



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:13 PM GMT

PDB ID : 3WFP
Title : tRNA processing enzyme (apo form 2)
Authors : Yamashita, S.; Takeshita, D.; Tomita, K.
Deposited on : 2013-07-23
Resolution : 4.00 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

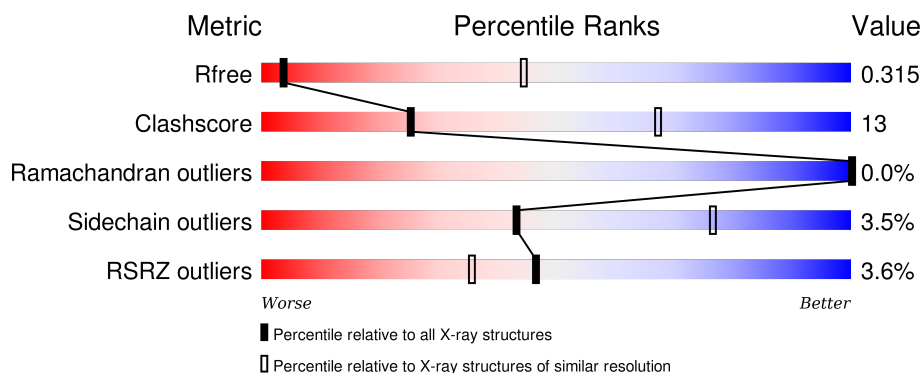
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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))
R_{free}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	<div> <div></div> <div> <div></div> <div>65%</div> <div>24%</div> <div>8%</div> </div> </div>
1	B	497	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>9%</div> </div> </div>
1	C	497	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>20%</div> <div>16%</div> </div> </div>
1	D	497	<div> <div></div> <div> <div></div> <div>64%</div> <div>19%</div> <div>16%</div> </div> </div>
1	E	497	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>21%</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	497	
1	G	497	
1	H	497	

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
2	SO4	B	1001	-	-	-	X
2	SO4	C	1001	-	-	X	X
2	SO4	G	1001	-	-	-	X
2	SO4	H	1001	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27564 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 Poly A polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3624	2334	624	659	7			
1	B	450	Total	C	N	O	S	0	0	0
			3568	2296	611	654	7			
1	C	419	Total	C	N	O	S	0	0	0
			3436	2222	588	619	7			
1	D	419	Total	C	N	O	S	0	0	0
			3436	2222	588	619	7			
1	E	411	Total	C	N	O	S	0	0	0
			3365	2175	572	611	7			
1	F	411	Total	C	N	O	S	0	0	0
			3365	2175	572	611	7			
1	G	411	Total	C	N	O	S	0	0	0
			3365	2175	572	611	7			
1	H	411	Total	C	N	O	S	0	0	0
			3365	2175	572	611	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	EXPRESSION TAG	UNP O67911
B	16	MET	-	EXPRESSION TAG	UNP O67911
C	16	MET	-	EXPRESSION TAG	UNP O67911
D	16	MET	-	EXPRESSION TAG	UNP O67911
E	16	MET	-	EXPRESSION TAG	UNP O67911
F	16	MET	-	EXPRESSION TAG	UNP O67911
G	16	MET	-	EXPRESSION TAG	UNP O67911
H	16	MET	-	EXPRESSION TAG	UNP O67911

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

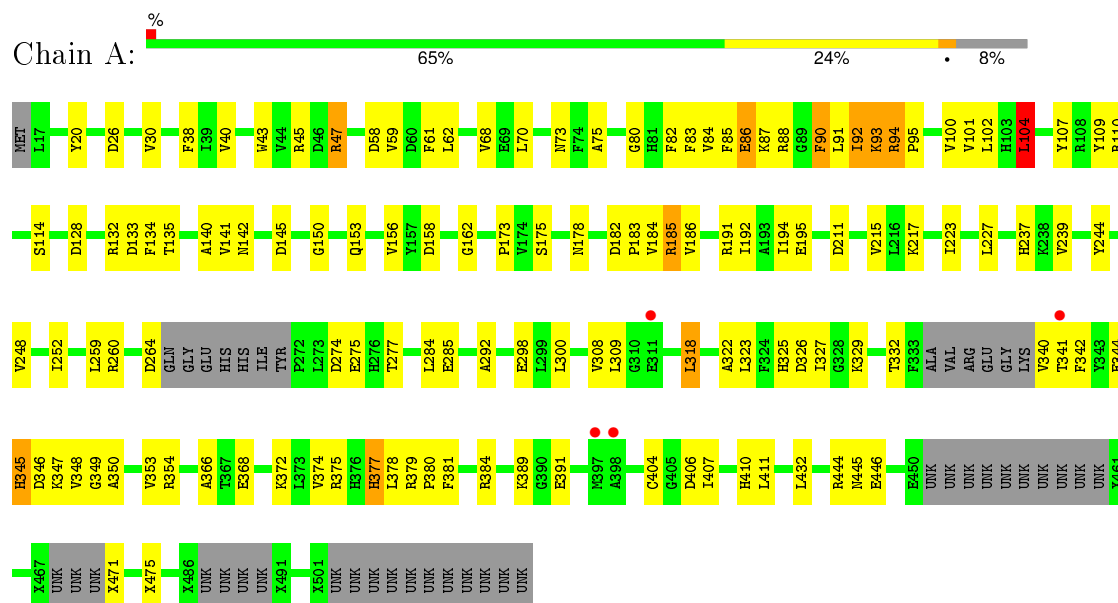


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

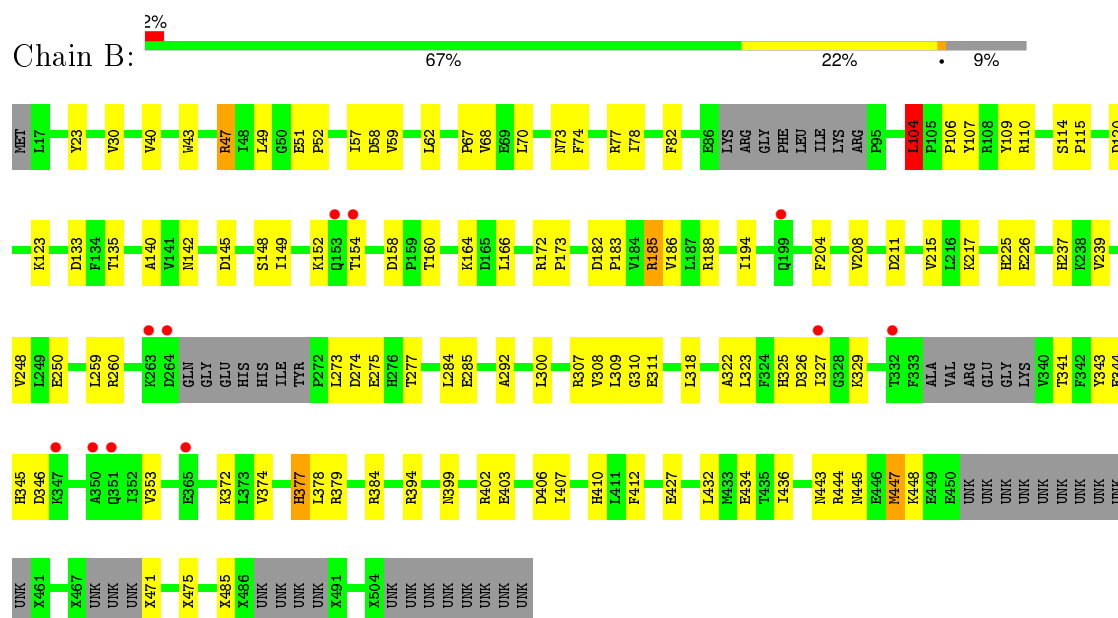
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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: Poly A polymerase



- Molecule 1: Poly A polymerase

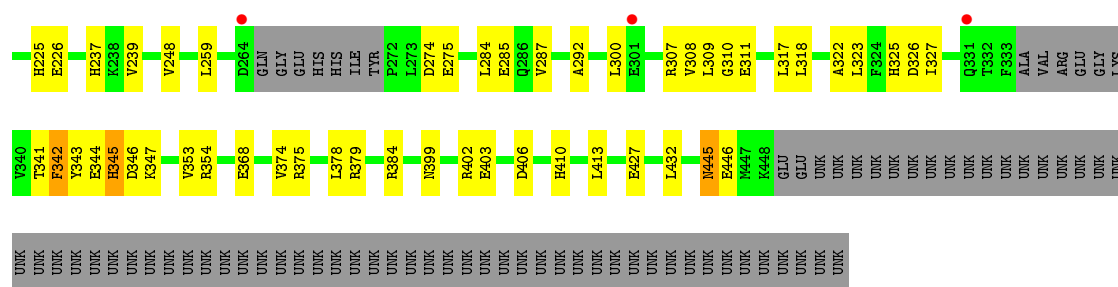


[illegible]

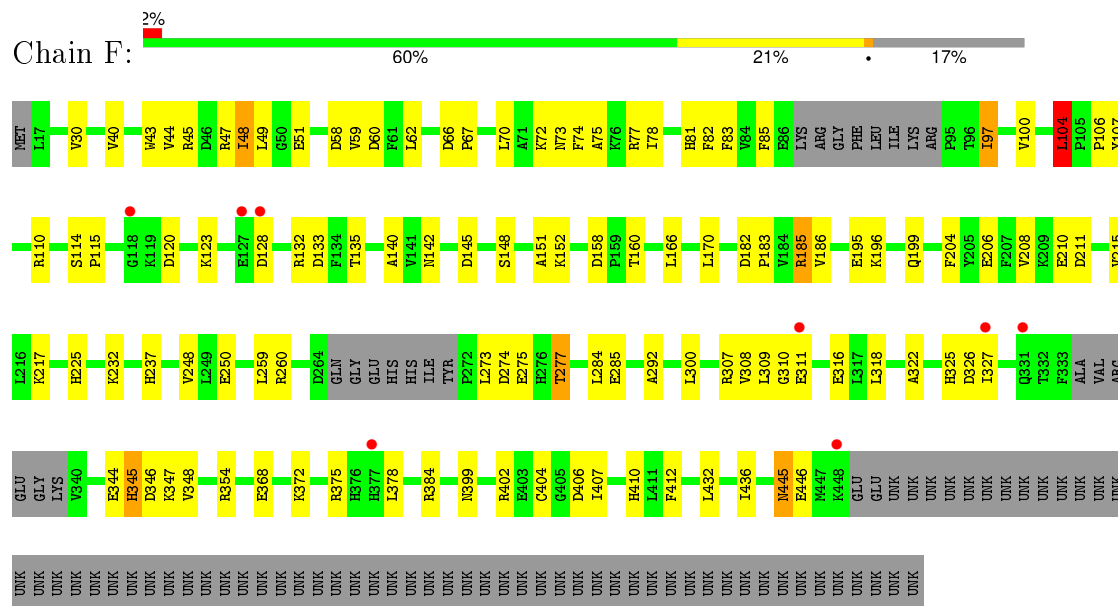
Chain D: 

Chain E:

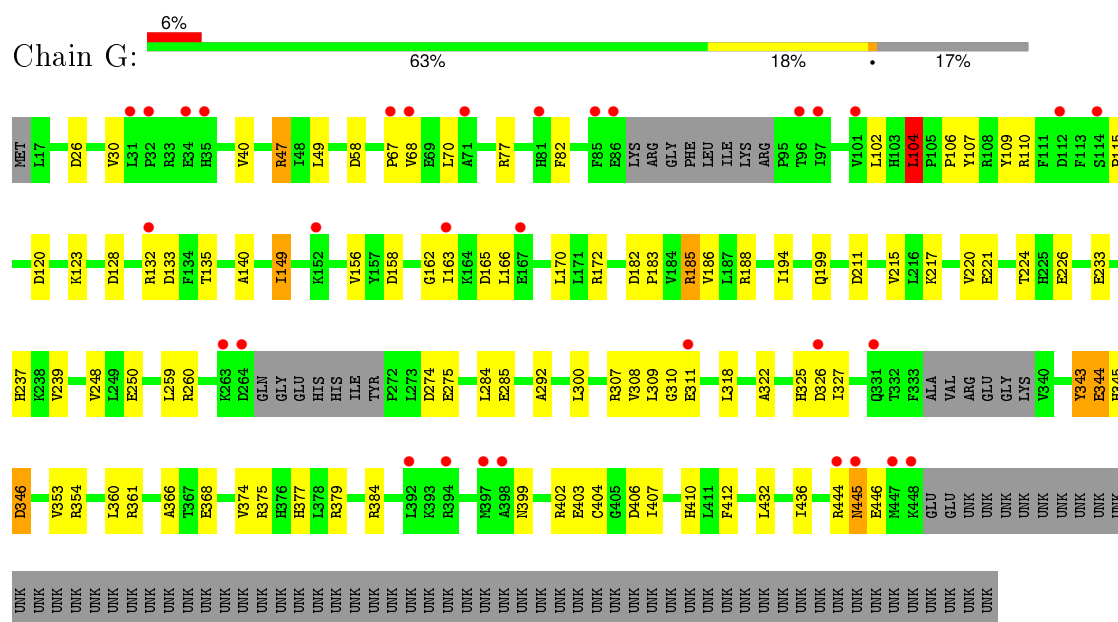
Sequence logo for Chain E showing amino acid frequencies across 100 positions. The y-axis represents frequency in bits (0.00 to 0.15). The x-axis shows positions 1 to 100. A color key at the top indicates: MET (grey), LYS (red), ARG (orange), GLY (yellow), PHE (green), LEU (blue), ILE (cyan), LYS (dark blue), ARG (dark green), and P95 (light green). The sequence is: MET, L17, D25, K29, V30, L31, P32, V40, P43, R47, L48, L49, D58, V59, D60, P61, L62, T63, T64, D65, P66, P67, V68, S69, L70, H81, F82, F85, E86, LYS, ARG, GLY, PHE, LEU, ILE, LYS, ARG, P95, V101, L102, L103, L104, P105, P106, Y107, Y108, Y109, R110, S114, R115. Notable peaks are at positions 17, 32, 47, 63, 86, and 104.



• Molecule 1: Poly A polymerase



• Molecule 1: Poly A polymerase



• Molecule 1: Poly A polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	126.91Å 138.36Å 147.62Å 90.00° 111.04° 90.00°	Depositor
Resolution (Å)	19.97 – 4.00 48.81 – 4.01	Depositor EDS
% Data completeness (in resolution range)	86.8 (19.97-4.00) 76.7 (48.81-4.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.258 , 0.314 0.260 , 0.315	Depositor DCC
R_{free} test set	1755 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 107.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	2 of 34980 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	27564	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: SO4

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	0.24	0/3527	0.42	1/4750 (0.0%)
1	B	0.23	0/3454	0.42	1/4653 (0.0%)
1	C	0.23	0/3509	0.42	1/4726 (0.0%)
1	D	0.26	0/3509	0.45	2/4726 (0.0%)
1	E	0.22	0/3436	0.40	2/4629 (0.0%)
1	F	0.27	0/3436	0.46	2/4629 (0.0%)
1	G	0.23	0/3436	0.42	2/4629 (0.0%)
1	H	0.22	0/3436	0.40	1/4629 (0.0%)
All	All	0.24	0/27743	0.42	12/37371 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	94	ARG	C-N-CD	5.83	140.64	128.40
1	B	104	LEU	CA-CB-CG	5.72	128.45	115.30
1	G	104	LEU	CA-CB-CG	5.71	128.43	115.30
1	F	104	LEU	CA-CB-CG	5.70	128.41	115.30
1	H	104	LEU	CA-CB-CG	5.70	128.41	115.30
1	D	104	LEU	CA-CB-CG	5.68	128.38	115.30
1	E	104	LEU	CA-CB-CG	5.68	128.37	115.30
1	E	85	PHE	CB-CA-C	-5.64	99.12	110.40
1	C	104	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	104	LEU	CA-CB-CG	5.48	127.90	115.30
1	F	48	ILE	CG1-CB-CG2	-5.40	99.52	111.40
1	G	346	ASP	CB-CA-C	-5.07	100.25	110.40

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	3624	0	3522	107	0
1	B	3568	0	3439	80	0
1	C	3436	0	3470	104	0
1	D	3436	0	3470	107	0
1	E	3365	0	3384	76	0
1	F	3365	0	3384	96	0
1	G	3365	0	3384	84	0
1	H	3365	0	3384	59	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	2	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
2	G	5	0	0	0	0
2	H	5	0	0	2	0
All	All	27564	0	27437	690	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 13.

All (690) 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:92:ILE:HD12	1:A:93:LYS:N	1.27	1.41
1:C:345:HIS:HD2	1:C:346:ASP:N	1.30	1.28
1:C:345:HIS:CD2	1:C:346:ASP:H	1.57	1.20
1:A:92:ILE:CD1	1:A:93:LYS:H	1.55	1.19
1:C:345:HIS:CD2	1:C:346:ASP:N	2.10	1.16
1:D:86:GLU:HG3	1:D:94:ARG:HG3	1.28	1.15
1:D:308:VAL:HG12	1:D:309:LEU:HD13	1.27	1.14
1:D:133:ASP:HB3	1:D:185:ARG:HD3	1.25	1.14
1:F:347:LYS:HE3	1:F:375:ARG:HE	0.97	1.09
1:A:90:PHE:O	1:A:91:LEU:HG	1.56	1.05
1:E:308:VAL:HG12	1:E:309:LEU:HD13	1.37	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:LEU:HD11	1:F:196:LYS:HB3	1.40	1.04
1:G:325:HIS:CD2	1:G:377:HIS:HE1	1.77	1.03
1:D:90:PHE:CZ	1:D:222:ARG:HD3	1.93	1.03
1:G:221:GLU:HG3	1:G:361:ARG:HH11	1.21	1.02
1:A:92:ILE:CD1	1:A:93:LYS:N	2.20	0.99
1:F:347:LYS:HE3	1:F:375:ARG:NE	1.76	0.99
1:G:308:VAL:HG12	1:G:309:LEU:HD13	1.45	0.99
1:D:184:VAL:CG1	1:D:222:ARG:HH21	1.76	0.97
1:C:152:LYS:HE2	1:C:152:LYS:HA	1.46	0.97
1:C:308:VAL:HG12	1:C:309:LEU:HD13	1.46	0.96
1:E:347:LYS:HG2	1:E:375:ARG:NE	1.80	0.96
1:D:90:PHE:HE1	1:D:218:SER:CB	1.77	0.95
1:D:184:VAL:HG12	1:D:222:ARG:HH21	1.27	0.95
1:F:49:LEU:HD12	1:F:196:LYS:HD2	1.49	0.95
1:A:91:LEU:HB3	1:A:92:ILE:HA	1.49	0.95
1:D:183:PRO:HG3	1:D:217:LYS:HB2	1.46	0.94
1:C:155:ILE:HD12	1:C:156:VAL:H	1.33	0.94
1:G:325:HIS:CD2	1:G:377:HIS:CE1	2.56	0.93
1:D:90:PHE:CE2	1:D:222:ARG:HD3	2.05	0.92
1:C:155:ILE:HD12	1:C:156:VAL:N	1.85	0.91
1:D:90:PHE:CZ	1:D:222:ARG:CD	2.54	0.90
1:C:308:VAL:CG1	1:C:309:LEU:HD13	2.02	0.90
1:D:90:PHE:HE1	1:D:218:SER:HB2	1.38	0.89
1:C:183:PRO:HG3	1:C:217:LYS:HB2	1.53	0.88
1:F:347:LYS:CE	1:F:375:ARG:HE	1.85	0.88
1:F:44:VAL:HG12	1:F:48:ILE:HD12	1.56	0.88
1:E:341:THR:HG1	1:E:343:TYR:HE2	0.98	0.88
1:D:90:PHE:CZ	1:D:222:ARG:NE	2.42	0.87
1:F:346:ASP:OD1	1:F:347:LYS:N	2.08	0.86
1:G:325:HIS:HD2	1:G:377:HIS:CE1	1.92	0.86
1:F:49:LEU:CD1	1:F:196:LYS:HD2	2.05	0.85
1:F:75:ALA:HB3	1:F:82:PHE:CE1	2.11	0.85
1:D:133:ASP:CB	1:D:185:ARG:HD3	2.07	0.84
1:D:133:ASP:HB3	1:D:185:ARG:CD	2.06	0.84
1:B:341:THR:OG1	1:B:343:TYR:HE2	1.59	0.83
1:D:332:THR:OG1	1:D:342:PHE:HB3	1.79	0.83
1:B:341:THR:HG1	1:B:343:TYR:HE2	1.23	0.82
1:G:344:GLU:OE2	1:G:344:GLU:N	2.13	0.82
1:C:151:ALA:HB2	1:D:427:GLU:HG3	1.61	0.82
1:D:308:VAL:CG1	1:D:309:LEU:HD13	2.08	0.81
1:A:345:HIS:CE1	1:A:346:ASP:OD1	2.34	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:VAL:HG12	1:D:222:ARG:NH2	1.96	0.80
1:E:308:VAL:HG12	1:E:309:LEU:CD1	2.12	0.80
1:F:75:ALA:HA	1:F:78:ILE:HG12	1.62	0.80
1:D:308:VAL:HG12	1:D:309:LEU:CD1	2.11	0.79
1:D:184:VAL:CG1	1:D:222:ARG:NH2	2.46	0.79
1:E:183:PRO:HG3	1:E:217:LYS:HB2	1.64	0.79
1:D:86:GLU:CG	1:D:94:ARG:HG3	2.11	0.79
1:B:183:PRO:HG3	1:B:217:LYS:HB2	1.65	0.78
1:G:183:PRO:HG3	1:G:217:LYS:HB2	1.65	0.78
1:A:183:PRO:HG3	1:A:217:LYS:HB2	1.66	0.77
1:F:49:LEU:HB3	1:F:51:GLU:HG3	1.67	0.77
1:G:221:GLU:CG	1:G:361:ARG:HH11	1.98	0.77
1:D:90:PHE:HZ	1:D:222:ARG:HD3	1.49	0.77
1:H:183:PRO:HG3	1:H:217:LYS:HB2	1.68	0.76
1:F:44:VAL:HG12	1:F:48:ILE:CD1	2.14	0.76
1:C:149:ILE:HD13	1:C:149:ILE:H	1.51	0.76
1:B:447:MET:SD	1:B:447:MET:N	2.58	0.76
1:F:347:LYS:HG2	1:F:375:ARG:NE	2.01	0.75
1:G:308:VAL:HG12	1:G:309:LEU:CD1	2.15	0.75
1:A:90:PHE:O	1:A:91:LEU:CG	2.31	0.75
1:E:308:VAL:CG1	1:E:309:LEU:HD13	2.15	0.75
1:B:225:HIS:NE2	1:B:311:GLU:OE2	2.20	0.75
1:G:346:ASP:O	1:G:375:ARG:HA	1.86	0.75
1:F:345:HIS:O	1:F:346:ASP:C	2.23	0.74
1:E:347:LYS:HG2	1:E:375:ARG:CD	2.16	0.74
1:D:184:VAL:HG23	1:D:187:LEU:HD12	1.70	0.74
1:C:225:HIS:NE2	1:C:311:GLU:OE2	2.21	0.74
1:C:345:HIS:HD2	1:C:346:ASP:H	0.77	0.74
1:E:341:THR:OG1	1:E:343:TYR:HE2	1.71	0.73
1:D:90:PHE:CE1	1:D:218:SER:HB2	2.22	0.73
1:E:225:HIS:NE2	1:E:311:GLU:OE2	2.21	0.73
1:E:309:LEU:HD12	1:E:309:LEU:N	2.02	0.73
1:C:151:ALA:HB2	1:D:427:GLU:CG	2.19	0.73
1:B:308:VAL:HG12	1:B:309:LEU:HD13	1.70	0.73
1:D:91:LEU:O	1:D:91:LEU:HG	1.89	0.72
1:C:215:VAL:HG21	1:C:248:VAL:HG13	1.72	0.72
1:G:343:TYR:C	1:G:344:GLU:OE2	2.29	0.71
1:B:148:SER:OG	1:B:152:LYS:NZ	2.22	0.71
1:H:250:GLU:OE2	1:H:260:ARG:NH2	2.20	0.71
1:C:71:ALA:HB3	1:C:82:PHE:HE1	1.56	0.70
1:G:221:GLU:HG3	1:G:361:ARG:NH1	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:ASP:O	1:G:375:ARG:HD2	1.92	0.69
1:D:86:GLU:HG3	1:D:94:ARG:CG	2.17	0.69
1:D:90:PHE:CE2	1:D:222:ARG:CD	2.76	0.69
1:D:90:PHE:CD2	1:D:94:ARG:NH2	2.61	0.69
1:B:309:LEU:N	1:B:309:LEU:HD12	2.07	0.68
1:E:308:VAL:CG1	1:E:309:LEU:CD1	2.72	0.68
1:D:250:GLU:OE2	1:D:260:ARG:NH2	2.27	0.68
1:F:237:HIS:ND1	1:F:285:GLU:OE1	2.26	0.68
1:F:183:PRO:HG3	1:F:217:LYS:HB2	1.75	0.68
1:F:345:HIS:O	1:F:348:VAL:N	2.27	0.68
1:F:83:PHE:HB3	1:F:85:PHE:HE2	1.59	0.68
1:G:325:HIS:HB2	1:G:377:HIS:CE1	2.29	0.67
1:C:149:ILE:HG12	1:C:150:GLY:N	2.10	0.67
1:F:30:VAL:HG13	1:F:73:ASN:HB2	1.75	0.67
1:A:332:THR:CG2	1:A:345:HIS:HB3	2.24	0.67
1:D:346:ASP:N	1:D:346:ASP:OD1	2.22	0.67
1:D:345:HIS:HD2	1:D:346:ASP:N	1.93	0.67
1:E:354:ARG:NH1	1:E:368:GLU:OE1	2.28	0.67
1:C:82:PHE:CZ	1:C:84:VAL:HG21	2.30	0.67
1:C:151:ALA:O	1:C:152:LYS:HB2	1.95	0.67
1:D:225:HIS:NE2	1:D:311:GLU:OE2	2.27	0.67
1:F:49:LEU:HD11	1:F:196:LYS:CB	2.20	0.67
1:G:308:VAL:CG1	1:G:309:LEU:HD13	2.23	0.66
1:A:298:GLU:CD	1:A:444:ARG:HD2	2.16	0.66
1:D:89:GLY:O	1:D:94:ARG:HD3	1.95	0.66
1:C:309:LEU:HD12	1:C:309:LEU:N	2.11	0.66
1:B:448:LYS:HB3	1:B:448:LYS:HZ2	1.59	0.65
1:A:308:VAL:HG12	1:A:309:LEU:HD12	1.79	0.65
1:C:153:GLN:HA	1:C:153:GLN:OE1	1.97	0.64
1:D:215:VAL:HG21	1:D:248:VAL:HG13	1.79	0.64
1:D:90:PHE:CE1	1:D:218:SER:CB	2.70	0.64
1:F:347:LYS:HG2	1:F:375:ARG:CD	2.28	0.64
1:D:237:HIS:ND1	1:D:285:GLU:OE1	2.29	0.64
1:A:347:LYS:HG2	1:A:375:ARG:CZ	2.28	0.64
1:A:347:LYS:HG2	1:A:375:ARG:NE	2.13	0.63
1:C:250:GLU:OE2	1:C:260:ARG:NH2	2.27	0.63
1:C:71:ALA:CB	1:C:82:PHE:HE1	2.12	0.63
1:H:30:VAL:HG12	1:H:70:LEU:HD12	1.79	0.63
1:D:90:PHE:HZ	1:D:222:ARG:CD	2.07	0.63
1:B:448:LYS:HB3	1:B:448:LYS:NZ	2.13	0.63
1:A:308:VAL:HG11	1:A:366:ALA:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:LEU:HD22	1:E:322:ALA:HB2	1.81	0.63
1:H:40:VAL:HG13	1:H:140:ALA:HB2	1.81	0.63
1:D:184:VAL:HG11	1:D:222:ARG:HH21	1.61	0.63
1:F:284:LEU:HD22	1:F:322:ALA:HB2	1.80	0.63
1:F:225:HIS:NE2	1:F:311:GLU:OE2	2.32	0.63
1:A:445:ASN:ND2	1:B:77:ARG:O	2.27	0.62
1:G:284:LEU:HD22	1:G:322:ALA:HB2	1.81	0.62
1:B:284:LEU:HD22	1:B:322:ALA:HB2	1.81	0.62
1:F:250:GLU:OE2	1:F:260:ARG:NH2	2.30	0.62
1:C:30:VAL:HG12	1:C:70:LEU:HD12	1.81	0.62
1:C:151:ALA:HB2	1:D:427:GLU:CD	2.20	0.62
1:F:30:VAL:HG21	1:F:74:PHE:HA	1.81	0.62
1:F:40:VAL:HG13	1:F:140:ALA:HB2	1.82	0.62
1:E:341:THR:OG1	1:E:343:TYR:CE2	2.43	0.62
1:G:343:TYR:HB3	1:G:344:GLU:OE2	2.00	0.61
1:A:128:ASP:OD1	1:A:132:ARG:NH1	2.32	0.61
1:G:237:HIS:ND1	1:G:285:GLU:OE1	2.31	0.61
1:B:30:VAL:HG12	1:B:70:LEU:HD12	1.82	0.61
1:F:44:VAL:O	1:F:48:ILE:HG13	1.99	0.61
1:G:221:GLU:HG3	1:G:361:ARG:HD2	1.83	0.61
1:B:308:VAL:CG1	1:B:309:LEU:HD13	2.31	0.61
1:G:445:ASN:OD1	1:H:77:ARG:NH2	2.34	0.61
1:C:284:LEU:HD22	1:C:322:ALA:HB2	1.81	0.61
1:H:225:HIS:NE2	1:H:311:GLU:OE2	2.34	0.61
1:G:379:ARG:NH1	1:G:403:GLU:OE1	2.29	0.61
1:C:345:HIS:O	1:C:346:ASP:C	2.37	0.61
1:A:345:HIS:O	1:A:348:VAL:N	2.34	0.60
1:A:94:ARG:HD3	1:A:95:PRO:HD2	1.83	0.60
1:G:250:GLU:OE2	1:G:260:ARG:NH2	2.27	0.60
1:A:26:ASP:OD1	1:B:444:ARG:NH2	2.31	0.60
1:D:30:VAL:HG12	1:D:70:LEU:HD12	1.83	0.60
1:G:346:ASP:HB3	1:G:375:ARG:O	2.01	0.60
1:C:237:HIS:ND1	1:C:285:GLU:OE1	2.32	0.60
1:C:40:VAL:HG13	1:C:140:ALA:HB2	1.81	0.60
1:H:284:LEU:HD22	1:H:322:ALA:HB2	1.83	0.60
1:A:345:HIS:O	1:A:348:VAL:HB	2.02	0.60
1:F:62:LEU:HD23	1:F:114:SER:HB2	1.84	0.60
1:E:237:HIS:ND1	1:E:285:GLU:OE1	2.32	0.60
1:D:284:LEU:HD22	1:D:322:ALA:HB2	1.82	0.60
1:D:182:ASP:OD1	1:D:222:ARG:NH2	2.34	0.59
1:G:307:ARG:NH2	1:G:310:GLY:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:PHE:HB2	1:C:94:ARG:HB2	1.84	0.59
1:C:427:GLU:HB3	1:D:149:ILE:O	2.01	0.59
1:C:49:LEU:HD21	1:C:166:LEU:HD22	1.84	0.59
1:F:49:LEU:HD12	1:F:51:GLU:CD	2.22	0.59
1:B:399:ASN:OD1	1:B:402:ARG:NH2	2.36	0.59
1:G:40:VAL:HG13	1:G:140:ALA:HB2	1.84	0.59
1:E:347:LYS:CG	1:E:375:ARG:NE	2.63	0.59
1:C:84:VAL:O	1:C:84:VAL:HG12	2.02	0.59
1:C:345:HIS:CD2	1:C:346:ASP:OD1	2.56	0.59
1:E:40:VAL:HG13	1:E:140:ALA:HB2	1.85	0.59
1:D:90:PHE:CZ	1:D:222:ARG:CZ	2.85	0.59
1:C:82:PHE:CZ	1:C:84:VAL:CG2	2.85	0.59
1:H:237:HIS:ND1	1:H:285:GLU:OE1	2.34	0.59
1:E:30:VAL:HG12	1:E:70:LEU:HD12	1.84	0.58
1:H:307:ARG:NH2	1:H:310:GLY:O	2.36	0.58
1:A:92:ILE:O	1:A:93:LYS:C	2.42	0.58
1:F:259:LEU:HD21	1:F:327:ILE:HD12	1.84	0.58
1:C:344:GLU:HG3	1:C:344:GLU:O	2.02	0.58
1:B:40:VAL:HG13	1:B:140:ALA:HB2	1.85	0.58
1:H:45:ARG:NH2	2:H:1001:SO4:O1	2.32	0.58
1:G:67:PRO:HG2	1:G:115:PRO:HG3	1.86	0.58
1:F:354:ARG:NH1	1:F:368:GLU:OE1	2.37	0.58
1:C:81:HIS:N	1:C:101:VAL:O	2.35	0.58
1:C:151:ALA:CB	1:D:427:GLU:HG3	2.33	0.58
1:A:444:ARG:NH2	1:B:78:ILE:O	2.37	0.57
1:A:308:VAL:HG12	1:A:309:LEU:CD1	2.35	0.57
1:C:384:ARG:HD3	1:C:432:LEU:HB2	1.86	0.57
1:E:399:ASN:OD1	1:E:402:ARG:NH2	2.37	0.57
1:E:345:HIS:HD2	1:E:346:ASP:H	1.51	0.57
1:C:82:PHE:CE2	1:C:84:VAL:HG23	2.39	0.57
1:C:47:ARG:NH1	1:C:51:GLU:O	2.38	0.57
1:D:307:ARG:NH2	1:D:310:GLY:O	2.34	0.57
1:E:345:HIS:CD2	1:E:346:ASP:N	2.73	0.57
1:F:72:LYS:HA	1:F:82:PHE:CE1	2.39	0.57
1:C:345:HIS:O	1:C:348:VAL:N	2.37	0.56
1:B:250:GLU:OE2	1:B:260:ARG:NH2	2.38	0.56
1:A:90:PHE:C	1:A:91:LEU:HG	2.25	0.56
1:D:342:PHE:CD2	1:D:342:PHE:N	2.73	0.56
1:G:30:VAL:HG12	1:G:70:LEU:HD12	1.86	0.56
1:A:237:HIS:ND1	1:A:285:GLU:OE1	2.36	0.56
1:D:40:VAL:HG13	1:D:140:ALA:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:PHE:CE1	1:D:218:SER:HA	2.40	0.56
1:G:183:PRO:HB2	1:G:215:VAL:HA	1.88	0.56
1:C:82:PHE:CE2	1:C:84:VAL:CG2	2.88	0.56
1:E:342:PHE:CD2	1:E:342:PHE:N	2.73	0.56
1:D:345:HIS:CD2	1:D:346:ASP:N	2.73	0.56
1:E:384:ARG:HD3	1:E:432:LEU:HB2	1.87	0.56
1:E:307:ARG:NH2	1:E:310:GLY:O	2.36	0.56
1:G:77:ARG:NH2	1:H:445:ASN:OD1	2.38	0.56
1:F:345:HIS:ND1	1:F:346:ASP:N	2.53	0.55
1:C:307:ARG:NH2	1:C:310:GLY:O	2.37	0.55
1:E:67:PRO:HG2	1:E:115:PRO:HG3	1.87	0.55
1:A:354:ARG:NH1	1:A:368:GLU:OE1	2.40	0.55
1:A:133:ASP:N	1:A:133:ASP:OD1	2.40	0.55
1:A:332:THR:HG21	1:A:345:HIS:HB3	1.88	0.55
1:A:284:LEU:HD22	1:A:322:ALA:HB2	1.88	0.55
1:F:307:ARG:NH2	1:F:310:GLY:O	2.34	0.55
1:B:406:ASP:N	1:B:406:ASP:OD1	2.39	0.55
1:H:399:ASN:OD1	1:H:402:ARG:NH2	2.39	0.55
1:D:309:LEU:N	1:D:309:LEU:HD12	2.21	0.55
1:F:58:ASP:OD2	1:F:110:ARG:HD3	2.07	0.55
1:F:97:ILE:HG22	1:F:114:SER:HA	1.89	0.55
1:B:341:THR:OG1	1:B:343:TYR:CE2	2.41	0.55
1:B:183:PRO:HB2	1:B:215:VAL:HA	1.89	0.54
1:D:399:ASN:OD1	1:D:402:ARG:NH2	2.40	0.54
1:D:318:LEU:HG	1:D:410:HIS:HB3	1.88	0.54
1:F:399:ASN:OD1	1:F:402:ARG:NH2	2.40	0.54
1:C:332:THR:OG1	1:C:342:PHE:HB3	2.07	0.54
1:D:156:VAL:HG21	1:D:163:ILE:HD11	1.88	0.54
1:A:347:LYS:HD3	1:A:375:ARG:NH2	2.22	0.54
1:C:58:ASP:OD2	1:C:110:ARG:HD3	2.07	0.54
1:B:318:LEU:HG	1:B:410:HIS:HB3	1.89	0.54
1:H:384:ARG:HD3	1:H:432:LEU:HB2	1.89	0.54
1:G:345:HIS:O	1:G:346:ASP:HB2	2.07	0.54
1:A:318:LEU:HG	1:A:410:HIS:HB3	1.90	0.54
1:F:384:ARG:HD3	1:F:432:LEU:HB2	1.87	0.54
1:G:26:ASP:OD1	1:H:444:ARG:NH2	2.41	0.54
1:A:329:LYS:HE3	1:A:342:PHE:CD2	2.42	0.54
1:D:67:PRO:HG2	1:D:115:PRO:HG3	1.89	0.54
1:C:345:HIS:HD2	1:C:346:ASP:CA	2.17	0.54
1:D:353:VAL:HG21	1:D:374:VAL:HG21	1.89	0.54
1:G:308:VAL:CG1	1:G:309:LEU:CD1	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LYS:HA	1:A:345:HIS:HD2	1.73	0.54
1:F:308:VAL:HG12	1:F:309:LEU:HD13	1.90	0.54
1:A:43:TRP:CD1	1:A:59:VAL:HG22	2.43	0.53
1:B:346:ASP:N	1:B:346:ASP:OD1	2.40	0.53
1:C:345:HIS:NE2	1:C:346:ASP:OD1	2.42	0.53
1:B:49:LEU:HD21	1:B:166:LEU:HD22	1.90	0.53
1:G:399:ASN:OD1	1:G:402:ARG:NH2	2.41	0.53
1:A:91:LEU:HB3	1:A:92:ILE:CA	2.31	0.53
1:D:346:ASP:CG	1:D:378:LEU:HD21	2.29	0.53
1:A:372:LYS:HG2	1:A:407:ILE:HD13	1.91	0.53
1:D:90:PHE:HE1	1:D:218:SER:CA	2.20	0.53
1:F:211:ASP:OD1	1:F:211:ASP:N	2.42	0.53
1:G:220:VAL:HG13	1:G:361:ARG:HD2	1.91	0.53
1:B:394:ARG:HH12	1:B:485:UNK:HA	1.74	0.53
1:F:67:PRO:HG2	1:F:115:PRO:HG3	1.90	0.53
1:F:45:ARG:NH2	2:F:1001:SO4:O2	2.42	0.53
1:F:75:ALA:HB3	1:F:82:PHE:HE1	1.73	0.53
1:H:318:LEU:HG	1:H:410:HIS:HB3	1.90	0.53
1:F:406:ASP:OD1	1:F:406:ASP:N	2.39	0.53
1:D:90:PHE:CE1	1:D:218:SER:CA	2.92	0.52
1:H:49:LEU:HD21	1:H:166:LEU:HD22	1.91	0.52
1:B:133:ASP:OD1	1:B:133:ASP:N	2.42	0.52
1:C:378:LEU:HD12	1:C:381:PHE:HD2	1.74	0.52
1:C:214:ILE:O	1:C:217:LYS:HG2	2.08	0.52
1:B:164:LYS:HZ2	1:E:81:HIS:CE1	2.26	0.52
1:H:135:THR:HG22	1:H:160:THR:HB	1.92	0.52
1:A:40:VAL:HG13	1:A:140:ALA:HB2	1.90	0.52
1:D:49:LEU:HD21	1:D:166:LEU:HD22	1.91	0.52
1:C:133:ASP:OD1	1:C:133:ASP:N	2.42	0.52
1:C:152:LYS:O	1:C:153:GLN:HG2	2.09	0.52
1:D:104:LEU:HD23	1:D:106:PRO:HD2	1.90	0.52
1:B:237:HIS:ND1	1:B:285:GLU:OE1	2.38	0.52
1:H:133:ASP:OD1	1:H:133:ASP:N	2.42	0.52
1:E:133:ASP:N	1:E:133:ASP:OD1	2.42	0.52
1:A:141:VAL:HG12	1:A:156:VAL:HG12	1.90	0.52
1:F:72:LYS:HA	1:F:82:PHE:CZ	2.45	0.52
1:A:104:LEU:HD22	1:A:107:TYR:H	1.74	0.52
1:C:309:LEU:CD1	1:C:309:LEU:N	2.73	0.52
1:E:58:ASP:OD2	1:E:110:ARG:HD3	2.08	0.52
1:C:308:VAL:CG1	1:C:309:LEU:CD1	2.83	0.52
1:D:104:LEU:HD22	1:D:107:TYR:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:ASN:OD1	1:C:402:ARG:NH2	2.41	0.52
1:D:133:ASP:OD1	1:D:133:ASP:N	2.42	0.52
1:F:104:LEU:HD22	1:F:107:TYR:H	1.75	0.52
1:F:133:ASP:OD1	1:F:133:ASP:N	2.43	0.52
1:A:329:LYS:HE3	1:A:342:PHE:CE2	2.45	0.52
1:E:345:HIS:CD2	1:E:346:ASP:H	2.27	0.52
1:C:308:VAL:HG13	1:C:309:LEU:HD13	1.88	0.52
1:D:142:ASN:HB3	1:D:145:ASP:OD2	2.10	0.52
1:B:58:ASP:OD2	1:B:110:ARG:HD3	2.10	0.52
1:G:406:ASP:OD1	1:G:406:ASP:N	2.39	0.52
1:H:379:ARG:NH1	1:H:403:GLU:OE1	2.37	0.51
1:D:92:ILE:O	1:D:92:ILE:HG22	2.10	0.51
1:G:133:ASP:OD1	1:G:133:ASP:N	2.42	0.51
1:F:135:THR:HG22	1:F:160:THR:HB	1.93	0.51
1:B:104:LEU:HD22	1:B:107:TYR:H	1.76	0.51
1:B:379:ARG:NH1	1:B:403:GLU:OE1	2.37	0.51
1:H:104:LEU:HD22	1:H:107:TYR:H	1.75	0.51
1:D:184:VAL:HG11	1:D:222:ARG:NH2	2.23	0.51
1:F:104:LEU:HD23	1:F:106:PRO:HD2	1.92	0.51
1:A:391:GLU:CG	1:D:258:ARG:HH12	2.24	0.51
1:C:318:LEU:HG	1:C:410:HIS:HB3	1.92	0.51
1:B:104:LEU:HD23	1:B:106:PRO:HD2	1.92	0.51
1:F:182:ASP:OD2	1:F:185:ARG:HD3	2.11	0.51
1:F:49:LEU:CD1	1:F:51:GLU:OE2	2.58	0.51
1:G:308:VAL:C	1:G:310:GLY:H	2.13	0.51
1:E:104:LEU:HD23	1:E:106:PRO:HD2	1.91	0.51
1:A:191:ARG:NH1	1:A:195:GLU:OE1	2.44	0.51
1:A:215:VAL:HG21	1:A:248:VAL:HG13	1.92	0.51
1:D:188:ARG:HG2	1:D:226:GLU:OE2	2.11	0.51
1:G:104:LEU:HD23	1:G:106:PRO:HD2	1.93	0.51
1:B:292:ALA:HA	1:B:300:LEU:HD11	1.93	0.51
1:G:346:ASP:O	1:G:375:ARG:CD	2.59	0.51
1:A:30:VAL:HG12	1:A:70:LEU:HD12	1.92	0.51
1:C:104:LEU:HD23	1:C:106:PRO:HD2	1.93	0.51
1:F:49:LEU:HD12	1:F:51:GLU:OE2	2.10	0.51
1:A:345:HIS:O	1:A:349:GLY:N	2.38	0.51
1:G:354:ARG:NH1	1:G:368:GLU:OE1	2.44	0.51
1:F:142:ASN:HB3	1:F:145:ASP:OD2	2.10	0.50
1:A:62:LEU:HD23	1:A:114:SER:HB2	1.93	0.50
1:B:309:LEU:N	1:B:309:LEU:CD1	2.73	0.50
1:C:104:LEU:HD22	1:C:107:TYR:H	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ARG:HG3	1:C:188:ARG:HD3	1.93	0.50
1:B:67:PRO:HG2	1:B:115:PRO:HG3	1.92	0.50
1:E:309:LEU:CD1	1:E:309:LEU:N	2.73	0.50
1:F:148:SER:HB3	1:F:152:LYS:HD2	1.93	0.50
1:G:353:VAL:HG21	1:G:374:VAL:HG21	1.94	0.50
1:A:90:PHE:O	1:A:91:LEU:CD2	2.60	0.50
1:E:215:VAL:HG21	1:E:248:VAL:HG13	1.91	0.50
1:G:58:ASP:OD2	1:G:110:ARG:HD3	2.12	0.50
1:E:49:LEU:HD21	1:E:166:LEU:HD22	1.94	0.50
1:G:308:VAL:HG11	1:G:366:ALA:HB2	1.93	0.50
1:G:104:LEU:HD22	1:G:107:TYR:H	1.76	0.50
1:A:353:VAL:HG21	1:A:374:VAL:HG21	1.92	0.50
1:B:68:VAL:HG13	1:B:82:PHE:HZ	1.76	0.50
1:F:49:LEU:CB	1:F:51:GLU:HG3	2.39	0.49
1:A:329:LYS:CA	1:A:345:HIS:HD2	2.25	0.49
1:F:73:ASN:O	1:F:77:ARG:HG3	2.12	0.49
1:H:58:ASP:OD2	1:H:110:ARG:HD3	2.11	0.49
1:E:104:LEU:HD22	1:E:107:TYR:H	1.78	0.49
1:B:384:ARG:HD3	1:B:432:LEU:HB2	1.93	0.49
1:C:258:ARG:NH1	1:C:331:GLN:HE22	2.11	0.49
1:G:221:GLU:CG	1:G:361:ARG:HD2	2.42	0.49
1:F:30:VAL:HG12	1:F:70:LEU:HD12	1.95	0.49
1:F:120:ASP:HB3	1:F:123:LYS:HB3	1.94	0.49
1:E:259:LEU:HD21	1:E:327:ILE:HD12	1.95	0.49
1:G:318:LEU:HG	1:G:410:HIS:HB3	1.95	0.49
1:A:58:ASP:OD2	1:A:110:ARG:HD3	2.13	0.49
1:F:318:LEU:HG	1:F:410:HIS:HB3	1.93	0.49
1:B:344:GLU:O	1:B:346:ASP:N	2.45	0.49
1:H:104:LEU:HD23	1:H:106:PRO:HD2	1.94	0.49
1:G:182:ASP:OD2	1:G:185:ARG:HD3	2.13	0.49
1:C:68:VAL:HG22	1:C:84:VAL:HG11	1.94	0.49
1:F:49:LEU:HD11	1:F:196:LYS:HD2	1.91	0.48
1:F:45:ARG:HA	1:F:48:ILE:HB	1.95	0.48
1:D:91:LEU:O	1:D:91:LEU:CG	2.60	0.48
1:H:215:VAL:HG21	1:H:248:VAL:HG13	1.96	0.48
1:G:384:ARG:HD3	1:G:432:LEU:HB2	1.93	0.48
1:H:332:THR:HG1	1:H:342:PHE:HD1	1.60	0.48
1:G:325:HIS:HB2	1:G:377:HIS:ND1	2.29	0.48
1:H:284:LEU:HD21	1:H:318:LEU:HD22	1.95	0.48
1:C:120:ASP:HB3	1:C:123:LYS:HB3	1.94	0.48
1:G:120:ASP:HB3	1:G:123:LYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:OE1	1:A:444:ARG:HD2	2.13	0.48
1:G:325:HIS:CG	1:G:377:HIS:CE1	3.01	0.48
1:C:182:ASP:OD2	1:C:185:ARG:HD3	2.14	0.48
1:H:142:ASN:HB3	1:H:145:ASP:OD2	2.12	0.48
1:C:292:ALA:HA	1:C:300:LEU:HD11	1.96	0.48
1:H:406:ASP:OD1	1:H:406:ASP:N	2.39	0.48
1:D:120:ASP:HB3	1:D:123:LYS:HE3	1.95	0.48
1:E:62:LEU:HD23	1:E:114:SER:HB2	1.95	0.48
1:C:71:ALA:HB3	1:C:82:PHE:CE1	2.42	0.47
1:B:182:ASP:OD2	1:B:185:ARG:HD3	2.14	0.47
1:A:347:LYS:HA	1:A:375:ARG:HD3	1.96	0.47
1:B:394:ARG:HH12	1:B:485:UNK:C	2.27	0.47
1:E:68:VAL:HG13	1:E:82:PHE:HZ	1.80	0.47
1:G:47:ARG:HA	1:G:47:ARG:HD3	1.76	0.47
1:C:67:PRO:HG2	1:C:115:PRO:HG3	1.96	0.47
1:A:274:ASP:OD1	1:A:275:GLU:N	2.46	0.47
1:B:274:ASP:OD1	1:B:275:GLU:N	2.48	0.47
1:A:142:ASN:HB3	1:A:145:ASP:OD2	2.14	0.47
1:D:184:VAL:CG2	1:D:187:LEU:HD12	2.43	0.47
1:A:329:LYS:N	1:A:345:HIS:HD2	2.12	0.47
1:A:404:CYS:HB2	1:A:407:ILE:HG12	1.95	0.47
1:C:182:ASP:OD2	1:C:185:ARG:NH1	2.47	0.47
1:G:135:THR:HB	1:G:162:GLY:HA2	1.97	0.47
1:F:404:CYS:HB2	1:F:407:ILE:HG12	1.97	0.47
1:G:308:VAL:C	1:G:310:GLY:N	2.68	0.47
1:A:345:HIS:CE1	1:A:346:ASP:CG	2.88	0.47
1:F:215:VAL:HG21	1:F:248:VAL:HG13	1.95	0.47
1:F:30:VAL:HG11	1:F:70:LEU:O	2.15	0.47
1:A:298:GLU:OE2	1:A:444:ARG:HD2	2.14	0.47
1:A:444:ARG:NH1	1:B:23:TYR:OH	2.48	0.47
1:H:353:VAL:HG21	1:H:374:VAL:HG21	1.97	0.47
1:B:135:THR:HG22	1:B:160:THR:HB	1.96	0.47
1:D:308:VAL:C	1:D:310:GLY:H	2.17	0.47
1:E:292:ALA:HA	1:E:300:LEU:HD11	1.97	0.47
1:C:135:THR:HG22	1:C:160:THR:HB	1.96	0.47
1:C:72:LYS:N	1:C:82:PHE:CE1	2.83	0.47
1:F:284:LEU:HD21	1:F:318:LEU:HD22	1.97	0.46
1:C:353:VAL:HG21	1:C:374:VAL:HG21	1.96	0.46
1:D:62:LEU:HD23	1:D:114:SER:HB2	1.97	0.46
1:F:44:VAL:O	1:F:48:ILE:CG1	2.63	0.46
1:H:274:ASP:OD1	1:H:275:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:ALA:HA	1:D:300:LEU:HD11	1.96	0.46
1:D:86:GLU:O	1:D:86:GLU:HG3	2.15	0.46
1:G:221:GLU:HG3	1:G:361:ARG:CD	2.43	0.46
1:D:58:ASP:OD2	1:D:110:ARG:HD3	2.15	0.46
1:A:244:TYR:OH	1:A:260:ARG:CG	2.63	0.46
1:B:443:ASN:HA	1:B:447:MET:SD	2.55	0.46
1:C:185:ARG:HE	1:C:188:ARG:HH11	1.64	0.46
1:C:142:ASN:HB3	1:C:145:ASP:OD2	2.15	0.46
1:D:332:THR:O	1:D:342:PHE:HD1	1.99	0.46
1:B:372:LYS:HG2	1:B:407:ILE:HD13	1.98	0.46
1:H:292:ALA:HA	1:H:300:LEU:HD11	1.97	0.46
1:B:142:ASN:HB3	1:B:145:ASP:OD2	2.14	0.46
1:G:292:ALA:HA	1:G:300:LEU:HD11	1.98	0.46
1:B:471:UNK:O	1:B:475:UNK:N	2.48	0.46
1:B:62:LEU:HD23	1:B:114:SER:HB2	1.96	0.46
1:C:308:VAL:HG13	1:C:309:LEU:CD1	2.43	0.46
1:C:30:VAL:HG21	1:C:74:PHE:HA	1.98	0.46
1:A:384:ARG:HD3	1:A:432:LEU:HB2	1.97	0.46
1:A:298:GLU:OE1	1:A:444:ARG:NH1	2.49	0.46
1:G:274:ASP:OD1	1:G:275:GLU:N	2.48	0.46
1:A:378:LEU:HD12	1:A:381:PHE:HD2	1.81	0.46
1:B:194:ILE:HG13	1:B:239:VAL:HG22	1.97	0.46
1:D:308:VAL:O	1:D:309:LEU:HB2	2.16	0.46
1:E:308:VAL:O	1:E:309:LEU:HB2	2.15	0.46
1:F:274:ASP:OD1	1:F:275:GLU:N	2.49	0.45
1:A:182:ASP:OD2	1:A:185:ARG:HD3	2.15	0.45
1:F:128:ASP:OD1	1:F:132:ARG:NH1	2.49	0.45
1:A:345:HIS:ND1	1:A:346:ASP:N	2.64	0.45
1:E:194:ILE:HG13	1:E:239:VAL:HG22	1.97	0.45
1:B:30:VAL:HG21	1:B:74:PHE:HA	1.98	0.45
1:A:175:SER:OG	1:A:178:ASN:OD1	2.29	0.45
1:E:200:LEU:HD13	1:E:204:PHE:CE2	2.51	0.45
1:H:184:VAL:HG23	1:H:223:ILE:HD13	1.98	0.45
1:F:195:GLU:OE2	1:F:196:LYS:NZ	2.49	0.45
1:G:284:LEU:HD21	1:G:318:LEU:HD22	1.99	0.45
1:B:259:LEU:HD21	1:B:327:ILE:HD12	1.97	0.45
1:E:142:ASN:HB3	1:E:145:ASP:OD2	2.16	0.45
1:A:75:ALA:HB2	1:A:100:VAL:HG22	1.98	0.45
1:C:86:GLU:OE2	1:C:94:ARG:CZ	2.64	0.45
1:G:259:LEU:HD21	1:G:327:ILE:HD12	1.99	0.45
1:D:194:ILE:HG13	1:D:239:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:VAL:HG21	1:B:374:VAL:HG21	1.97	0.45
1:A:406:ASP:N	1:A:406:ASP:OD1	2.43	0.45
1:A:158:ASP:N	1:A:158:ASP:OD1	2.50	0.45
1:E:353:VAL:HG21	1:E:374:VAL:HG21	1.99	0.45
1:G:194:ILE:HG13	1:G:239:VAL:HG22	1.98	0.45
1:A:377:HIS:HA	1:A:411:LEU:HD11	1.98	0.45
1:H:68:VAL:HG13	1:H:82:PHE:HZ	1.82	0.45
1:D:90:PHE:HE2	1:D:222:ARG:HD3	1.74	0.45
1:A:332:THR:HG1	1:A:342:PHE:HD1	1.64	0.45
1:E:183:PRO:HB2	1:E:215:VAL:HA	1.97	0.45
1:G:165:ASP:OD1	1:G:172:ARG:NH2	2.43	0.45
1:F:325:HIS:CG	1:F:326:ASP:N	2.85	0.45
1:A:332:THR:HG23	1:A:345:HIS:HB3	1.96	0.45
1:A:150:GLY:HA2	1:B:427:GLU:OE1	2.17	0.45
1:A:259:LEU:HD21	1:A:327:ILE:HD12	1.98	0.45
1:D:379:ARG:NH1	1:D:403:GLU:OE1	2.43	0.45
1:E:347:LYS:CG	1:E:375:ARG:CZ	2.95	0.45
1:F:83:PHE:HB3	1:F:85:PHE:CE2	2.45	0.45
1:C:284:LEU:HD21	1:C:318:LEU:HD22	1.99	0.45
1:H:325:HIS:CG	1:H:326:ASP:N	2.84	0.45
1:C:274:ASP:OD1	1:C:275:GLU:N	2.48	0.45
1:D:345:HIS:CD2	1:D:346:ASP:OD1	2.70	0.44
1:F:206:GLU:O	1:F:210:GLU:HG3	2.17	0.44
1:B:47:ARG:HA	1:B:47:ARG:HD3	1.71	0.44
1:D:346:ASP:OD2	1:D:378:LEU:HD21	2.17	0.44
1:A:184:VAL:HG23	1:A:223:ILE:HD13	1.99	0.44
1:F:232:LYS:HA	1:F:316:GLU:OE2	2.17	0.44
1:C:85:PHE:O	1:C:85:PHE:CD2	2.70	0.44
1:C:152:LYS:CA	1:C:152:LYS:HE2	2.32	0.44
1:H:183:PRO:HB2	1:H:215:VAL:HA	2.00	0.44
1:C:82:PHE:CE2	1:C:84:VAL:HG21	2.51	0.44
1:E:318:LEU:HG	1:E:410:HIS:HB3	2.00	0.44
1:A:389:LYS:O	1:D:258:ARG:NH1	2.49	0.44
1:H:194:ILE:HG13	1:H:239:VAL:HG22	1.99	0.44
1:H:308:VAL:HG21	1:H:317:LEU:HD11	1.99	0.44
1:A:347:LYS:HG2	1:A:375:ARG:CD	2.48	0.44
1:G:120:ASP:HB3	1:G:123:LYS:HE3	1.99	0.44
1:E:120:ASP:HB3	1:E:123:LYS:HE3	1.99	0.44
1:G:325:HIS:CG	1:G:326:ASP:N	2.85	0.44
1:A:284:LEU:HD21	1:A:318:LEU:HD22	1.99	0.44
1:F:292:ALA:HA	1:F:300:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:CYS:HB2	1:D:407:ILE:HG12	1.98	0.44
1:E:325:HIS:CG	1:E:326:ASP:N	2.85	0.44
1:H:47:ARG:HD3	1:H:47:ARG:HA	1.77	0.44
1:D:273:LEU:HD13	1:D:329:LYS:NZ	2.32	0.44
1:D:274:ASP:OD1	1:D:275:GLU:N	2.49	0.44
1:A:325:HIS:CG	1:A:326:ASP:N	2.85	0.44
1:H:354:ARG:NH1	1:H:368:GLU:OE1	2.50	0.44
1:H:188:ARG:HG2	1:H:226:GLU:OE2	2.17	0.44
1:G:128:ASP:OD1	1:G:132:ARG:NH1	2.50	0.44
1:F:75:ALA:HB2	1:F:100:VAL:CG1	2.48	0.44
1:C:188:ARG:NH2	2:C:1001:SO4:O2	2.50	0.44
1:D:120:ASP:HB3	1:D:123:LYS:HB3	1.99	0.44
1:F:49:LEU:HD23	1:F:49:LEU:HA	1.86	0.44
1:F:72:LYS:O	1:F:82:PHE:CZ	2.71	0.44
1:E:284:LEU:HD21	1:E:318:LEU:HD22	1.99	0.44
1:A:87:LYS:HD3	1:A:87:LYS:HA	1.79	0.44
1:G:149:ILE:HA	1:H:430:LYS:HE3	2.00	0.44
1:E:188:ARG:NH2	2:E:1001:SO4:O2	2.51	0.44
1:C:151:ALA:CB	1:D:427:GLU:CD	2.85	0.44
1:C:62:LEU:HD23	1:C:114:SER:HB2	2.00	0.44
1:E:120:ASP:HB3	1:E:123:LYS:HB3	1.99	0.44
1:C:325:HIS:CG	1:C:326:ASP:N	2.85	0.44
1:E:135:THR:HG22	1:E:160:THR:HB	1.99	0.44
1:H:120:ASP:HB3	1:H:123:LYS:HB3	2.00	0.44
1:C:185:ARG:NE	1:C:188:ARG:HH11	2.14	0.43
1:F:120:ASP:HB3	1:F:123:LYS:HE3	2.00	0.43
1:A:378:LEU:HG	1:A:378:LEU:O	2.18	0.43
1:E:379:ARG:NH1	1:E:403:GLU:OE1	2.42	0.43
1:A:471:UNK:O	1:A:475:UNK:N	2.51	0.43
1:F:75:ALA:HB2	1:F:100:VAL:HG13	1.99	0.43
1:C:82:PHE:O	1:C:83:PHE:CD1	2.70	0.43
1:F:60:ASP:OD2	1:F:132:ARG:NH2	2.51	0.43
1:A:47:ARG:HA	1:A:47:ARG:HD3	1.72	0.43
1:C:120:ASP:HB3	1:C:123:LYS:HE3	2.00	0.43
1:A:45:ARG:NH1	1:A:192:ILE:HD13	2.33	0.43
1:D:325:HIS:CG	1:D:326:ASP:N	2.85	0.43
1:B:120:ASP:HB3	1:B:123:LYS:HB3	1.99	0.43
1:A:94:ARG:HA	1:A:94:ARG:HD3	1.81	0.43
1:B:120:ASP:HB3	1:B:123:LYS:HE3	1.99	0.43
1:B:325:HIS:CG	1:B:326:ASP:N	2.87	0.43
1:C:92:ILE:HG12	1:C:93:LYS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:ARG:HG2	1:G:226:GLU:OE2	2.18	0.43
1:F:49:LEU:CD1	1:F:196:LYS:CD	2.87	0.43
1:A:347:LYS:O	1:A:350:ALA:HB3	2.18	0.43
1:C:30:VAL:HG13	1:C:73:ASN:HB2	2.00	0.43
1:B:43:TRP:CD1	1:B:59:VAL:HG22	2.54	0.43
1:F:170:LEU:HD23	1:F:199:GLN:HB3	2.01	0.43
1:A:194:ILE:HG13	1:A:239:VAL:HG22	2.00	0.43
1:C:47:ARG:HA	1:C:47:ARG:HD3	1.65	0.43
1:C:92:ILE:HG23	1:C:93:LYS:HD3	2.01	0.43
1:E:427:GLU:HG3	1:F:151:ALA:HA	2.01	0.43
1:G:377:HIS:O	1:G:377:HIS:CD2	2.71	0.43
1:G:343:TYR:CB	1:G:344:GLU:OE2	2.66	0.43
1:A:347:LYS:HD3	1:A:375:ARG:CZ	2.49	0.43
1:C:378:LEU:O	1:C:378:LEU:HG	2.19	0.43
1:D:92:ILE:CG2	1:D:92:ILE:O	2.67	0.43
1:D:135:THR:HB	1:D:162:GLY:HA2	2.00	0.43
1:C:158:ASP:OD1	1:C:158:ASP:N	2.52	0.43
1:F:30:VAL:HG21	1:F:74:PHE:CA	2.48	0.43
1:B:412:PHE:HB3	1:B:436:ILE:HD13	2.01	0.43
1:F:158:ASP:OD1	1:F:158:ASP:N	2.52	0.43
1:C:183:PRO:HG2	1:C:218:SER:HB3	2.01	0.42
1:G:404:CYS:HB2	1:G:407:ILE:HG12	2.01	0.42
1:E:182:ASP:OD2	1:E:185:ARG:HD3	2.19	0.42
1:A:183:PRO:HB2	1:A:215:VAL:HA	2.00	0.42
1:C:114:SER:HA	1:C:115:PRO:HD3	1.89	0.42
1:F:372:LYS:HG2	1:F:407:ILE:HD13	2.00	0.42
1:D:135:THR:HG22	1:D:160:THR:HB	2.00	0.42
1:B:57:ILE:HD12	1:B:109:TYR:CE2	2.54	0.42
1:G:156:VAL:HG21	1:G:163:ILE:HD11	2.01	0.42
1:E:102:LEU:HB3	1:E:109:TYR:HB2	2.00	0.42
1:E:25:ASP:C	1:E:29:LYS:HZ3	2.23	0.42
1:G:215:VAL:HG21	1:G:248:VAL:HG13	2.01	0.42
1:H:30:VAL:HG13	1:H:73:ASN:HB2	2.01	0.42
1:D:92:ILE:O	1:D:93:LYS:CB	2.67	0.42
1:A:244:TYR:OH	1:A:260:ARG:HG2	2.19	0.42
1:B:326:ASP:OD1	1:B:377:HIS:NE2	2.52	0.42
1:G:224:THR:OG1	1:G:360:LEU:O	2.25	0.42
1:A:292:ALA:HA	1:A:300:LEU:HD11	2.01	0.42
1:D:384:ARG:HD3	1:D:432:LEU:HB2	2.00	0.42
1:B:323:LEU:HA	1:B:323:LEU:HD23	1.90	0.42
1:G:309:LEU:N	1:G:309:LEU:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:LYS:HG2	1:E:375:ARG:CZ	2.45	0.42
1:A:134:PHE:HA	1:A:173:PRO:HA	2.01	0.42
1:C:412:PHE:HB3	1:C:436:ILE:HD13	2.01	0.42
1:H:158:ASP:N	1:H:158:ASP:OD1	2.52	0.42
1:E:158:ASP:N	1:E:158:ASP:OD1	2.52	0.42
1:D:314:ASP:N	1:D:314:ASP:OD1	2.47	0.42
1:B:204:PHE:O	1:B:208:VAL:HG23	2.20	0.42
1:F:183:PRO:HB2	1:F:215:VAL:HA	2.01	0.42
1:E:188:ARG:HG2	1:E:226:GLU:OE2	2.18	0.42
1:G:158:ASP:OD1	1:G:158:ASP:N	2.52	0.42
1:D:323:LEU:HD23	1:D:323:LEU:HA	1.89	0.42
1:H:45:ARG:NH1	1:H:137:ASN:OD1	2.50	0.42
1:B:185:ARG:HE	1:B:188:ARG:HH11	1.67	0.42
1:H:185:ARG:HG3	1:H:188:ARG:HD3	2.00	0.42
1:G:49:LEU:HD21	1:G:166:LEU:HD22	2.02	0.42
1:E:274:ASP:OD1	1:E:275:GLU:N	2.50	0.42
1:D:309:LEU:CD1	1:D:309:LEU:N	2.82	0.42
1:B:30:VAL:HG13	1:B:73:ASN:HB2	2.02	0.42
1:E:43:TRP:CD1	1:E:59:VAL:HG22	2.55	0.42
1:H:57:ILE:HD12	1:H:109:TYR:CE2	2.55	0.42
1:F:43:TRP:CD1	1:F:59:VAL:HG22	2.54	0.42
1:D:158:ASP:OD1	1:D:158:ASP:N	2.52	0.42
1:G:412:PHE:HB3	1:G:436:ILE:HD13	2.01	0.42
1:H:60:ASP:OD2	1:H:132:ARG:NH2	2.53	0.42
1:F:204:PHE:O	1:F:208:VAL:HG23	2.20	0.42
1:F:412:PHE:HB3	1:F:436:ILE:HD13	2.02	0.42
1:H:191:ARG:NH2	2:H:1001:SO4:O2	2.47	0.41
1:B:188:ARG:NH2	2:B:1001:SO4:O1	2.53	0.41
1:A:20:TYR:CE1	1:B:434:GLU:HG2	2.54	0.41
1:H:67:PRO:HG2	1:H:115:PRO:HG3	2.01	0.41
1:F:166:LEU:HD23	1:F:166:LEU:HA	1.81	0.41
1:B:448:LYS:CB	1:B:448:LYS:NZ	2.81	0.41
1:D:92:ILE:O	1:D:93:LYS:HB3	2.19	0.41
1:C:20:TYR:CE1	1:D:434:GLU:HG2	2.55	0.41
1:G:221:GLU:CG	1:G:361:ARG:CD	2.99	0.41
1:A:227:LEU:HD11	1:A:252:ILE:HG21	2.03	0.41
1:D:86:GLU:O	1:D:94:ARG:CG	2.68	0.41
1:E:66:ASP:HA	1:E:67:PRO:HD3	1.92	0.41
1:C:133:ASP:HB3	1:C:185:ARG:HG2	2.03	0.41
1:B:185:ARG:HG3	1:B:188:ARG:HD3	2.02	0.41
1:G:233:GLU:OE2	1:G:239:VAL:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:THR:HB	1:A:162:GLY:HA2	2.01	0.41
1:E:60:ASP:OD2	1:E:132:ARG:NH2	2.53	0.41
1:A:68:VAL:HG13	1:A:84:VAL:HG21	2.01	0.41
1:B:307:ARG:NH2	1:B:310:GLY:O	2.47	0.41
1:F:273:LEU:O	1:F:277:THR:OG1	2.38	0.41
1:G:311:GLU:O	1:G:311:GLU:HG2	2.20	0.41
1:D:406:ASP:OD1	1:D:406:ASP:N	2.40	0.41
1:H:346:ASP:OD1	1:H:346:ASP:N	2.39	0.41
1:E:323:LEU:HA	1:E:323:LEU:HD23	1.89	0.41
1:H:404:CYS:HB2	1:H:407:ILE:HG12	2.03	0.41
1:C:149:ILE:N	1:C:149:ILE:HD13	2.29	0.41
1:E:81:HIS:N	1:E:101:VAL:O	2.33	0.41
1:A:38:PHE:O	1:A:61:PHE:HA	2.21	0.41
1:B:172:ARG:HA	1:B:173:PRO:HD2	1.94	0.41
1:B:158:ASP:OD1	1:B:158:ASP:N	2.53	0.41
1:A:30:VAL:HG13	1:A:73:ASN:HB2	2.02	0.41
1:G:170:LEU:HD23	1:G:199:GLN:HB3	2.03	0.41
1:H:24:PHE:HB3	1:H:143:LEU:HD11	2.03	0.41
1:F:345:HIS:O	1:F:347:LYS:N	2.53	0.41
1:B:215:VAL:HG21	1:B:248:VAL:HG13	2.03	0.41
1:A:445:ASN:HD21	1:B:77:ARG:C	2.19	0.41
1:A:86:GLU:HG2	1:A:95:PRO:O	2.21	0.41
1:C:191:ARG:NH2	2:C:1001:SO4:O1	2.47	0.41
1:G:444:ARG:NH2	1:H:26:ASP:OD1	2.54	0.41
1:E:126:ILE:HG23	1:E:159:PRO:HG3	2.03	0.41
1:A:340:VAL:HG12	1:A:341:THR:HG23	2.02	0.41
1:A:379:ARG:HB3	1:A:380:PRO:HD3	2.03	0.41
1:E:287:VAL:HG12	1:E:413:LEU:HD22	2.03	0.41
1:H:117:LYS:HB3	1:H:117:LYS:HE2	1.93	0.41
1:C:149:ILE:HG12	1:C:150:GLY:H	1.82	0.41
1:D:55:TYR:HB3	1:D:106:PRO:O	2.21	0.41
1:H:259:LEU:HD21	1:H:327:ILE:HD12	2.03	0.41
1:E:173:PRO:HD2	1:E:201:THR:HG22	2.02	0.41
1:G:102:LEU:HB3	1:G:109:TYR:HB2	2.03	0.41
1:A:43:TRP:CZ3	1:A:47:ARG:HG2	2.56	0.40
1:C:258:ARG:O	1:C:261:GLU:HG2	2.21	0.40
1:E:201:THR:OG1	1:E:202:GLU:N	2.54	0.40
1:D:43:TRP:CD1	1:D:59:VAL:HG22	2.56	0.40
1:H:141:VAL:HG12	1:H:156:VAL:HG12	2.02	0.40
1:G:68:VAL:HG13	1:G:82:PHE:HZ	1.86	0.40
1:B:51:GLU:HA	1:B:52:PRO:HD3	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:ILE:O	1:E:167:GLU:HG3	2.21	0.40
1:E:406:ASP:N	1:E:406:ASP:OD1	2.40	0.40
1:F:66:ASP:HA	1:F:67:PRO:HD3	1.96	0.40
1:A:80:GLY:HA2	1:A:101:VAL:O	2.21	0.40
1:F:44:VAL:HG12	1:F:48:ILE:HD11	1.99	0.40
1:B:284:LEU:HD21	1:B:318:LEU:HD22	2.03	0.40
1:A:94:ARG:HA	1:A:95:PRO:HD2	1.90	0.40
1:B:188:ARG:HG2	1:B:226:GLU:OE2	2.22	0.40
1:C:287:VAL:HG12	1:C:413:LEU:HD22	2.04	0.40
1:D:176:ILE:HD11	1:D:203:ASP:HB2	2.03	0.40
1:A:102:LEU:HB3	1:A:109:TYR:HB2	2.03	0.40
1:E:165:ASP:OD1	1:E:172:ARG:NH2	2.44	0.40
1:H:204:PHE:O	1:H:208:VAL:HG23	2.22	0.40
1:A:92:ILE:CG1	1:A:93:LYS:N	2.83	0.40
1:E:308:VAL:HG21	1:E:317:LEU:HD11	2.04	0.40
1:G:445:ASN:OD1	1:G:446:GLU:HG3	2.22	0.40
1:B:394:ARG:HH12	1:B:485:UNK:CA	2.33	0.40
1:H:379:ARG:HB3	1:H:380:PRO:HD3	2.04	0.40
1:H:372:LYS:HG2	1:H:407:ILE:HD13	2.04	0.40
1:F:445:ASN:OD1	1:F:446:GLU:HG3	2.20	0.40
1:B:273:LEU:HD13	1:B:329:LYS:NZ	2.37	0.40
1:E:47:ARG:HD3	1:E:47:ARG:HA	1.70	0.40
1:E:445:ASN:OD1	1:E:446:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/497 (84%)	409 (99%)	6 (1%)	0	100	100
1	B	405/497 (82%)	402 (99%)	2 (0%)	1 (0%)	52	86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	413/497 (83%)	407 (98%)	6 (2%)	0	100	100
1	D	413/497 (83%)	407 (98%)	6 (2%)	0	100	100
1	E	403/497 (81%)	402 (100%)	1 (0%)	0	100	100
1	F	403/497 (81%)	400 (99%)	3 (1%)	0	100	100
1	G	403/497 (81%)	400 (99%)	3 (1%)	0	100	100
1	H	403/497 (81%)	399 (99%)	4 (1%)	0	100	100
All	All	3258/3976 (82%)	3226 (99%)	31 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	345	HIS

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	367/378 (97%)	344 (94%)	23 (6%)	22	61
1	B	360/378 (95%)	348 (97%)	12 (3%)	45	77
1	C	365/378 (97%)	350 (96%)	15 (4%)	37	73
1	D	365/378 (97%)	354 (97%)	11 (3%)	48	78
1	E	358/378 (95%)	346 (97%)	12 (3%)	44	77
1	F	358/378 (95%)	347 (97%)	11 (3%)	47	78
1	G	358/378 (95%)	349 (98%)	9 (2%)	55	82
1	H	358/378 (95%)	349 (98%)	9 (2%)	55	82
All	All	2889/3024 (96%)	2787 (96%)	102 (4%)	43	76

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG

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Mol	Chain	Res	Type
1	A	82	PHE
1	A	83	PHE
1	A	85	PHE
1	A	86	GLU
1	A	88	ARG
1	A	90	PHE
1	A	92	ILE
1	A	93	LYS
1	A	94	ARG
1	A	104	LEU
1	A	153	GLN
1	A	185	ARG
1	A	186	VAL
1	A	211	ASP
1	A	264	ASP
1	A	277	THR
1	A	318	LEU
1	A	323	LEU
1	A	344	GLU
1	A	345	HIS
1	A	377	HIS
1	A	446	GLU
1	B	47	ARG
1	B	104	LEU
1	B	149	ILE
1	B	154	THR
1	B	185	ARG
1	B	186	VAL
1	B	211	ASP
1	B	277	THR
1	B	377	HIS
1	B	378	LEU
1	B	445	ASN
1	B	447	MET
1	C	47	ARG
1	C	85	PHE
1	C	86	GLU
1	C	87	LYS
1	C	93	LYS
1	C	104	LEU
1	C	148	SER
1	C	149	ILE

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Mol	Chain	Res	Type
1	C	155	ILE
1	C	185	ARG
1	C	186	VAL
1	C	211	ASP
1	C	345	HIS
1	C	377	HIS
1	C	445	ASN
1	D	47	ARG
1	D	87	LYS
1	D	94	ARG
1	D	104	LEU
1	D	186	VAL
1	D	211	ASP
1	D	342	PHE
1	D	345	HIS
1	D	346	ASP
1	D	378	LEU
1	D	445	ASN
1	E	47	ARG
1	E	104	LEU
1	E	149	ILE
1	E	153	GLN
1	E	185	ARG
1	E	186	VAL
1	E	211	ASP
1	E	342	PHE
1	E	344	GLU
1	E	345	HIS
1	E	378	LEU
1	E	445	ASN
1	F	47	ARG
1	F	81	HIS
1	F	97	ILE
1	F	104	LEU
1	F	185	ARG
1	F	186	VAL
1	F	277	THR
1	F	344	GLU
1	F	345	HIS
1	F	378	LEU
1	F	445	ASN
1	G	47	ARG

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Mol	Chain	Res	Type
1	G	104	LEU
1	G	149	ILE
1	G	185	ARG
1	G	186	VAL
1	G	211	ASP
1	G	343	TYR
1	G	344	GLU
1	G	445	ASN
1	H	47	ARG
1	H	104	LEU
1	H	149	ILE
1	H	154	THR
1	H	185	ARG
1	H	186	VAL
1	H	211	ASP
1	H	378	LEU
1	H	445	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	HIS
1	A	345	HIS
1	C	345	HIS
1	D	345	HIS
1	E	345	HIS
1	G	225	HIS
1	G	325	HIS
1	G	377	HIS

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 ⓘ

8 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	SO4	A	1001	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	B	1001	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	C	1001	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	D	1001	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	E	1001	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	F	1001	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	G	1001	-	4,4,4	1.48	0	6,6,6	1.71	1 (16%)
2	SO4	H	1001	-	4,4,4	0.24	0	6,6,6	0.08	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
2	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1001	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	G	1001	SO4	O4-S-O3	4.03	125.37	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	SO4	1	0
2	C	1001	SO4	2	0
2	E	1001	SO4	1	0
2	F	1001	SO4	1	0
2	H	1001	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	421/497 (84%)	-0.22	4 (0%) 84 77	51, 113, 166, 211	0
1	B	413/497 (83%)	-0.10	11 (2%) 58 46	62, 116, 177, 218	0
1	C	419/497 (84%)	0.03	15 (3%) 46 36	71, 139, 209, 259	0
1	D	419/497 (84%)	-0.03	7 (1%) 73 62	75, 133, 193, 243	0
1	E	411/497 (82%)	0.03	9 (2%) 65 54	83, 146, 198, 249	0
1	F	411/497 (82%)	-0.08	8 (1%) 70 59	65, 125, 176, 190	0
1	G	411/497 (82%)	0.33	32 (7%) 16 11	118, 167, 231, 259	0
1	H	411/497 (82%)	0.36	32 (7%) 16 11	102, 177, 223, 266	0
All	All	3316/3976 (83%)	0.04	118 (3%) 46 36	51, 140, 209, 266	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	264	ASP	6.4
1	H	264	ASP	5.6
1	C	264	ASP	5.5
1	G	31	LEU	5.3
1	E	180	LYS	4.7
1	G	394	ARG	4.2
1	G	32	PRO	4.2
1	C	35	HIS	4.2
1	D	35	HIS	4.1
1	H	366	ALA	4.0
1	H	233	GLU	4.0
1	E	119	LYS	4.0
1	G	444	ARG	3.9
1	H	361	ARG	3.9
1	G	163	ILE	3.9
1	E	118	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	264	ASP	3.7
1	C	36	TYR	3.7
1	H	394	ARG	3.7
1	H	448	LYS	3.6
1	H	311	GLU	3.6
1	C	217	LYS	3.5
1	G	67	PRO	3.5
1	H	86	GLU	3.5
1	G	132	ARG	3.5
1	G	397	MET	3.5
1	H	34	GLU	3.5
1	G	85	PHE	3.3
1	F	327	ILE	3.3
1	H	33	ARG	3.3
1	C	115	PRO	3.3
1	C	92	ILE	3.3
1	B	264	ASP	3.2
1	C	17	LEU	3.2
1	H	259	LEU	3.2
1	B	154	THR	3.1
1	H	103	HIS	3.1
1	E	32	PRO	3.1
1	C	71	ALA	3.1
1	G	398	ALA	3.1
1	F	331	GLN	3.0
1	C	114	SER	3.0
1	G	71	ALA	3.0
1	G	448	LYS	2.9
1	G	445	ASN	2.9
1	G	68	VAL	2.9
1	C	33	ARG	2.9
1	E	301	GLU	2.9
1	G	114	SER	2.9
1	F	118	GLY	2.8
1	H	362	TRP	2.8
1	H	340	VAL	2.8
1	H	105	PRO	2.8
1	G	81	HIS	2.8
1	H	395	ARG	2.7
1	H	330	PRO	2.7
1	D	180	LYS	2.7
1	A	311	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	263	LYS	2.7
1	H	406	ASP	2.6
1	G	112	ASP	2.6
1	H	365	GLU	2.6
1	A	398	ALA	2.6
1	H	32	PRO	2.6
1	C	93	LYS	2.6
1	H	327	ILE	2.6
1	G	34	GLU	2.5
1	G	86	GLU	2.5
1	H	389	LYS	2.5
1	H	132	ARG	2.5
1	B	332	THR	2.5
1	B	350	ALA	2.5
1	F	311	GLU	2.4
1	C	63	THR	2.4
1	G	392	LEU	2.4
1	G	35	HIS	2.4
1	H	363	GLY	2.3
1	G	167	GLU	2.3
1	B	263	LYS	2.3
1	H	341	THR	2.3
1	B	347	LYS	2.3
1	G	311	GLU	2.3
1	G	96	THR	2.3
1	H	364	ASP	2.3
1	E	86	GLU	2.3
1	H	331	GLN	2.3
1	F	377	HIS	2.3
1	A	397	MET	2.3
1	H	369	PHE	2.3
1	D	36	TYR	2.2
1	E	64	THR	2.2
1	H	373	LEU	2.2
1	C	31	LEU	2.2
1	D	311	GLU	2.2
1	A	341	THR	2.2
1	B	351	GLN	2.2
1	G	331	GLN	2.2
1	B	365	GLU	2.1
1	D	17	LEU	2.1
1	G	152	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	127	GLU	2.1
1	E	331	GLN	2.1
1	H	258	ARG	2.1
1	G	101	VAL	2.1
1	F	128	ASP	2.1
1	E	264	ASP	2.1
1	G	326	ASP	2.1
1	C	112	ASP	2.1
1	G	97	ILE	2.1
1	F	448	LYS	2.1
1	B	199	GLN	2.1
1	D	401	TRP	2.1
1	B	327	ILE	2.0
1	H	60	ASP	2.0
1	C	37	CYS	2.0
1	B	153	GLN	2.0
1	G	447	MET	2.0
1	H	402	ARG	2.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	B	1001	5/5	0.91	0.45	1.90	126,131,139,141	0
2	SO4	C	1001	5/5	0.73	0.49	1.48	162,165,166,172	0
2	SO4	H	1001	5/5	0.92	0.39	1.00	152,157,161,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	G	1001	5/5	0.92	0.43	0.42	172,174,178,186	0
2	SO4	A	1001	5/5	0.88	0.31	0.16	119,122,146,154	0
2	SO4	E	1001	5/5	0.95	0.24	-0.66	133,135,137,145	0
2	SO4	D	1001	5/5	0.94	0.29	-0.86	104,115,144,156	0
2	SO4	F	1001	5/5	0.94	0.16	-1.15	81,81,91,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.