



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:44 PM GMT

PDB ID : 4JC0  
Title : Crystal structure of Thermotoga maritima holo RimO in complex with penta-sulfide, Northeast Structural Genomics Consortium Target VR77  
Authors : Forouhar, F.; Hussain, M.; Seetharaman, J.; Fang, Y.; Chen, C.X.; Cunningham, K.; Conover, K.; Ma, L.-C.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2013-02-20  
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

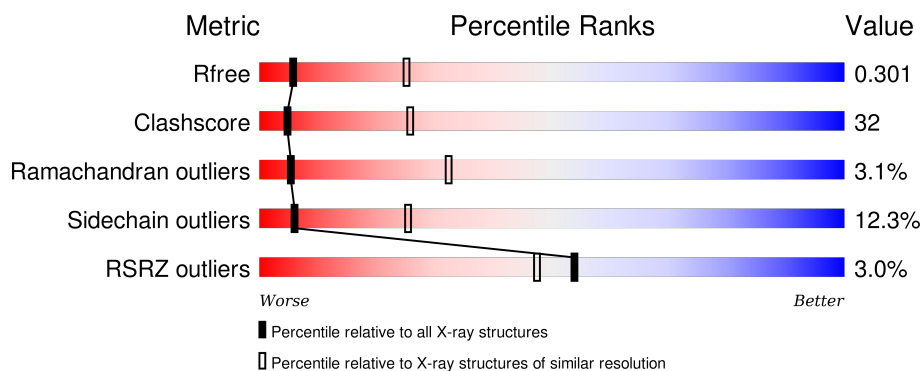
# 1 Overall quality at a glance

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	438	<div> <div>%</div> <div> <div></div> <div>41%</div> <div>47%</div> <div>9%</div> <div>.</div> </div> </div>
1	B	438	<div> <div>5%</div> <div> <div></div> <div>41%</div> <div>47%</div> <div>8%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6850 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.

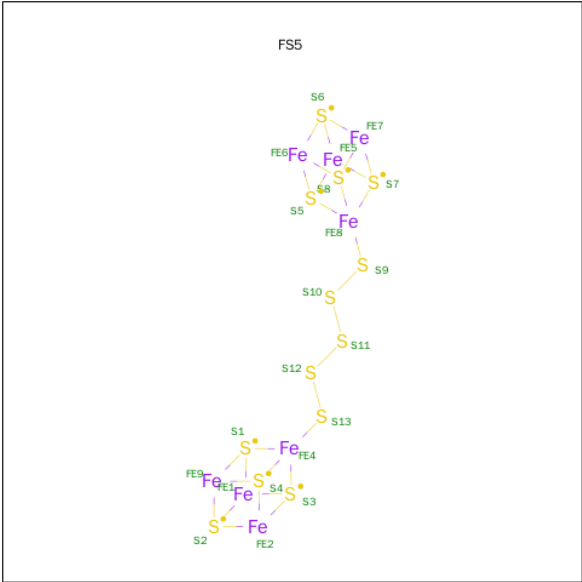
- Molecule 1 is a protein called Ribosomal protein S12 methylthiotransferase RimO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3419	2179	570	657	13			
1	B	421	Total	C	N	O	S	0	0	0
			3389	2162	562	652	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	LEU	-	EXPRESSION TAG	UNP Q9X2H6
A	432	GLU	-	EXPRESSION TAG	UNP Q9X2H6
A	433	HIS	-	EXPRESSION TAG	UNP Q9X2H6
A	434	HIS	-	EXPRESSION TAG	UNP Q9X2H6
A	435	HIS	-	EXPRESSION TAG	UNP Q9X2H6
A	436	HIS	-	EXPRESSION TAG	UNP Q9X2H6
A	437	HIS	-	EXPRESSION TAG	UNP Q9X2H6
A	438	HIS	-	EXPRESSION TAG	UNP Q9X2H6
B	431	LEU	-	EXPRESSION TAG	UNP Q9X2H6
B	432	GLU	-	EXPRESSION TAG	UNP Q9X2H6
B	433	HIS	-	EXPRESSION TAG	UNP Q9X2H6
B	434	HIS	-	EXPRESSION TAG	UNP Q9X2H6
B	435	HIS	-	EXPRESSION TAG	UNP Q9X2H6
B	436	HIS	-	EXPRESSION TAG	UNP Q9X2H6
B	437	HIS	-	EXPRESSION TAG	UNP Q9X2H6
B	438	HIS	-	EXPRESSION TAG	UNP Q9X2H6

- Molecule 2 is IRON/SULFUR PENTA-SULFIDE CONNECTED CLUSTERS (three-letter code: FS5) (formula: Fe<sub>8</sub>S<sub>13</sub>).

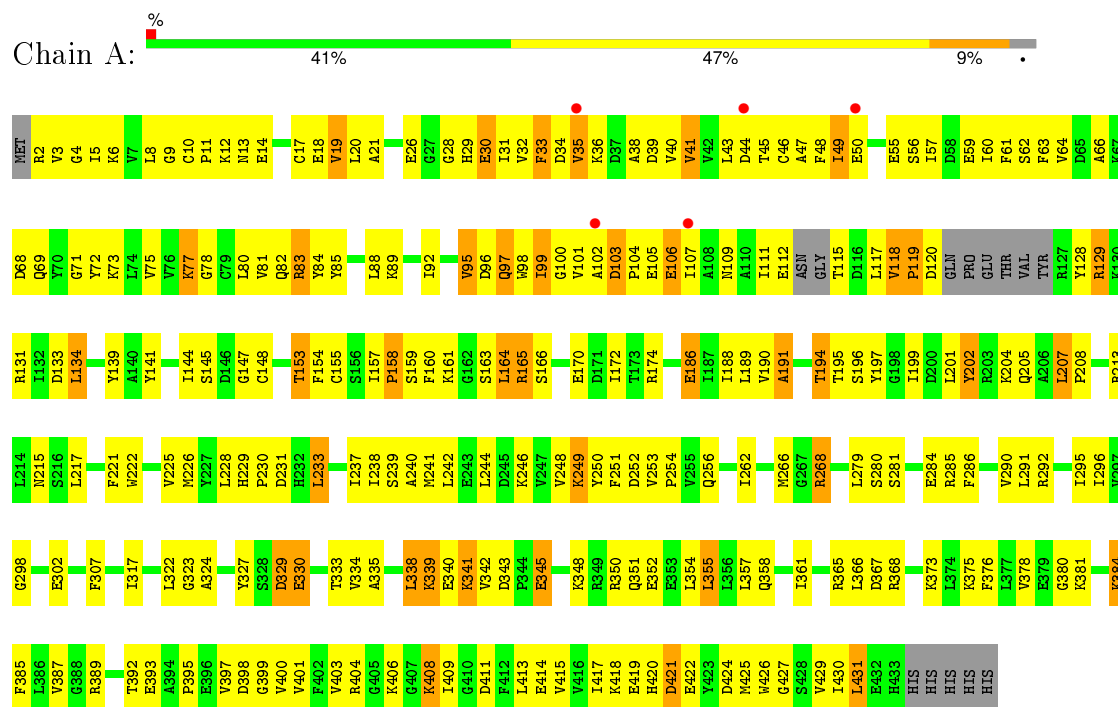


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			21	8	13		
2	B	1	Total	Fe	S	0	0
			21	8	13		

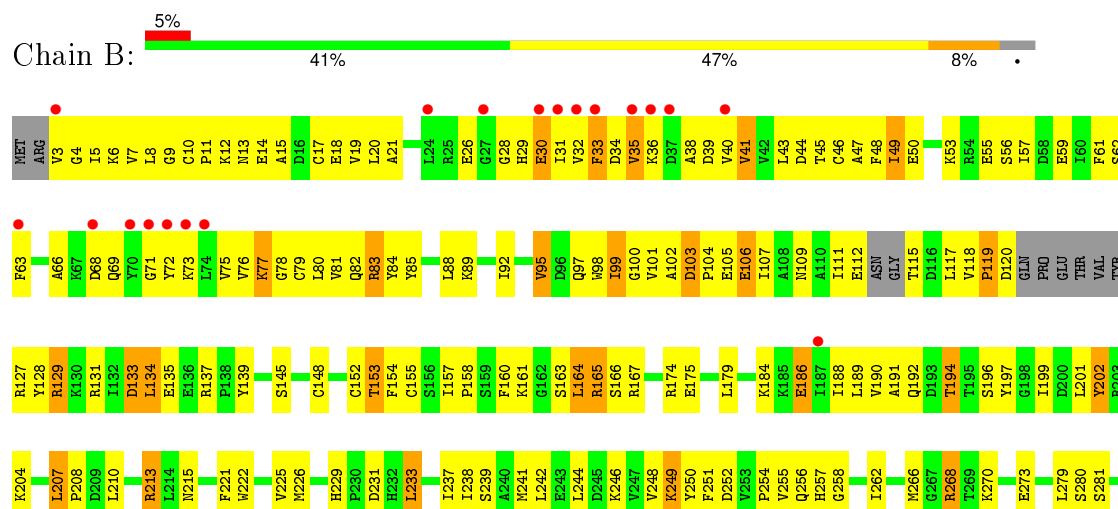
### 3 Residue-property plots

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: Ribosomal protein S12 methylthiotransferase RimO



- Molecule 1: Ribosomal protein S12 methylthiotransferase RimO



E284	D667	HIS
A285	R368	HIS
F286	K373	HIS
V290	L374	
L291	K375	
R292	F376	
T293	G380	
	K381	
L296	K384	
V297	F385	
G298	L386	
	V387	
E302	G388	
	R389	
F307		
	F313	
F313	T392	
	E393	
I317	A394	
Q318	F395	
	E396	
L322	V397	
G323	D398	
A324	G399	
	V400	
Y327	V401	
S328	F402	
D329	V403	
E330	R404	
	G405	
T333	K406	
V334	G407	
A335	K408	
	I409	
L338	G410	
K339	D411	
E340		
K341	E414	
V342	V415	
D343	V416	
P344	I417	
E345	K418	
	E419	
K348	R420	
R349	D421	
R350	E422	
Q351	Y423	
E352	D424	
E363	M425	
L354	W426	
L355	G427	
L356	S428	
L357	V429	
Q358	I430	
	L431	
T361	GLU	
	HIS	
R365	HIS	
L366	HIS	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.72Å 86.95Å 172.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.46 – 3.30 41.46 – 3.29	Depositor EDS
% Data completeness (in resolution range)	83.1 (41.46-3.30) 82.7 (41.46-3.29)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 3.32Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.245 , 0.296 0.247 , 0.301	Depositor DCC
$R_{free}$ test set	1344 reflections (12.75%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.3	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 60.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 13065 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6850	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: FS5

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	0.47	0/3476	0.59	0/4676
1	B	0.48	0/3445	0.59	0/4635
All	All	0.48	0/6921	0.59	0/9311

There are no bond length outliers.

There are no bond angle outliers.

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	3419	0	3420	207	0
1	B	3389	0	3394	228	0
2	A	21	0	0	2	0
2	B	21	0	0	5	0
All	All	6850	0	6814	432	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (432) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:VAL:HG21	1:B:38:ALA:HB2	1.38	1.06
1:A:32:VAL:HG21	1:A:38:ALA:HB2	1.38	1.04
1:B:81:VAL:HG21	1:B:99:ILE:O	1.66	0.94
1:B:131:ARG:HD3	1:B:179:LEU:HD21	1.48	0.92
1:A:81:VAL:HG21	1:A:99:ILE:O	1.73	0.89
1:A:322:LEU:HB3	1:A:358:GLN:HG2	1.55	0.87
1:B:9:GLY:HA2	1:B:46:CYS:HB2	1.59	0.85
1:A:408:LYS:HD3	1:A:409:ILE:H	1.43	0.84
1:B:40:VAL:HG13	1:B:73:LYS:HB3	1.59	0.83
1:A:9:GLY:HA2	1:A:46:CYS:HB2	1.60	0.83
1:B:13:ASN:ND2	2:B:501:FS5:S6	2.52	0.83
1:B:408:LYS:HD3	1:B:409:ILE:H	1.42	0.83
1:B:5:ILE:HD11	1:B:134:LEU:HD22	1.61	0.83
1:B:322:LEU:HB3	1:B:358:GLN:HG2	1.62	0.82
1:A:420:HIS:O	1:A:421:ASP:HB2	1.80	0.82
1:A:188:ILE:HD11	1:A:395:PRO:HG2	1.63	0.80
1:B:420:HIS:O	1:B:421:ASP:HB2	1.79	0.80
1:A:20:LEU:HD11	1:A:106:GLU:HB2	1.64	0.78
1:B:188:ILE:HD11	1:B:395:PRO:HG2	1.66	0.78
1:B:10:CYS:SG	1:B:12:LYS:HE3	2.24	0.77
1:B:5:ILE:HD12	1:B:17:CYS:HB3	1.67	0.76
1:A:279:LEU:HD12	1:A:317:ILE:HD13	1.67	0.76
1:A:40:VAL:HG13	1:A:73:LYS:HB3	1.66	0.76
1:A:128:TYR:CE2	1:A:174:ARG:HD2	2.22	0.75
1:A:32:VAL:HG21	1:A:38:ALA:CB	2.17	0.74
1:A:48:PHE:CE2	1:A:330:GLU:HG2	2.23	0.74
1:A:5:ILE:HD12	1:A:17:CYS:HB3	1.70	0.73
1:A:10:CYS:SG	1:A:12:LYS:HE3	2.27	0.73
1:B:32:VAL:HG21	1:B:38:ALA:CB	2.17	0.73
1:A:307:PHE:CE2	1:A:350:ARG:HB3	2.23	0.73
1:B:20:LEU:HD11	1:B:106:GLU:HB2	1.71	0.73
1:B:241:MET:HE3	1:B:251:PHE:CE2	2.23	0.72
1:A:103:ASP:HB3	1:A:104:PRO:HD3	1.69	0.72
1:B:417:ILE:HD12	1:B:425:MET:HB3	1.71	0.72
1:A:13:ASN:ND2	2:A:501:FS5:S6	2.60	0.71
1:B:251:PHE:HB2	1:B:291:LEU:HD23	1.73	0.70
1:B:6:LYS:HB3	1:B:43:LEU:HD12	1.73	0.70
1:A:417:ILE:HD12	1:A:425:MET:HB3	1.73	0.69
1:B:279:LEU:HD12	1:B:317:ILE:HD13	1.73	0.69
1:B:105:GLU:O	1:B:109:ASN:HB2	1.93	0.69
1:A:201:LEU:HB3	1:A:202:TYR:CD2	2.28	0.68
1:B:165:ARG:HB3	1:B:165:ARG:HH21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLU:HG3	1:B:418:LYS:HE3	1.76	0.68
1:A:201:LEU:HD23	1:A:202:TYR:CE2	2.29	0.68
1:B:307:PHE:CE2	1:B:350:ARG:HB3	2.29	0.68
1:A:201:LEU:HD23	1:A:202:TYR:HE2	1.59	0.68
1:A:268:ARG:HH11	1:A:268:ARG:HG2	1.60	0.67
1:B:201:LEU:HB3	1:B:202:TYR:CD2	2.30	0.67
1:B:268:ARG:HH11	1:B:268:ARG:HG2	1.60	0.67
1:B:79:CYS:SG	1:B:161:LYS:HE3	2.35	0.67
1:B:418:LYS:HD3	1:B:427:GLY:HA2	1.76	0.67
1:A:165:ARG:HB3	1:A:165:ARG:HH21	1.59	0.67
1:B:83:ARG:HB2	1:B:160:PHE:CE2	2.30	0.66
1:A:418:LYS:HD3	1:A:427:GLY:HA2	1.76	0.66
1:A:415:VAL:HG12	1:A:429:VAL:HG22	1.77	0.66
1:B:103:ASP:HB3	1:B:104:PRO:HD3	1.77	0.66
1:A:393:GLU:OE2	1:A:398:ASP:HB3	1.96	0.66
1:B:139:TYR:CB	1:B:186:GLU:HB3	2.27	0.65
1:A:194:THR:HG21	1:A:225:VAL:CG1	2.26	0.65
1:A:327:TYR:CE2	1:A:329:ASP:HB3	2.31	0.65
1:B:201:LEU:HD23	1:B:202:TYR:HE2	1.62	0.65
1:A:78:GLY:O	1:A:81:VAL:HG22	1.96	0.65
1:A:251:PHE:HB2	1:A:291:LEU:HD23	1.78	0.65
1:B:17:CYS:SG	1:B:44:ASP:CG	2.75	0.64
1:A:49:ILE:HG22	1:A:49:ILE:O	1.98	0.64
1:A:105:GLU:O	1:A:109:ASN:HB2	1.97	0.64
1:A:400:VAL:HG22	1:A:401:VAL:H	1.63	0.64
1:B:139:TYR:CE1	1:B:395:PRO:HB3	2.33	0.64
1:B:78:GLY:O	1:B:81:VAL:HG22	1.97	0.63
1:A:241:MET:HE3	1:A:251:PHE:CE2	2.33	0.63
1:A:215:ASN:ND2	1:A:244:LEU:HD22	2.14	0.63
1:A:415:VAL:HG12	1:A:429:VAL:CG2	2.28	0.63
1:A:148:CYS:HA	1:A:164:LEU:HD23	1.80	0.63
1:A:422:GLU:HG3	1:B:418:LYS:CE	2.29	0.63
1:B:194:THR:HG21	1:B:225:VAL:CG1	2.29	0.62
1:B:83:ARG:NE	1:B:83:ARG:HA	2.12	0.62
1:B:201:LEU:HD23	1:B:202:TYR:CE2	2.34	0.62
1:B:75:VAL:HG22	1:B:97:GLN:HB2	1.81	0.62
1:A:2:ARG:HA	1:A:30:GLU:O	1.99	0.62
1:A:222:TRP:HZ2	1:A:375:LYS:HB3	1.65	0.62
1:A:298:GLY:HA2	1:A:342:VAL:HG11	1.81	0.62
1:A:117:LEU:O	1:A:118:VAL:HG13	1.99	0.61
1:B:7:VAL:HG11	1:B:134:LEU:HD21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HD11	1:A:134:LEU:CD2	2.31	0.61
1:B:79:CYS:HB3	1:B:160:PHE:HZ	1.64	0.61
1:B:66:ALA:HB1	1:B:69:GLN:HG3	1.83	0.61
1:A:322:LEU:C	1:A:322:LEU:HD23	2.21	0.61
1:A:66:ALA:HB1	1:A:69:GLN:HG3	1.83	0.61
1:A:83:ARG:HA	1:A:83:ARG:NE	2.15	0.61
1:B:215:ASN:ND2	1:B:244:LEU:HD22	2.16	0.61
1:B:201:LEU:HB3	1:B:202:TYR:HD2	1.66	0.61
1:B:148:CYS:HA	1:B:164:LEU:HD23	1.83	0.60
1:B:79:CYS:HB3	1:B:160:PHE:CZ	2.37	0.60
1:A:400:VAL:HG22	1:A:401:VAL:N	2.16	0.60
1:B:12:LYS:HD3	1:B:191:ALA:C	2.22	0.60
1:B:242:LEU:HA	1:B:249:LYS:HE3	1.82	0.60
1:A:290:VAL:HG21	1:A:392:THR:HB	1.84	0.60
1:A:242:LEU:HA	1:A:249:LYS:HE3	1.84	0.60
1:B:32:VAL:HG11	1:B:38:ALA:HA	1.84	0.60
1:A:262:ILE:O	1:A:266:MET:HG3	2.02	0.60
1:B:207:LEU:HB3	1:B:208:PRO:HD3	1.84	0.60
1:A:75:VAL:HG22	1:A:97:GLN:HB2	1.83	0.59
1:B:327:TYR:OH	1:B:329:ASP:HB3	2.01	0.59
1:A:155:CYS:HB2	2:A:501:FS5:S3	2.41	0.59
1:A:166:SER:HB2	1:A:197:TYR:CD1	2.37	0.59
1:B:222:TRP:HZ2	1:B:375:LYS:HB3	1.67	0.59
1:A:279:LEU:CD1	1:A:317:ILE:HD13	2.32	0.59
1:B:393:GLU:OE2	1:B:398:ASP:HB3	2.01	0.59
1:B:233:LEU:HD22	1:B:238:ILE:HG13	1.84	0.59
1:B:17:CYS:SG	1:B:44:ASP:OD2	2.61	0.59
1:B:80:LEU:O	1:B:84:TYR:HB2	2.02	0.59
1:A:343:ASP:HB3	1:A:345:GLU:HG3	1.85	0.59
1:A:49:ILE:CG2	1:A:49:ILE:O	2.51	0.59
1:B:400:VAL:HG22	1:B:401:VAL:H	1.67	0.59
1:B:327:TYR:CE2	1:B:329:ASP:HB3	2.38	0.59
1:B:322:LEU:HD23	1:B:323:GLY:N	2.18	0.58
1:B:83:ARG:HB2	1:B:160:PHE:CD2	2.37	0.58
1:B:55:GLU:O	1:B:59:GLU:HB2	2.02	0.58
1:A:153:THR:OG1	1:A:266:MET:HA	2.03	0.58
1:A:207:LEU:HB3	1:A:208:PRO:HD3	1.84	0.58
1:B:21:ALA:O	1:B:31:ILE:HD11	2.04	0.58
1:B:49:ILE:HG22	1:B:49:ILE:O	2.03	0.58
1:A:408:LYS:HD3	1:A:409:ILE:N	2.18	0.58
1:B:408:LYS:HD3	1:B:409:ILE:N	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG11	1:A:38:ALA:HA	1.85	0.58
1:A:400:VAL:HG12	1:A:424:ASP:OD2	2.04	0.58
1:B:117:LEU:O	1:B:118:VAL:HG13	2.04	0.58
1:A:92:ILE:O	1:A:95:VAL:HG13	2.03	0.58
1:A:249:LYS:HG2	1:A:286:PHE:CD2	2.38	0.58
1:A:281:SER:O	1:A:285:ARG:HG3	2.03	0.58
1:A:5:ILE:HD11	1:A:134:LEU:HD22	1.85	0.58
1:B:186:GLU:OE1	1:B:222:TRP:HE3	1.87	0.57
1:B:322:LEU:C	1:B:322:LEU:HD23	2.24	0.57
1:B:290:VAL:HG21	1:B:392:THR:HB	1.85	0.57
1:A:322:LEU:HD23	1:A:323:GLY:N	2.19	0.57
1:A:201:LEU:HB3	1:A:202:TYR:HD2	1.70	0.57
1:B:3:VAL:HG23	1:B:40:VAL:O	2.04	0.57
1:A:109:ASN:C	1:A:111:ILE:H	2.06	0.57
1:B:32:VAL:C	1:B:34:ASP:H	2.08	0.57
1:A:80:LEU:O	1:A:84:TYR:HB2	2.04	0.57
1:B:112:GLU:HG3	1:B:115:THR:OG1	2.03	0.56
1:B:327:TYR:CZ	1:B:329:ASP:HB3	2.40	0.56
1:A:157:ILE:N	1:A:158:PRO:CD	2.68	0.56
1:B:157:ILE:N	1:B:158:PRO:CD	2.67	0.56
1:A:327:TYR:CZ	1:A:329:ASP:HB3	2.40	0.56
1:A:229:HIS:CE1	1:A:231:ASP:HB2	2.40	0.56
1:A:45:THR:HG22	1:A:77:LYS:O	2.06	0.56
1:A:9:GLY:CA	1:A:46:CYS:HB2	2.35	0.56
1:A:49:ILE:O	1:A:50:GLU:HG2	2.05	0.56
1:A:117:LEU:N	1:A:117:LEU:HD23	2.21	0.56
1:B:157:ILE:HG23	1:B:161:LYS:HB2	1.88	0.56
1:B:45:THR:HG22	1:B:77:LYS:O	2.05	0.56
1:A:48:PHE:O	1:A:49:ILE:HG12	2.06	0.56
1:A:186:GLU:OE1	1:A:222:TRP:HE3	1.89	0.56
1:B:81:VAL:CG2	1:B:99:ILE:O	2.47	0.55
1:A:55:GLU:O	1:A:59:GLU:HB2	2.05	0.55
1:B:279:LEU:CD1	1:B:317:ILE:HD13	2.36	0.55
1:B:109:ASN:C	1:B:111:ILE:H	2.09	0.55
1:B:17:CYS:SG	1:B:44:ASP:OD1	2.65	0.55
1:A:17:CYS:SG	1:A:44:ASP:CG	2.85	0.55
1:B:343:ASP:HB3	1:B:345:GLU:HG3	1.86	0.55
1:B:139:TYR:HB2	1:B:186:GLU:HG2	1.89	0.55
1:A:112:GLU:HG3	1:A:115:THR:OG1	2.06	0.55
1:A:6:LYS:HB3	1:A:43:LEU:HD12	1.87	0.55
1:B:129:ARG:HG2	1:B:129:ARG:HH11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:TYR:OH	1:A:329:ASP:HB3	2.06	0.55
1:A:233:LEU:HD22	1:A:238:ILE:HG13	1.89	0.55
1:B:49:ILE:O	1:B:49:ILE:CG2	2.55	0.55
1:B:192:GLN:O	2:B:501:FS5:S12	2.65	0.55
1:B:12:LYS:HD3	1:B:191:ALA:O	2.07	0.54
1:B:400:VAL:HG22	1:B:401:VAL:N	2.23	0.54
1:B:281:SER:O	1:B:285:ARG:HG3	2.07	0.54
1:B:400:VAL:HG12	1:B:424:ASP:OD2	2.06	0.54
1:B:202:TYR:CD2	1:B:202:TYR:N	2.76	0.54
1:A:57:ILE:CD1	1:A:80:LEU:HD21	2.36	0.54
1:A:389:ARG:NH2	1:A:395:PRO:HG3	2.23	0.54
1:A:32:VAL:C	1:A:34:ASP:H	2.10	0.54
1:B:92:ILE:O	1:B:95:VAL:HG13	2.08	0.54
1:A:81:VAL:CG2	1:A:99:ILE:O	2.52	0.54
1:B:153:THR:OG1	1:B:266:MET:HA	2.08	0.54
1:B:12:LYS:NZ	2:B:501:FS5:S11	2.80	0.54
1:B:324:ALA:HB2	1:B:354:LEU:HD23	1.90	0.54
1:B:49:ILE:O	1:B:50:GLU:HG2	2.08	0.53
1:A:21:ALA:O	1:A:31:ILE:HD11	2.07	0.53
1:A:188:ILE:CD1	1:A:395:PRO:HG2	2.37	0.53
1:A:420:HIS:O	1:A:421:ASP:CB	2.55	0.53
1:B:417:ILE:HD12	1:B:425:MET:CB	2.38	0.53
1:A:298:GLY:CA	1:A:342:VAL:HG11	2.38	0.53
1:A:351:GLN:O	1:A:355:LEU:HB2	2.07	0.53
1:B:139:TYR:HB3	1:B:186:GLU:HB3	1.90	0.53
1:B:221:PHE:O	1:B:246:LYS:HG2	2.08	0.53
1:A:11:PRO:HB3	1:A:141:TYR:CD2	2.44	0.53
1:B:117:LEU:N	1:B:117:LEU:HD23	2.24	0.52
1:B:133:ASP:OD1	1:B:184:LYS:HE2	2.08	0.52
1:B:18:GLU:OE1	1:B:134:LEU:HD23	2.09	0.52
1:B:57:ILE:CD1	1:B:80:LEU:HD21	2.40	0.52
1:B:48:PHE:O	1:B:49:ILE:HG12	2.09	0.52
1:B:53:LYS:NZ	1:B:330:GLU:OE1	2.42	0.52
1:B:128:TYR:CE2	1:B:175:GLU:HA	2.45	0.52
1:B:98:TRP:C	1:B:99:ILE:HG12	2.30	0.52
1:A:139:TYR:HA	1:A:186:GLU:HB3	1.92	0.52
1:A:18:GLU:OE1	1:A:133:ASP:HA	2.09	0.52
1:B:18:GLU:O	1:B:131:ARG:HB2	2.10	0.52
1:B:302:GLU:HG2	1:B:350:ARG:NH2	2.24	0.52
1:B:389:ARG:NH2	1:B:395:PRO:HG3	2.25	0.51
1:A:5:ILE:HG13	1:A:5:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:VAL:C	1:B:32:VAL:HG22	2.30	0.51
1:B:18:GLU:CD	1:B:134:LEU:HD23	2.31	0.51
1:B:421:ASP:O	1:B:422:GLU:HB2	2.11	0.51
1:A:221:PHE:O	1:A:246:LYS:HG2	2.11	0.51
1:A:366:LEU:HD23	1:A:366:LEU:N	2.26	0.51
1:A:403:VAL:HA	1:A:427:GLY:O	2.10	0.51
1:B:85:TYR:CD1	1:B:118:VAL:HG21	2.45	0.51
1:A:154:PHE:HZ	1:A:256:GLN:HG3	1.76	0.51
1:A:330:GLU:O	1:A:333:THR:HG23	2.10	0.51
1:B:39:ASP:O	1:B:72:TYR:HA	2.11	0.51
1:A:154:PHE:CZ	1:A:256:GLN:HG3	2.46	0.50
1:B:248:VAL:O	1:B:250:TYR:N	2.39	0.50
1:A:365:ARG:O	1:A:368:ARG:HG2	2.11	0.50
1:A:11:PRO:HB2	1:A:190:VAL:HG11	1.93	0.50
1:A:421:ASP:O	1:A:422:GLU:HB2	2.12	0.50
1:B:166:SER:HB2	1:B:197:TYR:CD1	2.46	0.50
1:A:139:TYR:HB3	1:A:186:GLU:HB3	1.93	0.50
1:A:157:ILE:HG23	1:A:161:LYS:HB2	1.93	0.50
1:B:229:HIS:CE1	1:B:231:ASP:HB2	2.46	0.50
1:A:207:LEU:HD12	1:A:237:ILE:HG23	1.94	0.50
1:B:250:TYR:OH	1:B:292:ARG:HD2	2.12	0.50
1:A:98:TRP:C	1:A:99:ILE:HG12	2.31	0.50
1:A:155:CYS:SG	1:A:157:ILE:HG12	2.52	0.50
1:A:39:ASP:O	1:A:72:TYR:HA	2.12	0.50
1:A:202:TYR:N	1:A:202:TYR:CD2	2.80	0.50
1:B:48:PHE:HE1	1:B:160:PHE:CG	2.30	0.50
1:B:82:GLN:OE1	1:B:100:GLY:HA3	2.12	0.50
1:B:365:ARG:O	1:B:368:ARG:HG2	2.11	0.50
1:B:351:GLN:O	1:B:355:LEU:HB2	2.11	0.50
1:B:242:LEU:HD21	1:B:251:PHE:CZ	2.48	0.49
1:B:207:LEU:HD12	1:B:237:ILE:HG23	1.94	0.49
1:B:420:HIS:O	1:B:421:ASP:CB	2.53	0.49
1:B:280:SER:O	1:B:284:GLU:HG3	2.12	0.49
1:A:139:TYR:CB	1:A:186:GLU:HB3	2.42	0.49
1:B:77:LYS:HA	1:B:99:ILE:O	2.12	0.49
1:B:48:PHE:HE1	1:B:160:PHE:CD2	2.29	0.49
1:B:152:CYS:HB2	2:B:501:FS5:S2	2.52	0.49
1:A:250:TYR:OH	1:A:292:ARG:HD2	2.13	0.49
1:B:226:MET:CE	1:B:250:TYR:HE2	2.25	0.49
1:A:196:SER:O	1:A:199:ILE:HG13	2.13	0.49
1:A:111:ILE:HG13	1:A:112:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:GLY:HA2	1:B:342:VAL:HG11	1.93	0.49
1:A:324:ALA:HB2	1:A:354:LEU:HD23	1.93	0.49
1:B:393:GLU:OE2	1:B:399:GLY:N	2.45	0.48
1:A:242:LEU:HD23	1:A:249:LYS:HG3	1.94	0.48
1:B:119:PRO:HG2	1:B:120:ASP:H	1.78	0.48
1:A:302:GLU:HG2	1:A:350:ARG:NH2	2.27	0.48
1:B:242:LEU:HD21	1:B:251:PHE:HZ	1.78	0.48
1:A:194:THR:HG21	1:A:225:VAL:HG11	1.94	0.48
1:A:30:GLU:HG3	1:A:31:ILE:N	2.28	0.48
1:A:82:GLN:OE1	1:A:118:VAL:HG12	2.14	0.48
1:B:128:TYR:HB2	1:B:167:ARG:NH1	2.28	0.48
1:A:393:GLU:OE2	1:A:399:GLY:N	2.42	0.48
1:A:11:PRO:CB	1:A:190:VAL:HG11	2.44	0.48
1:A:380:GLY:CA	1:A:387:VAL:HG12	2.43	0.48
1:B:14:GLU:O	1:B:18:GLU:HG2	2.14	0.48
1:A:95:VAL:HG21	1:A:98:TRP:CE2	2.49	0.48
1:A:85:TYR:CD1	1:A:118:VAL:HG21	2.49	0.48
1:B:257:HIS:ND1	1:B:258:GLY:N	2.58	0.48
1:A:82:GLN:OE1	1:A:100:GLY:HA3	2.13	0.47
1:B:330:GLU:O	1:B:333:THR:HG23	2.13	0.47
1:B:5:ILE:HG13	1:B:5:ILE:O	2.14	0.47
1:A:101:VAL:O	1:A:102:ALA:HB3	2.14	0.47
1:A:77:LYS:HA	1:A:99:ILE:O	2.13	0.47
1:B:381:LYS:NZ	1:B:406:LYS:HE3	2.29	0.47
1:A:3:VAL:HG23	1:A:40:VAL:O	2.14	0.47
1:A:17:CYS:SG	1:A:44:ASP:OD2	2.73	0.47
1:A:280:SER:O	1:A:284:GLU:HG3	2.14	0.47
1:B:157:ILE:HA	1:B:160:PHE:HB3	1.96	0.47
1:B:348:LYS:O	1:B:352:GLU:HG3	2.15	0.47
1:A:426:TRP:CH2	1:B:419:GLU:OE1	2.68	0.47
1:B:366:LEU:N	1:B:366:LEU:HD23	2.29	0.47
1:A:35:VAL:C	1:A:36:LYS:HG2	2.35	0.47
1:B:335:ALA:O	1:B:338:LEU:HB2	2.15	0.47
1:A:190:VAL:O	1:A:191:ALA:HB2	2.15	0.46
1:B:242:LEU:HD23	1:B:249:LYS:HG3	1.96	0.46
1:A:335:ALA:O	1:A:338:LEU:HB2	2.16	0.46
1:A:242:LEU:CD2	1:A:249:LYS:HG3	2.45	0.46
1:A:84:TYR:O	1:A:88:LEU:HG	2.15	0.46
1:A:381:LYS:NZ	1:A:406:LYS:HE3	2.29	0.46
1:A:329:ASP:OD1	1:A:329:ASP:N	2.49	0.46
1:A:119:PRO:HG2	1:A:120:ASP:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLY:O	1:A:148:CYS:HB2	2.14	0.46
1:A:14:GLU:O	1:A:18:GLU:HG2	2.15	0.46
1:B:95:VAL:HG21	1:B:98:TRP:CE2	2.51	0.46
1:B:9:GLY:O	1:B:10:CYS:HB3	2.14	0.46
1:B:365:ARG:CZ	1:B:368:ARG:HD3	2.45	0.46
1:B:417:ILE:HG23	1:B:425:MET:HB3	1.97	0.46
1:A:413:LEU:HD13	1:A:429:VAL:HG21	1.97	0.46
1:B:35:VAL:C	1:B:36:LYS:HG2	2.36	0.46
1:B:249:LYS:HG2	1:B:286:PHE:CD2	2.50	0.46
1:B:101:VAL:O	1:B:102:ALA:HB3	2.16	0.46
1:A:226:MET:CE	1:A:250:TYR:HE2	2.29	0.46
1:A:109:ASN:C	1:A:111:ILE:N	2.69	0.46
1:A:82:GLN:HB3	1:A:160:PHE:CE2	2.51	0.46
1:B:392:THR:OG1	1:B:393:GLU:N	2.49	0.46
1:B:57:ILE:HD13	1:B:80:LEU:HD21	1.98	0.46
1:A:35:VAL:HG22	1:A:35:VAL:O	2.16	0.46
1:B:241:MET:HE3	1:B:251:PHE:CD2	2.50	0.46
1:B:194:THR:HG21	1:B:225:VAL:HG11	1.98	0.46
1:B:329:ASP:N	1:B:329:ASP:OD1	2.47	0.46
1:B:5:ILE:CD1	1:B:134:LEU:HD22	2.41	0.45
1:B:403:VAL:HA	1:B:427:GLY:O	2.16	0.45
1:B:298:GLY:CA	1:B:342:VAL:HG11	2.46	0.45
1:A:228:LEU:O	1:A:254:PRO:HD2	2.16	0.45
1:A:57:ILE:HD13	1:A:80:LEU:HD21	1.98	0.45
1:B:18:GLU:OE2	1:B:137:ARG:NH2	2.50	0.45
1:B:82:GLN:OE1	1:B:118:VAL:HG12	2.16	0.45
1:B:155:CYS:HB2	2:B:501:FS5:S3	2.57	0.45
1:B:341:LYS:HB3	1:B:342:VAL:H	1.52	0.45
1:A:106:GLU:N	1:A:106:GLU:OE1	2.50	0.45
1:A:195:THR:O	1:A:205:GLN:NE2	2.45	0.45
1:B:139:TYR:CD2	1:B:139:TYR:C	2.90	0.45
1:B:84:TYR:O	1:B:88:LEU:HG	2.17	0.45
1:A:39:ASP:N	1:A:39:ASP:OD2	2.50	0.44
1:A:365:ARG:CZ	1:A:368:ARG:HD3	2.48	0.44
1:B:231:ASP:OD1	1:B:270:LYS:HB2	2.18	0.44
1:A:358:GLN:HA	1:A:361:ILE:HD12	1.99	0.44
1:A:40:VAL:HG12	1:A:41:VAL:N	2.31	0.44
1:A:28:GLY:C	1:A:30:GLU:H	2.21	0.44
1:A:248:VAL:O	1:A:250:TYR:N	2.46	0.44
1:B:9:GLY:CA	1:B:46:CYS:HB2	2.39	0.44
1:A:417:ILE:HD12	1:A:425:MET:CB	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:NH1	1:A:268:ARG:HG2	2.30	0.44
1:B:188:ILE:CD1	1:B:395:PRO:HG2	2.42	0.44
1:B:139:TYR:HA	1:B:186:GLU:HB3	2.00	0.44
1:B:32:VAL:O	1:B:34:ASP:N	2.48	0.44
1:B:30:GLU:HG3	1:B:31:ILE:N	2.30	0.44
1:B:89:LYS:HE3	1:B:89:LYS:HB3	1.77	0.44
1:B:39:ASP:N	1:B:39:ASP:OD2	2.51	0.43
1:A:48:PHE:HE2	1:A:330:GLU:HG2	1.81	0.43
1:B:242:LEU:CD2	1:B:251:PHE:HZ	2.31	0.43
1:A:139:TYR:CA	1:A:186:GLU:HB3	2.48	0.43
1:A:253:VAL:HG22	1:A:253:VAL:O	2.17	0.43
1:B:40:VAL:HG12	1:B:41:VAL:N	2.33	0.43
1:A:60:ILE:O	1:A:64:VAL:HG23	2.19	0.43
1:B:154:PHE:HZ	1:B:256:GLN:HG3	1.83	0.43
1:B:135:GLU:HG2	1:B:137:ARG:HD3	2.01	0.43
1:A:153:THR:HG22	1:A:334:VAL:HB	2.00	0.43
1:B:35:VAL:O	1:B:35:VAL:HG22	2.18	0.43
1:A:144:ILE:HG22	1:A:172:ILE:HD13	2.01	0.43
1:B:419:GLU:HG2	1:B:420:HIS:N	2.34	0.43
1:B:109:ASN:C	1:B:111:ILE:N	2.72	0.43
1:B:83:ARG:NE	1:B:83:ARG:CA	2.80	0.43
1:B:254:PRO:HA	1:B:293:THR:OG1	2.17	0.43
1:B:242:LEU:CD2	1:B:249:LYS:HG3	2.49	0.43
1:A:215:ASN:CG	1:A:244:LEU:HD22	2.39	0.43
1:B:342:VAL:HG13	1:B:342:VAL:O	2.18	0.43
1:A:348:LYS:O	1:A:352:GLU:HG3	2.19	0.43
1:B:135:GLU:HB3	1:B:137:ARG:NE	2.34	0.43
1:A:392:THR:OG1	1:A:393:GLU:N	2.51	0.43
1:A:83:ARG:CA	1:A:83:ARG:NE	2.81	0.43
1:B:76:VAL:HG12	1:B:81:VAL:CG1	2.48	0.42
1:A:17:CYS:SG	1:A:44:ASP:OD1	2.77	0.42
1:B:262:ILE:O	1:B:266:MET:HG3	2.19	0.42
1:A:217:LEU:HD23	1:A:217:LEU:N	2.34	0.42
1:B:210:LEU:O	1:B:213:ARG:HB3	2.19	0.42
1:A:95:VAL:HG23	1:A:96:ASP:N	2.33	0.42
1:A:295:ILE:CG2	1:A:296:ILE:N	2.82	0.42
1:A:19:VAL:HA	1:A:131:ARG:HB3	2.01	0.42
1:A:242:LEU:HD21	1:A:251:PHE:HZ	1.85	0.42
1:B:252:ASP:HA	1:B:292:ARG:O	2.20	0.42
1:A:338:LEU:HD13	1:A:339:LYS:H	1.83	0.42
1:A:103:ASP:C	1:A:105:GLU:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:SER:HB2	1:A:166:SER:CB	2.50	0.42
1:B:28:GLY:C	1:B:30:GLU:H	2.23	0.42
1:B:380:GLY:CA	1:B:387:VAL:HG12	2.49	0.42
1:B:154:PHE:CZ	1:B:256:GLN:HG3	2.55	0.42
1:A:104:PRO:HG3	1:A:129:ARG:NH1	2.34	0.42
1:B:83:ARG:HB2	1:B:160:PHE:HE2	1.77	0.42
1:B:47:ALA:HB2	1:B:80:LEU:N	2.34	0.42
1:A:157:ILE:O	1:A:159:SER:N	2.53	0.42
1:B:313:PHE:CZ	1:B:317:ILE:HD11	2.55	0.42
1:B:196:SER:O	1:B:199:ILE:HG13	2.19	0.42
1:A:12:LYS:HD3	1:A:191:ALA:C	2.40	0.41
1:B:111:ILE:HG13	1:B:112:GLU:OE1	2.20	0.41
1:A:242:LEU:HD21	1:A:251:PHE:CZ	2.55	0.41
1:A:57:ILE:HD12	1:A:80:LEU:HD21	2.01	0.41
1:B:145:SER:HB2	1:B:166:SER:CB	2.49	0.41
1:B:255:VAL:C	1:B:257:HIS:H	2.24	0.41
1:A:56:SER:O	1:A:60:ILE:HG13	2.19	0.41
1:B:11:PRO:HB2	1:B:190:VAL:HG11	2.02	0.41
1:B:139:TYR:CA	1:B:186:GLU:HB3	2.50	0.41
1:A:376:PHE:HE1	1:A:378:VAL:HG22	1.84	0.41
1:B:376:PHE:CB	1:B:415:VAL:HG13	2.50	0.41
1:B:45:THR:OG1	1:B:56:SER:HB3	2.20	0.41
1:B:268:ARG:NH1	1:B:268:ARG:HG2	2.33	0.41
1:B:273:GLU:CA	1:B:273:GLU:OE2	2.69	0.41
1:B:358:GLN:HA	1:B:361:ILE:HD12	2.03	0.41
1:A:237:ILE:O	1:A:240:ALA:HB3	2.20	0.41
1:A:351:GLN:O	1:A:351:GLN:HG2	2.19	0.41
1:A:417:ILE:HG23	1:A:425:MET:HB3	2.02	0.41
1:B:202:TYR:HD2	1:B:202:TYR:N	2.17	0.41
1:B:66:ALA:CB	1:B:69:GLN:HG3	2.48	0.41
1:B:338:LEU:HD13	1:B:339:LYS:H	1.86	0.41
1:B:415:VAL:HA	1:B:429:VAL:HA	2.02	0.41
1:A:373:LYS:HD2	1:A:414:GLU:OE1	2.20	0.41
1:A:322:LEU:CB	1:A:358:GLN:HG2	2.38	0.41
1:A:419:GLU:HG2	1:A:420:HIS:N	2.36	0.41
1:A:174:ARG:CZ	1:A:174:ARG:HB2	2.50	0.41
1:A:47:ALA:HB2	1:A:80:LEU:N	2.36	0.41
1:B:11:PRO:CB	1:B:190:VAL:HG11	2.51	0.41
1:A:89:LYS:HE3	1:A:89:LYS:HB3	1.82	0.41
1:B:106:GLU:N	1:B:106:GLU:OE1	2.53	0.41
1:B:3:VAL:HG22	1:B:4:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ALA:CB	1:A:69:GLN:HG3	2.49	0.41
1:B:384:LYS:NZ	1:B:404:ARG:NH1	2.69	0.41
1:A:61:PHE:C	1:A:63:PHE:N	2.75	0.41
1:B:6:LYS:HD2	1:B:6:LYS:HA	1.99	0.41
1:B:80:LEU:HG	1:B:88:LEU:HD11	2.02	0.41
1:A:230:PRO:HB3	1:A:253:VAL:CG2	2.51	0.41
1:B:174:ARG:CZ	1:B:174:ARG:HB2	2.50	0.41
1:B:174:ARG:HG3	1:B:174:ARG:HH11	1.86	0.41
1:A:3:VAL:HG22	1:A:4:GLY:N	2.36	0.40
1:A:341:LYS:HB3	1:A:342:VAL:H	1.55	0.40
1:B:215:ASN:CG	1:B:244:LEU:HD22	2.41	0.40
1:A:384:LYS:NZ	1:A:404:ARG:NH1	2.70	0.40
1:B:103:ASP:H	1:B:104:PRO:CD	2.35	0.40
1:B:61:PHE:C	1:B:63:PHE:N	2.74	0.40
1:B:317:ILE:O	1:B:318:GLN:HB2	2.21	0.40
1:B:256:GLN:OE1	1:B:296:ILE:HG13	2.22	0.40
1:B:273:GLU:HA	1:B:273:GLU:OE2	2.21	0.40
1:B:15:ALA:C	1:B:17:CYS:N	2.75	0.40
1:A:252:ASP:OD1	1:A:292:ARG:HG2	2.21	0.40
1:A:295:ILE:HG22	1:A:296:ILE:N	2.36	0.40
1:B:373:LYS:HD2	1:B:414:GLU:OE1	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	418/438 (95%)	351 (84%)	52 (12%)	15 (4%)	4	28
1	B	415/438 (95%)	348 (84%)	56 (14%)	11 (3%)	6	35
All	All	833/876 (95%)	699 (84%)	108 (13%)	26 (3%)	5	32

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	ILE
1	A	421	ASP
1	B	421	ASP
1	A	341	LYS
1	A	431	LEU
1	B	49	ILE
1	B	249	LYS
1	B	341	LYS
1	A	33	PHE
1	A	103	ASP
1	A	119	PRO
1	A	191	ALA
1	A	340	GLU
1	B	33	PHE
1	B	103	ASP
1	B	119	PRO
1	B	340	GLU
1	A	35	VAL
1	A	397	VAL
1	A	249	LYS
1	B	35	VAL
1	B	397	VAL
1	A	158	PRO
1	A	329	ASP
1	B	71	GLY
1	A	71	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	376/389 (97%)	329 (88%)	47 (12%)	6	24
1	B	373/389 (96%)	328 (88%)	45 (12%)	6	26
All	All	749/778 (96%)	657 (88%)	92 (12%)	6	25

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	19	VAL
1	A	26	GLU
1	A	29	HIS
1	A	30	GLU
1	A	33	PHE
1	A	41	VAL
1	A	62	SER
1	A	68	ASP
1	A	77	LYS
1	A	83	ARG
1	A	95	VAL
1	A	97	GLN
1	A	99	ILE
1	A	106	GLU
1	A	107	ILE
1	A	118	VAL
1	A	129	ARG
1	A	134	LEU
1	A	153	THR
1	A	163	SER
1	A	164	LEU
1	A	165	ARG
1	A	170	GLU
1	A	186	GLU
1	A	189	LEU
1	A	194	THR
1	A	202	TYR
1	A	204	LYS
1	A	207	LEU
1	A	213	ARG
1	A	233	LEU
1	A	239	SER
1	A	268	ARG
1	A	330	GLU
1	A	338	LEU
1	A	339	LYS
1	A	345	GLU
1	A	355	LEU
1	A	357	LEU
1	A	367	ASP
1	A	384	LYS

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Mol	Chain	Res	Type
1	A	385	PHE
1	A	408	LYS
1	A	411	ASP
1	A	430	ILE
1	A	431	LEU
1	B	8	LEU
1	B	19	VAL
1	B	26	GLU
1	B	29	HIS
1	B	30	GLU
1	B	33	PHE
1	B	41	VAL
1	B	62	SER
1	B	68	ASP
1	B	77	LYS
1	B	83	ARG
1	B	95	VAL
1	B	99	ILE
1	B	106	GLU
1	B	107	ILE
1	B	127	ARG
1	B	129	ARG
1	B	133	ASP
1	B	134	LEU
1	B	153	THR
1	B	163	SER
1	B	164	LEU
1	B	165	ARG
1	B	186	GLU
1	B	189	LEU
1	B	194	THR
1	B	202	TYR
1	B	204	LYS
1	B	207	LEU
1	B	213	ARG
1	B	233	LEU
1	B	239	SER
1	B	268	ARG
1	B	330	GLU
1	B	338	LEU
1	B	339	LYS
1	B	345	GLU

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Mol	Chain	Res	Type
1	B	355	LEU
1	B	357	LEU
1	B	367	ASP
1	B	384	LYS
1	B	385	PHE
1	B	408	LYS
1	B	411	ASP
1	B	429	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	B	192	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	FS5	A	501	1	2,30,30	0.78	0	1,59,59	2.53	1 (100%)
2	FS5	B	501	1	2,30,30	0.34	0	1,59,59	2.89	1 (100%)

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	FS5	A	501	1	-	0/0/118/118	0/12/10/10
2	FS5	B	501	1	-	0/0/118/118	0/12/10/10

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	501	FS5	S10-S11-S12	2.53	118.25	106.19
2	B	501	FS5	S10-S11-S12	2.89	120.00	106.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FS5	2	0
2	B	501	FS5	5	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	424/438 (96%)	0.04	5 (1%) 81 76	37, 94, 140, 201	0
1	B	421/438 (96%)	0.22	20 (4%) 34 28	45, 95, 140, 201	0
All	All	845/876 (96%)	0.13	25 (2%) 54 47	37, 94, 140, 201	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	VAL	5.5
1	B	72	TYR	5.4
1	B	31	ILE	4.7
1	B	27	GLY	4.6
1	B	30	GLU	4.5
1	A	35	VAL	4.5
1	B	33	PHE	3.6
1	A	50	GLU	3.4
1	B	35	VAL	3.4
1	B	70	TYR	3.2
1	B	3	VAL	3.1
1	B	63	PHE	3.1
1	B	74	LEU	3.0
1	B	36	LYS	3.0
1	B	73	LYS	2.9
1	B	37	ASP	2.7
1	B	187	ILE	2.7
1	A	44	ASP	2.6
1	A	102	ALA	2.5
1	B	40	VAL	2.5
1	B	71	GLY	2.2
1	A	107	ILE	2.1
1	B	406	LYS	2.1
1	B	68	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	24	LEU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
2	FS5	B	501	21/21	0.99	0.17	-1.19	51,68,84,93	5
2	FS5	A	501	21/21	0.99	0.14	-1.46	2,56,90,101	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.