2	1:B:1364:TYR:CE2	2.42	0.54
1:A:1288:ASP:OD1	1:A:1288:ASP:N	2.41	0.54
1:A:1465:ILE:HG12	3:A:600:MES:C2	2.38	0.54
1:B:1376:ILE:HB	1:B:1482:ASN:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1480:TYR:O	1:A:1481:LEU:HD12	2.08	0.53
1:A:1391:ILE:CG2	1:A:1391:ILE:O	2.56	0.53
1:B:80:THR:N	1:B:81:PRO:CD	2.71	0.53
1:A:199:ILE:HA	1:A:204:MET:O	2.08	0.53
1:A:1399:PRO:HD2	1:A:1419:ASP:HB3	1.91	0.53
1:A:1325:ARG:C	1:A:1327:PRO:HD2	2.29	0.53
1:A:80:THR:N	1:A:81:PRO:CD	2.72	0.53
1:A:62:TRP:HB3	1:A:67:PHE:HE1	1.74	0.53
1:A:1299:TYR:CE1	1:A:1362:LYS:HD2	2.44	0.53
1:A:1297:ARG:HG2	1:A:1364:TYR:CE2	2.44	0.53
1:A:1436:ILE:H	3:A:600:MES:H52	1.73	0.53
1:B:1359:THR:O	1:B:1448:TYR:CE2	2.62	0.53
1:B:198:LEU:HD13	1:B:204:MET:HE3	1.91	0.53
1:B:1408:LEU:HD12	1:B:1409:GLN:H	1.74	0.52
1:B:1325:ARG:O	1:B:1326:ASN:CB	2.56	0.52
1:A:1389:TYR:HE2	1:A:1390:ASN:CG	1.98	0.52
1:B:1423:HIS:O	1:B:1425:PRO:CD	2.46	0.52
1:B:1391:ILE:CG2	1:B:1391:ILE:O	2.56	0.52
1:A:179:LYS:HD2	1:A:1356:GLN:NE2	2.25	0.52
1:A:158:TRP:CD1	1:A:258:PHE:CD2	2.97	0.52
1:B:1299:TYR:CE1	1:B:1362:LYS:HD2	2.44	0.52
1:B:130:GLU:C	1:B:133:PRO:HD2	2.30	0.52
1:B:1324:SER:CB	1:B:1485:LYS:HA	2.40	0.52
1:A:1408:LEU:HD12	1:A:1409:GLN:N	2.25	0.52
1:B:198:LEU:HD13	1:B:204:MET:CE	2.40	0.52
1:A:132:ILE:N	1:A:133:PRO:HD2	2.24	0.52
1:A:1372:LYS:NZ	1:A:1488:VAL:O	2.42	0.52
1:B:340:TRP:CD1	2:B:500:MAL:H4	2.44	0.51
1:B:40:PRO:HG2	1:B:43:LEU:HB3	1.92	0.51
1:A:1379:VAL:HG21	1:A:1446:VAL:HG22	1.91	0.51
1:B:181:VAL:O	1:B:365:GLN:NE2	2.44	0.51
1:B:1398:GLN:HB3	1:B:1419:ASP:CB	2.41	0.51
1:B:1399:PRO:HD2	1:B:1419:ASP:HB3	1.92	0.51
1:B:1480:TYR:O	1:B:1481:LEU:HD12	2.10	0.51
1:A:1398:GLN:HB3	1:A:1419:ASP:CB	2.40	0.51
1:B:1379:VAL:HG21	1:B:1446:VAL:HG22	1.92	0.51
1:B:1449:GLU:OE1	1:B:1449:GLU:N	2.44	0.51
1:A:1366:GLU:O	1:A:1493:CYS:N	2.40	0.51
1:A:128:THR:OG1	1:A:130:GLU:OE1	2.25	0.51
1:A:1475:LYS:O	1:A:1477:VAL:HG13	2.10	0.51
1:A:159:PRO:HA	1:A:256:LYS:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1359:THR:O	1:A:1448:TYR:CD2	2.64	0.50
1:A:1378:GLY:HA3	1:A:1405:VAL:HA	1.92	0.50
1:A:1449:GLU:OE1	1:A:1449:GLU:N	2.43	0.50
1:A:1380:CYS:O	1:A:1478:PHE:O	2.29	0.50
1:B:1293:LEU:HG	1:B:1462:GLY:HA3	1.93	0.50
1:B:159:PRO:HA	1:B:256:LYS:O	2.11	0.50
1:B:1366:GLU:O	1:B:1493:CYS:N	2.35	0.50
1:B:1297:ARG:O	1:B:1300:TRP:HB2	2.12	0.50
1:A:1421:SER:HG	1:A:1424:THR:HG1	1.60	0.50
1:B:55:ASP:OD1	1:B:55:ASP:O	2.29	0.50
1:B:1303:VAL:O	1:B:1492:LEU:CD2	2.56	0.50
1:B:1435:VAL:HA	3:B:600:MES:C5	2.41	0.49
1:B:79:ILE:C	1:B:81:PRO:CD	2.81	0.49
1:A:199:ILE:HD13	1:A:351:ALA:HB1	1.94	0.49
1:B:1475:LYS:O	1:B:1477:VAL:HG13	2.11	0.49
1:B:62:TRP:HB3	1:B:67:PHE:HE1	1.77	0.49
1:B:199:ILE:HD13	1:B:351:ALA:HB1	1.94	0.49
1:A:1376:ILE:HB	1:A:1482:ASN:HB3	1.93	0.49
1:A:373:PHE:O	1:A:374:ARG:O	2.30	0.49
1:B:1358:ILE:HB	1:B:1477:VAL:HG23	1.94	0.49
1:A:129:TRP:HA	1:A:132:ILE:HD12	1.94	0.49
1:B:1303:VAL:CG1	1:B:1492:LEU:HD21	2.43	0.49
1:B:259:VAL:HB	1:B:329:ILE:HA	1.94	0.49
1:A:1385:SER:O	1:A:1386:ASP:CB	2.61	0.49
1:B:79:ILE:C	1:B:81:PRO:HD3	2.33	0.49
1:B:1451:CYS:HA	1:B:1473:PHE:CE2	2.48	0.49
1:A:1486:CYS:O	1:A:1487:THR:CB	2.61	0.49
1:A:1297:ARG:O	1:A:1300:TRP:HB2	2.13	0.48
1:A:135:LEU:O	1:A:139:LEU:HG	2.12	0.48
1:A:1376:ILE:HG13	1:A:1484:ARG:NH2	2.27	0.48
1:B:1422:SER:O	1:B:1425:PRO:HD3	2.12	0.48
1:B:132:ILE:N	1:B:133:PRO:HD2	2.29	0.48
1:A:1385:SER:O	1:A:1386:ASP:OD1	2.31	0.48
1:B:130:GLU:O	1:B:133:PRO:CG	2.61	0.48
1:A:1451:CYS:HA	1:A:1473:PHE:CE2	2.49	0.48
1:A:1376:ILE:HG12	1:A:1484:ARG:NH2	2.29	0.48
1:A:128:THR:HG23	1:A:131:GLU:H	1.79	0.48
1:B:122:LEU:HD21	1:B:126:PRO:HD3	1.95	0.48
1:A:259:VAL:HB	1:A:329:ILE:HA	1.95	0.48
1:B:176:TYR:N	4:B:2006:HOH:O	2.34	0.48
1:B:1372:LYS:HG2	1:B:1488:VAL:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ALA:O	1:A:181:VAL:HA	2.14	0.48
1:B:1287:LEU:CD2	1:B:1289:MET:O	2.62	0.48
1:A:1287:LEU:CG	1:A:1288:ASP:H	2.13	0.48
1:A:64:HIS:CE1	1:A:329:ILE:HD11	2.49	0.48
1:A:1293:LEU:HG	1:A:1462:GLY:HA3	1.95	0.48
1:B:168:ALA:O	1:B:181:VAL:HA	2.14	0.47
1:B:1385:SER:O	1:B:1386:ASP:CB	2.61	0.47
1:A:79:ILE:C	1:A:81:PRO:HD3	2.34	0.47
1:B:1385:SER:O	1:B:1386:ASP:OD1	2.32	0.47
1:B:1307:THR:CG2	1:B:1315:ILE:HD12	2.40	0.47
1:A:79:ILE:C	1:A:81:PRO:CD	2.83	0.47
1:B:1408:LEU:HD12	1:B:1409:GLN:N	2.29	0.47
1:B:28:GLU:O	1:B:32:GLY:N	2.42	0.47
1:B:45:GLU:O	1:B:48:PRO:HD2	2.15	0.47
1:A:1478:PHE:N	1:A:1478:PHE:CD1	2.82	0.46
1:A:1398:GLN:HB3	1:A:1419:ASP:HB3	1.96	0.46
1:A:89:LEU:HD23	1:A:304:LEU:CA	2.37	0.46
1:B:1359:THR:O	1:B:1448:TYR:CD2	2.68	0.46
1:A:1314:VAL:O	1:A:1322:VAL:HG23	2.15	0.46
1:A:1376:ILE:CG1	1:A:1484:ARG:HH21	2.29	0.46
1:A:1292:GLU:O	1:A:1295:ASP:HB3	2.16	0.46
1:B:1311:SER:O	1:B:1349:CYS:O	2.34	0.46
1:A:122:LEU:HD21	1:A:126:PRO:HD3	1.97	0.46
1:B:49:GLN:O	1:B:53:THR:CG2	2.63	0.46
1:B:1434:SER:O	3:B:600:MES:H51	2.16	0.46
1:B:132:ILE:HD12	1:B:133:PRO:N	2.31	0.45
1:B:179:LYS:HD2	1:B:1356:GLN:NE2	2.31	0.45
1:A:65:ASP:OD1	1:A:65:ASP:N	2.47	0.45
1:A:158:TRP:N	1:A:159:PRO:CD	2.80	0.45
1:A:1450:ALA:O	1:A:1451:CYS:HB2	2.17	0.45
1:B:1401:TYR:OH	1:B:1425:PRO:HB2	2.16	0.45
1:A:1367:VAL:HG21	1:A:1377:LEU:CD1	2.46	0.45
1:A:1397:TYR:HD1	1:A:1403:TYR:CG	2.34	0.45
1:B:1380:CYS:O	1:B:1478:PHE:O	2.34	0.45
1:B:111:GLU:HG2	1:B:260:GLY:O	2.17	0.45
1:A:1287:LEU:CG	1:A:1288:ASP:N	2.79	0.44
1:B:89:LEU:CD2	1:B:304:LEU:CA	2.95	0.44
1:A:18:ASN:HB2	4:A:2001:HOH:O	2.16	0.44
1:B:1314:VAL:O	1:B:1322:VAL:HG23	2.17	0.44
1:B:1380:CYS:HB3	1:B:1480:TYR:HB2	1.98	0.44
1:A:1416:VAL:HG12	1:A:1431:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:TYR:CE2	1:A:311:LEU:HD11	2.52	0.44
1:B:1299:TYR:O	1:B:1364:TYR:HB3	2.18	0.44
1:B:1398:GLN:HB3	1:B:1419:ASP:HB3	1.98	0.44
1:A:80:THR:N	1:A:81:PRO:HD3	2.33	0.44
1:A:1299:TYR:CZ	1:A:1362:LYS:HD2	2.52	0.44
1:A:139:LEU:HD12	1:A:146:ALA:HA	2.00	0.44
1:A:1400:LYS:HG3	1:A:1401:TYR:N	2.31	0.44
1:B:1357:SER:CB	1:B:1478:PHE:CE2	3.01	0.44
1:B:1435:VAL:HA	3:B:600:MES:H62	1.98	0.44
1:A:1424:THR:N	1:A:1425:PRO:HD3	2.17	0.44
1:B:1416:VAL:HG12	1:B:1431:VAL:HB	1.98	0.44
1:A:45:GLU:O	1:A:48:PRO:HD2	2.17	0.44
1:A:1295:ASP:O	1:A:1298:ARG:HB3	2.17	0.43
1:B:1299:TYR:CZ	1:B:1362:LYS:HD2	2.53	0.43
1:B:80:THR:N	1:B:81:PRO:HD3	2.34	0.43
1:B:1451:CYS:HB3	1:B:1471:CYS:O	2.18	0.43
1:A:68:GLY:HA3	1:A:332:ASN:O	2.18	0.43
1:B:1325:ARG:HG2	1:B:1326:ASN:H	1.84	0.43
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.54	0.43
1:B:1307:THR:C	1:B:1308:ASN:HD22	2.22	0.43
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.54	0.43
1:B:1450:ALA:O	1:B:1451:CYS:HB2	2.19	0.43
1:B:1397:TYR:HD1	1:B:1403:TYR:CG	2.36	0.43
1:B:1287:LEU:N	1:B:1287:LEU:CD1	2.82	0.43
1:B:47:PHE:N	1:B:48:PRO:CD	2.81	0.43
1:A:89:LEU:CD2	1:A:304:LEU:CA	2.96	0.42
1:A:109:ALA:O	1:A:261:VAL:HA	2.18	0.42
1:B:258:PHE:CE1	1:B:331:PRO:HD3	2.54	0.42
1:B:1381:ALA:HA	1:B:1477:VAL:HA	2.01	0.42
1:A:47:PHE:N	1:A:48:PRO:CD	2.82	0.42
1:B:136:ASP:O	1:B:140:LYS:HG2	2.19	0.42
1:A:1302:ASP:C	1:A:1302:ASP:OD1	2.57	0.42
1:A:1357:SER:CB	1:A:1478:PHE:CE2	3.02	0.42
1:B:130:GLU:O	1:B:133:PRO:HD2	2.18	0.42
1:A:1380:CYS:HB3	1:A:1480:TYR:HB2	1.97	0.42
1:B:1435:VAL:CA	3:B:600:MES:C6	2.97	0.42
1:A:1386:ASP:OD1	1:A:1387:ALA:N	2.53	0.42
1:B:68:GLY:HA3	1:B:332:ASN:O	2.19	0.42
1:B:158:TRP:N	1:B:159:PRO:CD	2.83	0.42
1:B:1302:ASP:OD1	1:B:1302:ASP:C	2.58	0.42
1:B:132:ILE:C	1:B:132:ILE:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASP:HB2	1:B:365:GLN:OE1	2.15	0.42
1:B:1386:ASP:OD1	1:B:1387:ALA:N	2.53	0.42
1:B:1435:VAL:CB	3:B:600:MES:C6	2.92	0.41
1:A:39:HIS:ND1	1:A:39:HIS:O	2.53	0.41
1:B:1400:LYS:HG3	1:B:1401:TYR:N	2.35	0.41
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.93	0.41
1:A:1325:ARG:CB	1:A:1327:PRO:HD2	2.49	0.41
1:A:287:ASP:OD1	1:A:306:SER:HB2	2.20	0.41
1:A:22:GLU:H	1:A:22:GLU:HG2	1.70	0.41
1:A:1431:VAL:HA	1:A:1432:PRO:HD2	1.86	0.41
1:B:1448:TYR:CE1	1:B:1473:PHE:HB3	2.55	0.41
1:A:1451:CYS:HB3	1:A:1471:CYS:O	2.21	0.41
1:B:1478:PHE:CD1	1:B:1478:PHE:N	2.89	0.41
1:B:126:PRO:HG2	1:B:132:ILE:HG22	2.02	0.41
1:B:64:HIS:CE1	1:B:329:ILE:HD11	2.56	0.41
1:A:1481:LEU:HD22	1:A:1492:LEU:HD11	2.01	0.41
1:A:1395:GLU:OE2	1:A:1484:ARG:NH1	2.54	0.41
1:A:261:VAL:HG23	1:A:329:ILE:HD11	2.03	0.41
1:B:15:LYS:NZ	2:B:500:MAL:O1'	2.54	0.41
1:A:67:PHE:HB3	1:A:104:ILE:HD12	2.02	0.40
1:B:307:TYR:CE2	1:B:311:LEU:HD11	2.56	0.40
1:A:1324:SER:HB2	1:A:1485:LYS:HA	2.03	0.40
1:B:1357:SER:HB2	1:B:1478:PHE:CE2	2.56	0.40
1:B:261:VAL:HG23	1:B:329:ILE:HD11	2.03	0.40
1:A:82:ASP:OD1	1:A:82:ASP:O	2.40	0.40
1:B:113:LEU:HA	1:B:113:LEU:HD23	1.94	0.40
1:A:28:GLU:O	1:A:32:GLY:N	2.49	0.40

All (1) 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:55:ASP:OD2	1:B:1291:ARG:NH1[2_555]	2.14	0.06

## 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	551/602 (92%)	526 (96%)	22 (4%)	3 (0%)	34	71
1	B	550/602 (91%)	525 (96%)	22 (4%)	3 (0%)	34	71
All	All	1101/1204 (91%)	1051 (96%)	44 (4%)	6 (0%)	34	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1424	THR
1	A	141	ALA
1	B	141	ALA
1	A	80	THR
1	B	80	THR
1	B	1424	THR

### 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	464/505 (92%)	464 (100%)	0	100	100
1	B	462/505 (92%)	461 (100%)	1 (0%)	95	98
All	All	926/1010 (92%)	925 (100%)	1 (0%)	95	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1287	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	201	ASN
1	A	1356	GLN
1	A	1460	ASN
1	B	173	ASN
1	B	201	ASN
1	B	218	ASN
1	B	282	ASN
1	B	1308	ASN
1	B	1356	GLN
1	B	1390	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	MAL	A	500	-	24,24,24	0.59	0	35,35,35	1.12	4 (11%)
3	MES	A	600	-	11,12,12	0.68	0	14,16,16	2.42	4 (28%)
2	MAL	B	500	-	24,24,24	0.52	0	35,35,35	1.31	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MES	B	600	-	11,12,12	0.84	0	14,16,16	2.30	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAL	A	500	-	-	0/8/48/48	0/2/2/2
3	MES	A	600	-	-	0/6/14/14	0/1/1/1
2	MAL	B	500	-	-	0/8/48/48	0/2/2/2
3	MES	B	600	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	MAL	O2'-C2'-C3'	-3.00	103.58	110.34
3	A	600	MES	O3S-S-O2S	-2.57	105.64	111.61
3	A	600	MES	O3S-S-O1S	-2.46	105.87	111.61
2	A	500	MAL	O5-C1-C2	-2.44	105.28	110.28
2	B	500	MAL	O2'-C2'-C1'	2.18	114.63	109.82
2	A	500	MAL	O5-C5-C4	2.21	113.82	109.68
2	A	500	MAL	O1'-C1'-C2'	2.33	115.46	109.21
2	A	500	MAL	C1'-C2'-C3'	2.53	114.19	110.43
2	B	500	MAL	C1'-C2'-C3'	2.97	114.84	110.43
2	B	500	MAL	O5'-C1'-C2'	3.29	115.04	109.80
3	A	600	MES	O2S-S-C8	4.57	110.81	106.91
3	B	600	MES	O1S-S-C8	5.53	111.62	106.91
3	B	600	MES	O2S-S-C8	5.95	111.99	106.91
3	A	600	MES	O1S-S-C8	6.59	112.53	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	MES	10	0
2	B	500	MAL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	600	MES	15	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	557/602 (92%)	0.24	11 (1%) 68 62	47, 83, 132, 202	0
1	B	556/602 (92%)	0.36	21 (3%) 44 37	48, 82, 132, 201	0
All	All	1113/1204 (92%)	0.30	32 (2%) 55 49	47, 82, 132, 202	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	141	ALA	5.8
1	B	1387	ALA	5.3
1	B	1386	ASP	5.1
1	A	1387	ALA	3.8
1	A	1385	SER	3.7
1	A	1386	ASP	3.7
1	B	144	LYS	3.5
1	B	1385	SER	3.5
1	B	143	GLY	3.3
1	A	194	PHE	3.1
1	B	1388	MET	3.1
1	B	197	ASP	2.9
1	B	1309	ASN	2.7
1	B	132	ILE	2.7
1	B	121	LEU	2.7
1	B	118	ASN	2.6
1	B	1313	ALA	2.6
1	B	1380	CYS	2.6
1	A	184	ASP	2.5
1	A	1384	GLN	2.4
1	A	129	TRP	2.4
1	B	241	ASN	2.4
1	B	1357	SER	2.3
1	B	217	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1309	ASN	2.3
1	A	164	ASP	2.2
1	A	250	PHE	2.2
1	B	140	LYS	2.2
1	A	193	THR	2.2
1	B	1473	PHE	2.1
1	B	204	MET	2.1
1	B	139	LEU	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MES	A	600	12/12	0.87	0.43	3.20	78,82,129,136	0
3	MES	B	600	12/12	0.85	0.36	2.41	67,73,127,130	0
2	MAL	A	500	23/23	0.96	0.25	1.06	55,64,70,73	0
2	MAL	B	500	23/23	0.97	0.22	-0.05	57,63,69,75	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.