



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:41 am GMT

PDB ID : 1IAS  
Title : CYTOPLASMIC DOMAIN OF UNPHOSPHORYLATED TYPE I TGF-BETA RECEPTOR CRYSTALLIZED WITHOUT FKBP12  
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Deposited on : 2001-03-23  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

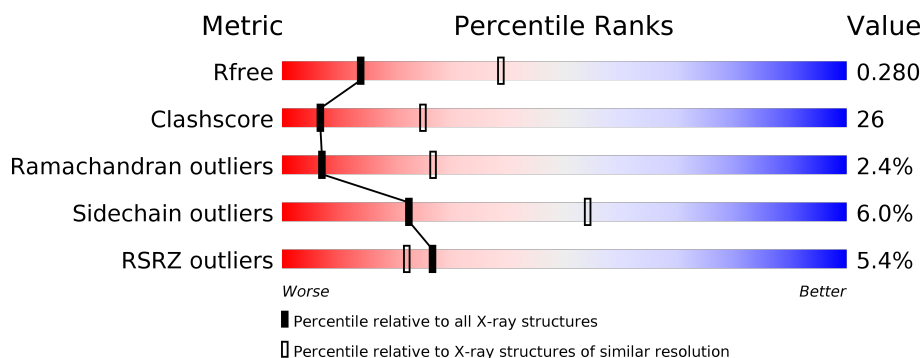
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	342	<div> <div>4%</div> <div> <div></div> <div>54%</div> <div>37%</div> <div>6%</div> </div> </div>
1	B	342	<div> <div>6%</div> <div> <div></div> <div>52%</div> <div>37%</div> <div>5%</div> <div>5%</div> </div> </div>
1	C	342	<div> <div>13%</div> <div> <div></div> <div>51%</div> <div>40%</div> <div>5%</div> </div> </div>
1	D	342	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>38%</div> <div>5%</div> </div> </div>
1	E	342	<div> <div>0%</div> <div> <div></div> <div>55%</div> <div>36%</div> <div>6%</div> </div> </div>

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	E	1	-	-	X	-

## 2 Entry composition [i](#)

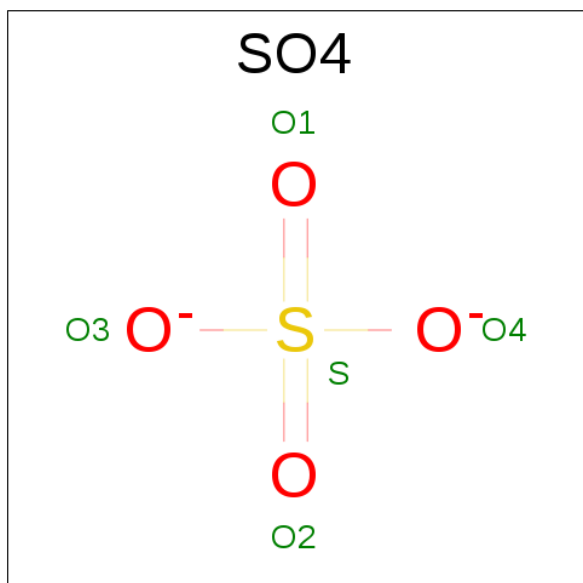
There are 2 unique types of molecules in this entry. The entry contains 13181 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TGF-BETA RECEPTOR TYPE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	B	324	Total	C	N	O	S	0	0	0
			2590	1636	463	475	16			
1	C	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	D	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	E	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		

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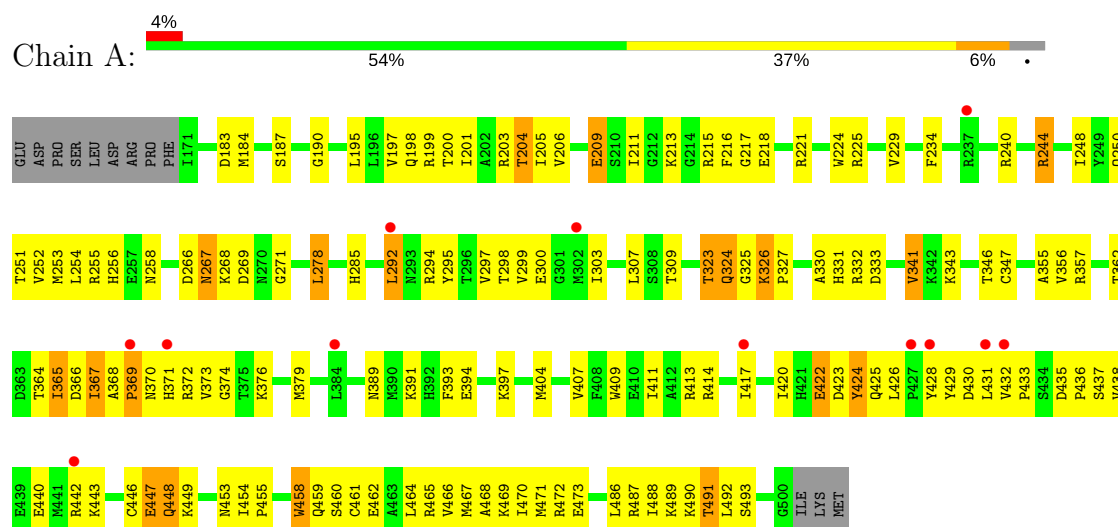
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0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

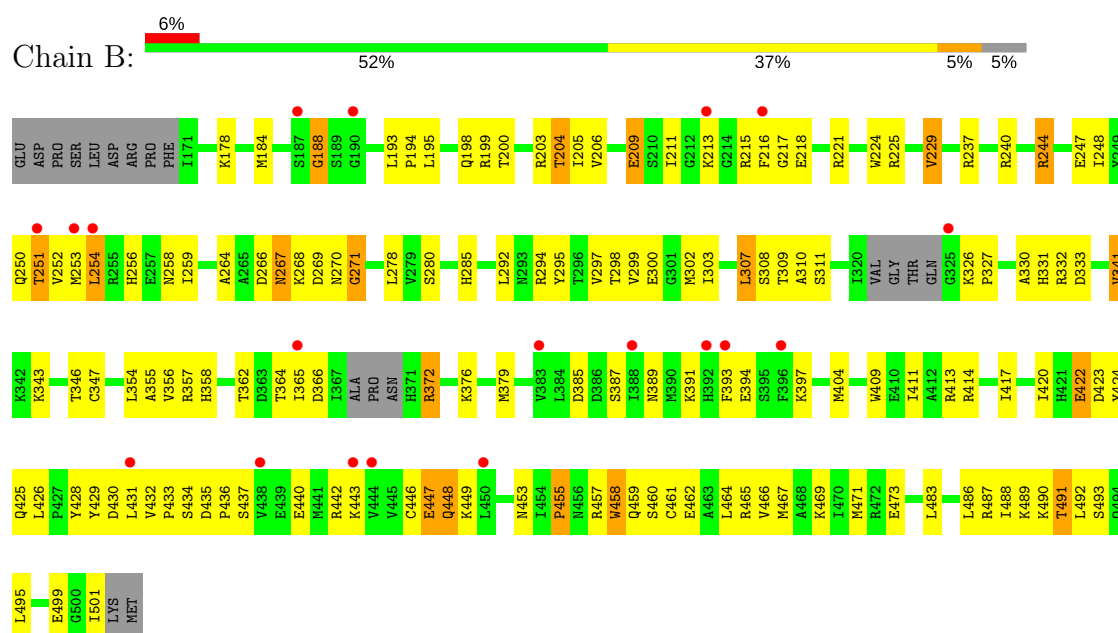
### 3 Residue-property plots

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

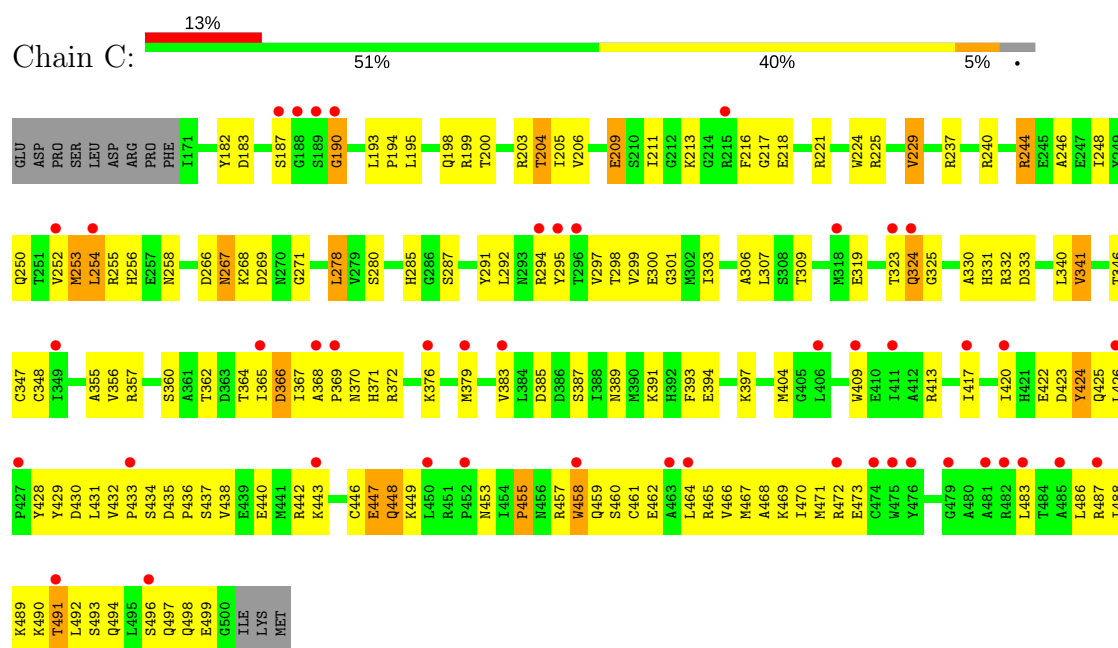
#### • Molecule 1: TGF-BETA RECEPTOR TYPE I



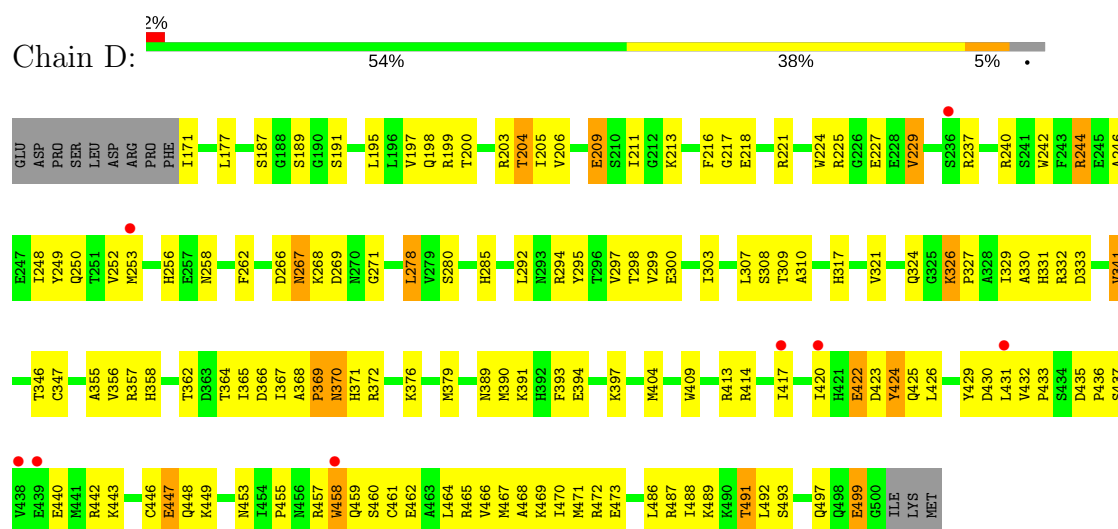
#### • Molecule 1: TGF-BETA RECEPTOR TYPE I



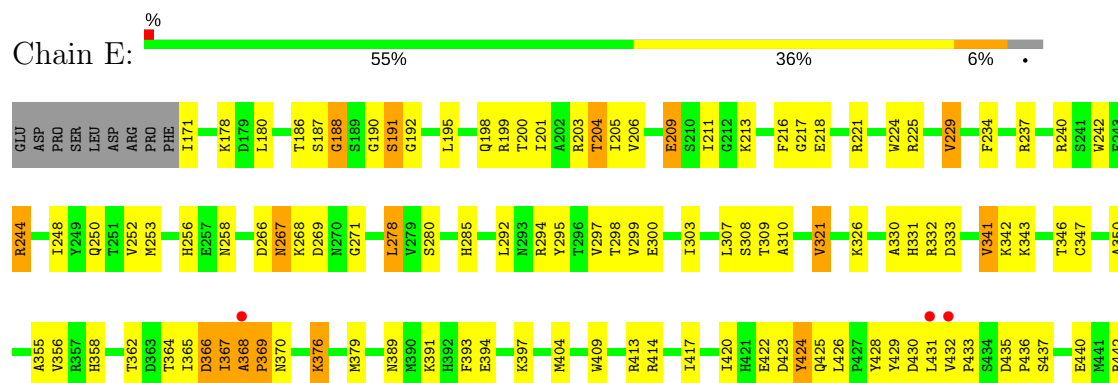
#### • Molecule 1: TGF-BETA RECEPTOR TYPE I

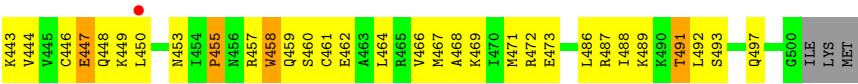


• Molecule 1: TGF-BETA RECEPTOR TYPE I



• Molecule 1: TGF-BETA RECEPTOR TYPE I







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.56Å 251.62Å 140.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 63.45 – 2.91	Depositor EDS
% Data completeness (in resolution range)	85.9 (30.00-2.90) 86.0 (63.45-2.91)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.81 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.255 , 0.284 0.254 , 0.280	Depositor DCC
$R_{free}$ test set	5833 reflections (10.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.3	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	13181	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.40	0/2682	0.63	1/3622 (0.0%)
1	B	0.44	0/2640	0.63	1/3560 (0.0%)
1	C	0.41	0/2682	0.63	1/3622 (0.0%)
1	D	0.45	1/2682 (0.0%)	0.66	2/3622 (0.1%)
1	E	0.43	0/2682	0.65	2/3622 (0.1%)
All	All	0.43	1/13368 (0.0%)	0.64	7/18048 (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	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	499	GLU	CG-CD	6.04	1.61	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	321	VAL	N-CA-C	5.44	125.70	111.00
1	E	268	LYS	N-CA-C	5.44	125.68	111.00
1	D	268	LYS	N-CA-C	5.19	125.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	499	GLU	N-CA-CB	5.17	119.91	110.60
1	B	268	LYS	N-CA-C	5.16	124.92	111.00
1	A	268	LYS	N-CA-C	5.15	124.90	111.00
1	C	268	LYS	N-CA-C	5.05	124.64	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	424	TYR	Sidechain
1	C	424	TYR	Sidechain
1	D	424	TYR	Sidechain
1	E	424	TYR	Sidechain

## 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	2629	0	2631	134	0
1	B	2590	0	2595	129	0
1	C	2629	0	2631	149	0
1	D	2629	0	2631	142	0
1	E	2629	0	2631	135	1
2	A	15	0	0	1	0
2	B	15	0	0	1	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
2	E	15	0	0	2	0
All	All	13181	0	13119	682	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 26.

All (682) 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:E:191:SER:HB2	1:E:253:MET:HA	1.31	1.12
1:E:368:ALA:HB3	1:E:369:PRO:HD3	1.37	1.05
1:A:298:THR:HG22	1:A:300:GLU:H	1.26	1.00
1:B:298:THR:HG22	1:B:300:GLU:H	1.27	0.98
1:C:298:THR:HG22	1:C:300:GLU:H	1.27	0.96
1:D:368:ALA:HB2	1:E:178:LYS:HE2	1.44	0.95
1:E:298:THR:HG22	1:E:300:GLU:H	1.26	0.95
1:A:332:ARG:NH2	1:A:369:PRO:HG2	1.82	0.94
1:E:211:ILE:HD11	1:E:221:ARG:HB2	1.50	0.94
1:E:368:ALA:CB	1:E:369:PRO:HD3	1.99	0.92
1:D:298:THR:HG22	1:D:300:GLU:H	1.30	0.91
1:C:211:ILE:HD11	1:C:221:ARG:HB2	1.51	0.91
1:D:267:ASN:H	1:D:267:ASN:HD22	1.21	0.89
1:D:211:ILE:HD11	1:D:221:ARG:HB2	1.54	0.88
1:B:211:ILE:HD11	1:B:221:ARG:HB2	1.55	0.87
1:C:372:ARG:NH2	1:C:438:VAL:HG11	1.90	0.86
1:E:191:SER:HB2	1:E:253:MET:CA	2.04	0.86
1:B:443:LYS:HG2	1:B:448:GLN:HE21	1.39	0.86
1:D:252:VAL:O	1:D:253:MET:HG2	1.74	0.86
1:A:211:ILE:HD11	1:A:221:ARG:HB2	1.57	0.86
1:D:443:LYS:HG2	1:D:448:GLN:HE21	1.41	0.86
1:A:332:ARG:HH22	1:A:369:PRO:HG2	1.40	0.86
1:C:372:ARG:HH22	1:C:438:VAL:HG11	1.38	0.86
1:E:443:LYS:HG2	1:E:448:GLN:HE21	1.40	0.86
1:A:443:LYS:HG2	1:A:448:GLN:HE21	1.38	0.85
1:C:443:LYS:HG2	1:C:448:GLN:HE21	1.42	0.85
1:E:204:THR:CG2	1:E:224:TRP:HE1	1.90	0.85
1:A:267:ASN:H	1:A:267:ASN:HD22	1.25	0.83
1:B:178:LYS:HE2	1:C:369:PRO:CD	2.09	0.83
1:B:267:ASN:HD22	1:B:267:ASN:H	1.27	0.82
1:D:252:VAL:HG13	1:D:326:LYS:HB2	1.61	0.82
1:C:204:THR:CG2	1:C:224:TRP:HE1	1.93	0.81
1:E:332:ARG:NH2	1:E:369:PRO:HD2	1.95	0.81
1:C:267:ASN:HD22	1:C:267:ASN:H	1.26	0.81
1:E:298:THR:HG22	1:E:300:GLU:N	1.96	0.80
1:B:178:LYS:HE2	1:C:369:PRO:HD3	1.63	0.80
1:A:298:THR:HG22	1:A:300:GLU:N	1.97	0.80
1:B:309:THR:HG22	1:B:404:MET:HE2	1.62	0.79
1:B:204:THR:CG2	1:B:224:TRP:HE1	1.96	0.79
1:C:298:THR:HG22	1:C:300:GLU:N	1.97	0.79
1:A:372:ARG:NH1	1:A:438:VAL:HG11	1.98	0.79
1:B:298:THR:HG22	1:B:300:GLU:N	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ARG:HD2	1:C:203:ARG:CZ	2.13	0.79
1:E:267:ASN:H	1:E:267:ASN:HD22	1.27	0.79
1:A:204:THR:CG2	1:A:224:TRP:HE1	1.96	0.78
1:D:204:THR:CG2	1:D:224:TRP:HE1	1.96	0.78
1:A:368:ALA:HB3	1:A:369:PRO:HD3	1.66	0.78
1:C:182:TYR:CD1	1:E:366:ASP:HB2	2.18	0.78
1:E:199:ARG:HD2	1:E:203:ARG:CZ	2.12	0.78
1:E:368:ALA:HB3	1:E:369:PRO:CD	2.14	0.78
1:D:256:HIS:CD2	1:D:258:ASN:H	2.03	0.76
1:E:256:HIS:CD2	1:E:258:ASN:H	2.02	0.76
1:B:199:ARG:HD2	1:B:203:ARG:CZ	2.15	0.76
1:C:256:HIS:CD2	1:C:258:ASN:H	2.03	0.76
1:D:294:ARG:HD2	1:D:295:TYR:CE1	2.21	0.76
1:D:365:ILE:HG23	1:D:367:ILE:H	1.51	0.76
1:C:368:ALA:HB3	1:C:369:PRO:HD3	1.68	0.76
1:B:256:HIS:CD2	1:B:258:ASN:H	2.05	0.75
1:D:199:ARG:HD2	1:D:203:ARG:CZ	2.16	0.75
1:D:298:THR:HG22	1:D:300:GLU:N	1.99	0.75
1:A:256:HIS:CD2	1:A:258:ASN:H	2.03	0.75
1:C:309:THR:HG22	1:C:404:MET:HE2	1.68	0.74
1:E:332:ARG:HH22	1:E:369:PRO:HD2	1.53	0.74
1:B:294:ARG:HD2	1:B:295:TYR:CE1	2.22	0.74
1:C:252:VAL:O	1:C:253:MET:HB3	1.88	0.74
1:C:294:ARG:HD2	1:C:295:TYR:CE1	2.23	0.74
1:D:417:ILE:O	1:D:420:ILE:HG12	1.88	0.73
1:B:417:ILE:O	1:B:420:ILE:HG12	1.88	0.73
1:E:417:ILE:O	1:E:420:ILE:HG12	1.89	0.73
1:D:267:ASN:N	1:D:267:ASN:HD22	1.85	0.73
1:A:294:ARG:HD2	1:A:295:TYR:CE1	2.23	0.72
1:A:199:ARG:HD2	1:A:203:ARG:CZ	2.19	0.72
1:C:417:ILE:O	1:C:420:ILE:HG12	1.89	0.72
1:C:248:ILE:HD13	1:C:355:ALA:HB3	1.69	0.72
1:E:309:THR:HG22	1:E:404:MET:HE2	1.71	0.72
1:E:437:SER:OG	1:E:440:GLU:HG3	1.89	0.72
1:B:437:SER:OG	1:B:440:GLU:HG3	1.90	0.72
1:D:309:THR:HG22	1:D:404:MET:HE2	1.72	0.71
1:E:294:ARG:HD2	1:E:295:TYR:CE1	2.24	0.71
1:A:417:ILE:O	1:A:420:ILE:HG12	1.89	0.71
1:D:368:ALA:HB2	1:E:178:LYS:CE	2.17	0.71
1:C:453:ASN:O	1:C:455:PRO:HD3	1.90	0.71
1:B:216:PHE:CD1	1:B:217:GLY:N	2.59	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:453:ASN:O	1:E:455:PRO:HD3	1.91	0.70
1:C:437:SER:OG	1:C:440:GLU:HG3	1.90	0.70
1:D:453:ASN:O	1:D:455:PRO:HD3	1.92	0.70
1:A:453:ASN:O	1:A:455:PRO:HD3	1.92	0.70
1:D:216:PHE:CD1	1:D:217:GLY:N	2.60	0.70
1:A:437:SER:OG	1:A:440:GLU:HG3	1.91	0.70
1:C:216:PHE:CD1	1:C:217:GLY:N	2.61	0.69
1:A:267:ASN:N	1:A:267:ASN:HD22	1.90	0.69
1:D:267:ASN:ND2	1:D:267:ASN:H	1.90	0.68
1:C:190:GLY:HA3	1:C:324:GLN:HE22	1.57	0.68
1:E:216:PHE:CD1	1:E:217:GLY:N	2.61	0.68
1:A:372:ARG:HG2	1:A:379:MET:HE1	1.75	0.67
1:C:461:CYS:SG	1:C:464:LEU:HD23	2.34	0.67
1:E:461:CYS:SG	1:E:464:LEU:HD23	2.34	0.67
1:A:216:PHE:CD1	1:A:217:GLY:N	2.62	0.67
1:C:371:HIS:CG	1:C:372:ARG:H	2.12	0.67
1:D:253:MET:O	1:D:253:MET:HG3	1.95	0.67
1:B:453:ASN:O	1:B:455:PRO:HD3	1.95	0.67
1:D:248:ILE:HD13	1:D:355:ALA:HB3	1.77	0.67
1:D:437:SER:OG	1:D:440:GLU:HG3	1.94	0.67
1:E:256:HIS:HD2	1:E:258:ASN:H	1.41	0.67
1:E:367:ILE:HG12	1:E:370:ASN:HD21	1.60	0.67
1:C:365:ILE:HG22	1:C:366:ASP:N	2.10	0.67
1:D:244:ARG:HH22	1:D:366:ASP:CG	1.98	0.66
1:C:498:GLN:O	1:C:499:GLU:HG3	1.95	0.66
1:B:267:ASN:HD22	1:B:267:ASN:N	1.92	0.66
1:D:267:ASN:N	1:D:267:ASN:ND2	2.44	0.66
1:A:254:LEU:HD12	1:A:255:ARG:H	1.59	0.66
1:D:357:ARG:HB2	1:D:366:ASP:HB2	1.78	0.66
1:E:204:THR:CG2	1:E:224:TRP:NE1	2.59	0.65
1:A:309:THR:HG22	1:A:404:MET:HE2	1.77	0.65
1:B:309:THR:HG22	1:B:404:MET:CE	2.26	0.65
1:D:461:CYS:SG	1:D:464:LEU:HD23	2.36	0.65
1:A:309:THR:HG22	1:A:404:MET:CE	2.27	0.65
1:E:267:ASN:N	1:E:267:ASN:HD22	1.93	0.65
1:B:365:ILE:O	1:B:365:ILE:HG13	1.95	0.65
1:C:357:ARG:H	1:C:366:ASP:HB2	1.62	0.65
1:B:251:THR:HG21	1:B:357:ARG:NH1	2.11	0.65
1:C:368:ALA:HB3	1:C:369:PRO:CD	2.27	0.64
1:C:285:HIS:HB2	1:C:341:VAL:O	1.97	0.64
1:D:256:HIS:HD2	1:D:258:ASN:H	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:ILE:HD11	1:D:393:PHE:HD1	1.62	0.64
1:E:209:GLU:OE2	1:E:221:ARG:NH1	2.28	0.64
1:C:332:ARG:NH2	1:C:367:ILE:HD12	2.13	0.64
1:B:267:ASN:H	1:B:267:ASN:ND2	1.95	0.64
1:A:365:ILE:HD12	1:A:365:ILE:N	2.12	0.63
1:C:309:THR:HG22	1:C:404:MET:CE	2.28	0.63
1:A:267:ASN:ND2	1:A:267:ASN:H	1.94	0.63
1:A:209:GLU:OE2	1:A:221:ARG:NH1	2.27	0.63
1:C:256:HIS:HD2	1:C:258:ASN:H	1.45	0.63
1:A:256:HIS:HD2	1:A:258:ASN:H	1.43	0.63
1:E:267:ASN:H	1:E:267:ASN:ND2	1.95	0.63
1:C:267:ASN:H	1:C:267:ASN:ND2	1.95	0.63
1:A:447:GLU:O	1:A:449:LYS:HG3	1.98	0.63
1:C:447:GLU:O	1:C:449:LYS:HG3	1.99	0.63
1:E:309:THR:HG22	1:E:404:MET:CE	2.29	0.63
1:C:209:GLU:OE2	1:C:221:ARG:NH1	2.28	0.62
1:D:209:GLU:OE2	1:D:221:ARG:NH1	2.27	0.62
1:D:376:LYS:HA	1:D:379:MET:HG3	1.82	0.62
1:C:204:THR:CG2	1:C:224:TRP:NE1	2.63	0.62
1:A:409:TRP:CD1	1:A:471:MET:HE1	2.34	0.62
1:D:409:TRP:CD1	1:D:471:MET:HE1	2.35	0.62
1:E:200:THR:O	1:E:204:THR:HB	2.00	0.62
1:D:204:THR:CG2	1:D:224:TRP:NE1	2.63	0.61
1:B:331:HIS:HD2	1:B:333:ASP:H	1.49	0.61
1:C:248:ILE:CD1	1:C:355:ALA:HB3	2.30	0.61
1:E:447:GLU:O	1:E:449:LYS:HG3	2.01	0.61
1:E:409:TRP:CD1	1:E:471:MET:HE1	2.36	0.61
1:B:200:THR:O	1:B:204:THR:HB	2.01	0.61
1:E:252:VAL:O	1:E:253:MET:HB3	2.01	0.61
1:B:199:ARG:HD3	1:B:266:ASP:OD2	1.99	0.61
1:D:447:GLU:O	1:D:449:LYS:HG3	2.01	0.61
1:B:267:ASN:N	1:B:267:ASN:ND2	2.49	0.60
1:E:362:THR:HG22	1:E:364:THR:HG23	1.83	0.60
1:B:461:CYS:SG	1:B:464:LEU:HD23	2.40	0.60
1:A:297:VAL:HG22	1:A:298:THR:N	2.16	0.60
1:B:447:GLU:O	1:B:449:LYS:HG3	2.02	0.60
1:E:430:ASP:OD1	1:E:431:LEU:HG	2.00	0.60
1:D:368:ALA:CB	1:E:178:LYS:HE2	2.27	0.60
1:E:244:ARG:HH11	1:E:244:ARG:HG2	1.67	0.60
1:A:409:TRP:HD1	1:A:471:MET:HE1	1.66	0.60
1:B:297:VAL:HG22	1:B:298:THR:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:VAL:HG22	1:C:298:THR:N	2.17	0.60
1:B:204:THR:CG2	1:B:224:TRP:NE1	2.64	0.60
1:D:326:LYS:HB2	1:D:327:PRO:HD2	1.84	0.59
1:A:267:ASN:N	1:A:267:ASN:ND2	2.48	0.59
1:A:461:CYS:SG	1:A:464:LEU:HD23	2.42	0.59
1:B:209:GLU:OE2	1:B:221:ARG:NH1	2.29	0.59
1:E:422:GLU:OE1	1:E:422:GLU:N	2.35	0.59
1:B:244:ARG:HG2	1:B:244:ARG:HH11	1.67	0.59
1:B:256:HIS:HD2	1:B:258:ASN:H	1.47	0.59
1:A:204:THR:CG2	1:A:224:TRP:NE1	2.65	0.59
1:A:323:THR:C	1:A:325:GLY:H	2.06	0.59
1:A:367:ILE:HD12	1:A:370:ASN:OD1	2.03	0.59
1:B:362:THR:HG22	1:B:364:THR:HG23	1.85	0.59
1:D:297:VAL:HG22	1:D:298:THR:N	2.18	0.59
1:E:198:GLN:HE22	1:E:250:GLN:NE2	2.01	0.59
1:A:369:PRO:HB2	1:A:373:VAL:HG11	1.85	0.59
1:B:409:TRP:CD1	1:B:471:MET:HE1	2.38	0.58
1:E:204:THR:HG22	1:E:224:TRP:HE1	1.67	0.58
1:E:297:VAL:HG22	1:E:298:THR:N	2.18	0.58
1:C:244:ARG:NH2	1:C:366:ASP:HB3	2.17	0.58
1:A:430:ASP:OD1	1:A:431:LEU:HG	2.03	0.58
1:C:331:HIS:HD2	1:C:333:ASP:H	1.51	0.58
1:C:362:THR:HG22	1:C:364:THR:HG23	1.85	0.58
1:C:430:ASP:OD1	1:C:431:LEU:HG	2.04	0.58
1:B:294:ARG:HD2	1:B:295:TYR:CZ	2.38	0.58
1:B:422:GLU:N	1:B:422:GLU:OE1	2.36	0.58
1:C:365:ILE:HG22	1:C:366:ASP:H	1.67	0.58
1:E:180:LEU:HD13	1:E:201:ILE:HD11	1.86	0.58
1:C:182:TYR:CE1	1:E:366:ASP:HB2	2.38	0.58
1:E:409:TRP:HD1	1:E:471:MET:HE1	1.69	0.58
1:D:309:THR:HG22	1:D:404:MET:CE	2.32	0.58
1:E:343:LYS:HB2	2:E:1:SO4:O2	2.03	0.58
1:A:190:GLY:HA3	1:A:253:MET:SD	2.44	0.58
1:D:430:ASP:OD1	1:D:431:LEU:HG	2.03	0.57
1:A:422:GLU:N	1:A:422:GLU:OE1	2.37	0.57
1:D:409:TRP:HD1	1:D:471:MET:HE1	1.68	0.57
1:D:200:THR:O	1:D:204:THR:HB	2.04	0.57
1:C:253:MET:O	1:C:253:MET:HG2	2.05	0.57
1:C:422:GLU:OE1	1:C:422:GLU:N	2.38	0.57
1:A:200:THR:O	1:A:204:THR:HB	2.04	0.57
1:B:252:VAL:HG13	1:B:327:PRO:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:TRP:CD1	1:C:471:MET:HE1	2.39	0.57
1:E:248:ILE:HD13	1:E:355:ALA:HB3	1.86	0.57
1:C:200:THR:O	1:C:204:THR:HB	2.04	0.57
1:A:376:LYS:HA	1:A:379:MET:HG3	1.86	0.57
1:D:253:MET:O	1:D:253:MET:CG	2.53	0.57
1:B:376:LYS:HA	1:B:379:MET:HG3	1.87	0.57
1:B:430:ASP:OD1	1:B:431:LEU:HG	2.04	0.57
1:D:199:ARG:HD3	1:D:266:ASP:OD2	2.04	0.57
1:E:331:HIS:HD2	1:E:333:ASP:H	1.52	0.57
1:B:229:VAL:HG22	1:B:280:SER:O	2.05	0.57
1:A:254:LEU:HD12	1:A:255:ARG:N	2.19	0.56
1:C:376:LYS:HA	1:C:379:MET:HG3	1.86	0.56
1:E:199:ARG:HD3	1:E:266:ASP:OD2	2.05	0.56
1:B:409:TRP:HB2	1:B:471:MET:HE3	1.87	0.56
1:D:294:ARG:HD2	1:D:295:TYR:CZ	2.39	0.56
1:B:198:GLN:HE22	1:B:250:GLN:NE2	2.03	0.56
1:C:267:ASN:N	1:C:267:ASN:ND2	2.50	0.56
1:C:389:ASN:HD21	1:C:391:LYS:HB3	1.71	0.56
1:E:267:ASN:N	1:E:267:ASN:ND2	2.50	0.56
1:B:258:ASN:ND2	1:B:311:SER:HB2	2.21	0.56
1:A:190:GLY:HA3	1:A:253:MET:CE	2.36	0.56
1:B:330:ALA:HB3	1:B:356:VAL:HG22	1.88	0.56
1:D:177:LEU:N	1:D:227:GLU:OE1	2.34	0.56
1:B:251:THR:HG21	1:B:357:ARG:HH12	1.70	0.55
1:B:487:ARG:O	1:B:491:THR:HG23	2.06	0.55
1:B:443:LYS:HG2	1:B:448:GLN:NE2	2.17	0.55
1:D:389:ASN:HD21	1:D:391:LYS:HB3	1.72	0.55
1:A:244:ARG:HG2	1:A:244:ARG:HH11	1.71	0.55
1:A:332:ARG:NH2	1:A:369:PRO:CG	2.65	0.55
1:B:409:TRP:HD1	1:B:471:MET:HE1	1.71	0.55
1:D:248:ILE:CD1	1:D:355:ALA:HB3	2.36	0.55
1:E:248:ILE:O	1:E:252:VAL:HG22	2.07	0.55
1:E:294:ARG:HD2	1:E:295:TYR:CZ	2.41	0.55
1:A:362:THR:HG22	1:A:364:THR:HG23	1.88	0.55
1:B:372:ARG:O	1:B:372:ARG:HG3	2.06	0.55
1:D:422:GLU:OE1	1:D:422:GLU:N	2.40	0.55
1:C:204:THR:HG22	1:C:224:TRP:HE1	1.70	0.55
1:D:204:THR:HG22	1:D:224:TRP:HE1	1.71	0.55
1:A:204:THR:HG22	1:A:224:TRP:HE1	1.71	0.55
1:C:240:ARG:O	1:C:244:ARG:HB2	2.07	0.55
1:C:498:GLN:C	1:C:499:GLU:HG3	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:TYR:OH	1:D:426:LEU:HD23	2.07	0.55
1:D:466:VAL:O	1:D:469:LYS:HB3	2.07	0.55
1:E:186:THR:HG22	1:E:187:SER:N	2.22	0.55
1:A:184:MET:HE2	1:A:255:ARG:HH12	1.70	0.54
1:C:487:ARG:O	1:C:491:THR:HG23	2.07	0.54
1:E:389:ASN:HD21	1:E:391:LYS:HB3	1.72	0.54
1:A:435:ASP:N	1:A:436:PRO:HD3	2.22	0.54
1:C:294:ARG:HD2	1:C:295:TYR:CZ	2.42	0.54
1:D:244:ARG:HG2	1:D:244:ARG:HH11	1.72	0.54
1:D:198:GLN:HE22	1:D:250:GLN:NE2	2.05	0.54
1:B:248:ILE:HD13	1:B:355:ALA:HB3	1.89	0.54
1:A:331:HIS:HD2	1:A:333:ASP:H	1.54	0.54
1:C:198:GLN:HE22	1:C:250:GLN:NE2	2.04	0.54
1:C:413:ARG:NH1	1:C:423:ASP:O	2.40	0.54
1:D:462:GLU:O	1:D:466:VAL:HG23	2.08	0.54
1:E:413:ARG:NH1	1:E:423:ASP:O	2.40	0.54
1:A:198:GLN:HE22	1:A:250:GLN:NE2	2.06	0.54
1:E:213:LYS:HG2	1:E:218:GLU:HG2	1.88	0.54
1:C:488:ILE:O	1:C:492:LEU:HB2	2.08	0.54
1:A:372:ARG:HG2	1:A:379:MET:CE	2.38	0.54
1:A:424:TYR:OH	1:A:426:LEU:HD23	2.07	0.54
1:C:244:ARG:HH22	1:C:366:ASP:HB3	1.71	0.54
1:D:362:THR:O	1:D:362:THR:HG22	2.08	0.54
1:D:362:THR:HG22	1:D:364:THR:HG23	1.89	0.54
1:D:365:ILE:HD11	1:D:393:PHE:CD1	2.42	0.54
1:E:409:TRP:HB2	1:E:471:MET:HE3	1.89	0.54
1:A:330:ALA:HB3	1:A:356:VAL:CG2	2.38	0.54
1:A:213:LYS:HG2	1:A:218:GLU:HG2	1.90	0.53
1:A:248:ILE:HD13	1:A:355:ALA:HB3	1.90	0.53
1:A:330:ALA:HB3	1:A:356:VAL:HG22	1.91	0.53
1:B:204:THR:HG22	1:B:224:TRP:HE1	1.70	0.53
1:D:368:ALA:C	1:D:370:ASN:H	2.09	0.53
1:E:362:THR:HG22	1:E:362:THR:O	2.08	0.53
1:E:443:LYS:HG2	1:E:448:GLN:NE2	2.18	0.53
1:B:330:ALA:HB3	1:B:356:VAL:CG2	2.38	0.53
1:B:389:ASN:HD21	1:B:391:LYS:HB3	1.72	0.53
1:A:326:LYS:NZ	1:A:327:PRO:O	2.42	0.53
1:B:394:GLU:OE2	1:B:397:LYS:HD2	2.09	0.53
1:C:330:ALA:HB3	1:C:356:VAL:HG22	1.91	0.53
1:D:331:HIS:HD2	1:D:333:ASP:H	1.56	0.53
1:A:389:ASN:HD21	1:A:391:LYS:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ARG:NH1	1:A:423:ASP:O	2.42	0.53
1:B:413:ARG:NH1	1:B:423:ASP:O	2.42	0.53
1:E:376:LYS:HA	1:E:379:MET:HG3	1.89	0.53
1:B:254:LEU:HD21	1:B:259:ILE:HD12	1.91	0.53
1:D:213:LYS:HG2	1:D:218:GLU:HG2	1.89	0.53
1:D:326:LYS:HG2	1:D:327:PRO:O	2.09	0.53
1:E:204:THR:HG21	1:E:224:TRP:HE1	1.71	0.53
1:E:240:ARG:O	1:E:244:ARG:HB2	2.09	0.53
1:C:372:ARG:CZ	1:C:438:VAL:HG11	2.39	0.52
1:D:369:PRO:O	1:D:371:HIS:N	2.43	0.52
1:C:204:THR:HG21	1:C:224:TRP:HE1	1.74	0.52
1:E:285:HIS:HB2	1:E:341:VAL:O	2.10	0.52
1:C:424:TYR:OH	1:C:426:LEU:HD23	2.10	0.52
1:E:487:ARG:O	1:E:491:THR:HG23	2.08	0.52
1:D:413:ARG:NH1	1:D:423:ASP:O	2.43	0.52
1:A:466:VAL:O	1:A:469:LYS:HB3	2.08	0.52
1:A:184:MET:CE	1:A:255:ARG:NH1	2.73	0.52
1:A:294:ARG:HD2	1:A:295:TYR:CZ	2.44	0.52
1:B:435:ASP:N	1:B:436:PRO:HD3	2.24	0.52
1:C:435:ASP:N	1:C:436:PRO:HD3	2.24	0.52
1:A:413:ARG:NH1	1:A:422:GLU:HB3	2.25	0.52
1:C:299:VAL:O	1:C:303:ILE:HG13	2.10	0.52
1:D:285:HIS:HB2	1:D:341:VAL:O	2.10	0.52
1:D:413:ARG:NH1	1:D:422:GLU:HB3	2.25	0.52
1:C:199:ARG:HD3	1:C:266:ASP:OD2	2.10	0.52
1:C:362:THR:O	1:C:362:THR:HG22	2.10	0.52
1:D:240:ARG:O	1:D:244:ARG:HB2	2.10	0.52
1:D:435:ASP:N	1:D:436:PRO:HD3	2.25	0.52
1:C:213:LYS:HG2	1:C:218:GLU:HG2	1.92	0.51
1:A:184:MET:HE2	1:A:255:ARG:NH1	2.25	0.51
1:C:330:ALA:HB3	1:C:356:VAL:CG2	2.40	0.51
1:A:488:ILE:O	1:A:492:LEU:HB2	2.10	0.51
1:C:267:ASN:HD22	1:C:267:ASN:N	1.91	0.51
1:D:330:ALA:HB3	1:D:356:VAL:HG22	1.93	0.51
1:D:330:ALA:HB3	1:D:356:VAL:CG2	2.40	0.51
1:E:413:ARG:NH1	1:E:422:GLU:HB3	2.26	0.51
1:C:462:GLU:O	1:C:466:VAL:HG23	2.09	0.51
1:E:424:TYR:OH	1:E:426:LEU:HD23	2.10	0.51
1:A:443:LYS:HG2	1:A:448:GLN:NE2	2.17	0.51
1:B:213:LYS:HG2	1:B:218:GLU:HG2	1.92	0.51
1:E:435:ASP:N	1:E:436:PRO:HD3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:ARG:H	1:D:366:ASP:HB3	1.76	0.51
1:E:330:ALA:HB3	1:E:356:VAL:HG22	1.93	0.51
1:A:298:THR:HG22	1:A:299:VAL:N	2.26	0.51
1:A:462:GLU:O	1:A:466:VAL:HG23	2.11	0.51
1:A:487:ARG:O	1:A:491:THR:HG23	2.10	0.51
1:B:240:ARG:O	1:B:244:ARG:HB2	2.11	0.51
1:D:367:ILE:HG13	1:D:369:PRO:HD3	1.91	0.51
1:B:466:VAL:O	1:B:469:LYS:HB3	2.11	0.50
1:D:487:ARG:O	1:D:491:THR:HG23	2.10	0.50
1:E:413:ARG:HG2	1:E:422:GLU:HB2	1.92	0.50
1:B:362:THR:O	1:B:362:THR:HG22	2.10	0.50
1:D:204:THR:HG21	1:D:224:TRP:HE1	1.75	0.50
1:A:409:TRP:HB2	1:A:471:MET:HE3	1.93	0.50
1:B:244:ARG:HG2	1:B:244:ARG:NH1	2.27	0.50
1:C:244:ARG:HH11	1:C:244:ARG:HG2	1.75	0.50
1:D:443:LYS:HG2	1:D:448:GLN:NE2	2.20	0.50
1:A:323:THR:O	1:A:325:GLY:N	2.42	0.50
1:C:356:VAL:HG23	1:C:393:PHE:HE1	1.76	0.50
1:C:413:ARG:NH1	1:C:422:GLU:HB3	2.27	0.50
1:D:409:TRP:HB2	1:D:471:MET:HE3	1.94	0.50
1:D:488:ILE:O	1:D:492:LEU:HB2	2.11	0.50
1:B:251:THR:HG22	1:B:252:VAL:HG23	1.94	0.50
1:E:298:THR:HG22	1:E:299:VAL:N	2.25	0.50
1:E:462:GLU:O	1:E:466:VAL:HG23	2.11	0.50
1:B:413:ARG:NH1	1:B:422:GLU:HB3	2.26	0.50
1:D:246:ALA:HB2	1:D:278:LEU:HD11	1.92	0.50
1:E:488:ILE:O	1:E:492:LEU:HB2	2.12	0.50
1:B:413:ARG:HG2	1:B:422:GLU:HB2	1.94	0.49
1:C:298:THR:HG22	1:C:299:VAL:N	2.27	0.49
1:B:298:THR:HG22	1:B:299:VAL:N	2.27	0.49
1:B:331:HIS:HD2	1:B:333:ASP:N	2.10	0.49
1:C:319:GLU:OE1	1:C:360:SER:HB3	2.12	0.49
1:C:332:ARG:HH21	1:C:367:ILE:HD12	1.77	0.49
1:E:224:TRP:CH2	1:E:225:ARG:HD2	2.48	0.49
1:D:369:PRO:HB2	1:D:390:MET:SD	2.53	0.49
1:A:190:GLY:O	1:A:253:MET:HB2	2.12	0.49
1:A:362:THR:O	1:A:362:THR:HG22	2.13	0.49
1:A:413:ARG:HG2	1:A:422:GLU:HB2	1.93	0.49
1:C:331:HIS:HD2	1:C:333:ASP:N	2.10	0.49
1:E:244:ARG:NH1	1:E:244:ARG:HG2	2.25	0.49
1:C:494:GLN:O	1:C:497:GLN:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:HIS:CG	1:C:372:ARG:N	2.80	0.49
1:D:299:VAL:O	1:D:303:ILE:HG13	2.12	0.49
1:E:205:ILE:CG2	1:E:206:VAL:N	2.76	0.49
1:A:248:ILE:O	1:A:252:VAL:HG22	2.13	0.49
1:C:285:HIS:HB3	1:C:341:VAL:HG13	1.95	0.49
1:E:466:VAL:O	1:E:469:LYS:HB3	2.13	0.49
1:A:184:MET:CE	1:A:255:ARG:HH12	2.25	0.49
1:A:215:ARG:HH12	1:A:374:GLY:HA2	1.77	0.49
1:E:331:HIS:HD2	1:E:333:ASP:N	2.11	0.49
1:B:300:GLU:HG3	1:B:501:ILE:HG12	1.93	0.48
1:E:330:ALA:HB3	1:E:356:VAL:CG2	2.44	0.48
1:B:285:HIS:HB2	1:B:341:VAL:O	2.13	0.48
1:C:409:TRP:HD1	1:C:471:MET:HE1	1.76	0.48
1:A:199:ARG:HD3	1:A:266:ASP:OD2	2.13	0.48
1:D:413:ARG:HG2	1:D:422:GLU:HB2	1.95	0.48
1:E:394:GLU:OE2	1:E:397:LYS:HD2	2.13	0.48
1:B:488:ILE:O	1:B:492:LEU:HB2	2.13	0.48
1:C:443:LYS:HG2	1:C:448:GLN:NE2	2.21	0.48
1:D:298:THR:HG22	1:D:299:VAL:N	2.28	0.48
1:D:372:ARG:HD3	1:D:379:MET:CE	2.43	0.48
1:E:342:LYS:HA	2:E:1:SO4:O4	2.13	0.48
1:E:346:THR:HG22	1:E:347:CYS:H	1.78	0.48
1:B:204:THR:HG21	1:B:224:TRP:HE1	1.76	0.48
1:C:303:ILE:HG21	1:C:496:SER:HB2	1.95	0.48
1:D:467:MET:O	1:D:471:MET:HG3	2.14	0.48
1:A:425:GLN:HB3	1:A:429:TYR:CD2	2.49	0.48
1:D:394:GLU:OE2	1:D:397:LYS:HD2	2.13	0.48
1:A:244:ARG:HG2	1:A:244:ARG:NH1	2.29	0.48
1:C:409:TRP:HB2	1:C:471:MET:HE3	1.96	0.48
1:C:303:ILE:CG2	1:C:496:SER:HB2	2.43	0.48
1:B:425:GLN:HB3	1:B:429:TYR:CD2	2.48	0.48
1:C:394:GLU:OE2	1:C:397:LYS:HD2	2.14	0.47
1:C:413:ARG:HG2	1:C:422:GLU:HB2	1.96	0.47
1:C:442:ARG:O	1:C:446:CYS:HB2	2.14	0.47
1:A:251:THR:HG21	1:A:357:ARG:HH12	1.79	0.47
1:E:489:LYS:O	1:E:493:SER:HB2	2.15	0.47
1:D:248:ILE:O	1:D:252:VAL:HB	2.15	0.47
1:E:442:ARG:O	1:E:446:CYS:HB2	2.14	0.47
1:A:356:VAL:HG23	1:A:393:PHE:HE1	1.79	0.47
1:B:198:GLN:HB3	1:B:264:ALA:HB1	1.97	0.47
1:C:323:THR:C	1:C:325:GLY:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:SER:OG	1:D:347:CYS:HB2	2.15	0.47
1:D:369:PRO:C	1:D:371:HIS:H	2.18	0.47
1:D:442:ARG:O	1:D:446:CYS:HB2	2.14	0.47
1:A:365:ILE:H	1:A:365:ILE:HD12	1.78	0.47
1:C:183:ASP:O	1:C:187:SER:HB2	2.15	0.47
1:C:425:GLN:HB3	1:C:429:TYR:CD2	2.50	0.47
1:D:204:THR:HG22	1:D:224:TRP:NE1	2.30	0.47
1:B:424:TYR:OH	1:B:426:LEU:HD23	2.14	0.47
1:D:224:TRP:CH2	1:D:225:ARG:HD2	2.50	0.47
1:A:394:GLU:OE2	1:A:397:LYS:HD2	2.15	0.47
1:A:346:THR:HG22	1:A:347:CYS:H	1.80	0.47
1:E:234:PHE:CE1	1:E:278:LEU:HD22	2.50	0.47
1:E:467:MET:O	1:E:471:MET:HG3	2.15	0.47
1:D:244:ARG:HG2	1:D:244:ARG:NH1	2.30	0.46
1:E:242:TRP:CD1	1:E:278:LEU:HD13	2.51	0.46
1:E:365:ILE:HG22	1:E:367:ILE:HG23	1.97	0.46
1:E:468:ALA:O	1:E:472:ARG:HG3	2.16	0.46
1:C:199:ARG:HD2	1:C:203:ARG:NE	2.29	0.46
1:C:365:ILE:CG2	1:C:366:ASP:N	2.78	0.46
1:D:249:TYR:CD2	1:D:262:PHE:HB2	2.50	0.46
1:A:299:VAL:O	1:A:303:ILE:HG13	2.15	0.46
1:B:442:ARG:O	1:B:446:CYS:HB2	2.15	0.46
1:A:459:GLN:NE2	1:A:465:ARG:CG	2.79	0.46
1:A:469:LYS:O	1:A:473:GLU:HG3	2.16	0.46
1:D:205:ILE:CG2	1:D:206:VAL:N	2.78	0.46
1:E:229:VAL:HG22	1:E:280:SER:O	2.16	0.46
1:A:459:GLN:HE22	1:A:465:ARG:HG2	1.81	0.46
1:B:204:THR:HG22	1:B:224:TRP:NE1	2.31	0.46
1:C:466:VAL:O	1:C:469:LYS:HB3	2.16	0.46
1:E:248:ILE:CD1	1:E:355:ALA:HB3	2.45	0.46
1:A:297:VAL:CG2	1:A:298:THR:N	2.79	0.46
1:E:299:VAL:O	1:E:303:ILE:HG13	2.14	0.46
1:E:367:ILE:CG1	1:E:370:ASN:HD21	2.26	0.46
1:A:240:ARG:O	1:A:244:ARG:HB2	2.16	0.46
1:B:299:VAL:O	1:B:303:ILE:HG13	2.16	0.46
1:D:372:ARG:HG2	1:D:379:MET:CE	2.45	0.46
1:E:497:GLN:O	1:E:497:GLN:HG2	2.15	0.46
1:B:310:ALA:HA	1:B:404:MET:CE	2.46	0.46
1:C:252:VAL:O	1:C:253:MET:CB	2.60	0.46
1:D:189:SER:C	1:D:191:SER:H	2.19	0.46
1:D:285:HIS:HB3	1:D:341:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:ILE:HG13	1:D:420:ILE:O	2.16	0.46
1:E:367:ILE:HG12	1:E:370:ASN:ND2	2.29	0.46
1:B:224:TRP:CH2	1:B:225:ARG:HD2	2.50	0.46
1:B:298:THR:CG2	1:B:299:VAL:N	2.79	0.46
1:B:420:ILE:HG13	1:B:420:ILE:O	2.16	0.46
1:C:409:TRP:HA	1:C:471:MET:HE1	1.97	0.46
1:C:492:LEU:HD12	1:C:492:LEU:HA	1.84	0.46
1:D:253:MET:CE	1:D:324:GLN:HA	2.46	0.46
1:D:425:GLN:HB3	1:D:429:TYR:CD2	2.50	0.46
1:E:367:ILE:HD12	1:E:367:ILE:H	1.81	0.46
1:A:372:ARG:CG	1:A:379:MET:CE	2.94	0.46
1:C:346:THR:HG22	1:C:347:CYS:H	1.80	0.46
1:C:385:ASP:OD1	1:C:387:SER:N	2.49	0.46
1:E:171:ILE:HD12	1:E:200:THR:CG2	2.46	0.46
1:A:234:PHE:CE1	1:A:278:LEU:HD22	2.51	0.45
1:A:298:THR:CG2	1:A:299:VAL:N	2.79	0.45
1:A:331:HIS:HD2	1:A:333:ASP:N	2.12	0.45
1:A:343:LYS:HB2	2:A:9:SO4:O3	2.17	0.45
1:A:467:MET:O	1:A:471:MET:HG3	2.15	0.45
1:B:247:GLU:O	1:B:251:THR:HB	2.16	0.45
1:C:297:VAL:CG2	1:C:298:THR:N	2.79	0.45
1:C:489:LYS:O	1:C:493:SER:HB2	2.16	0.45
1:D:365:ILE:HG23	1:D:366:ASP:N	2.30	0.45
1:E:298:THR:CG2	1:E:299:VAL:N	2.78	0.45
1:C:469:LYS:O	1:C:473:GLU:HG3	2.16	0.45
1:A:248:ILE:CD1	1:A:355:ALA:HB3	2.47	0.45
1:A:459:GLN:HA	1:A:459:GLN:NE2	2.31	0.45
1:D:469:LYS:O	1:D:473:GLU:HG3	2.16	0.45
1:D:489:LYS:O	1:D:493:SER:HB2	2.16	0.45
1:E:469:LYS:O	1:E:473:GLU:HG3	2.16	0.45
1:B:205:ILE:CG2	1:B:206:VAL:N	2.80	0.45
1:B:240:ARG:NH1	1:B:240:ARG:HB2	2.32	0.45
1:C:199:ARG:NH1	1:C:203:ARG:NH2	2.64	0.45
1:E:432:VAL:HA	1:E:433:PRO:HD3	1.81	0.45
1:C:205:ILE:CG2	1:C:206:VAL:N	2.79	0.45
1:C:420:ILE:O	1:C:420:ILE:HG13	2.15	0.45
1:D:294:ARG:HD3	1:D:294:ARG:O	2.17	0.45
1:D:346:THR:HG22	1:D:347:CYS:H	1.81	0.45
1:E:199:ARG:NH1	1:E:203:ARG:NH2	2.65	0.45
1:B:346:THR:HG22	1:B:347:CYS:H	1.81	0.45
1:D:297:VAL:CG2	1:D:298:THR:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:GLY:O	1:E:192:GLY:N	2.49	0.45
1:A:442:ARG:O	1:A:446:CYS:HB2	2.16	0.45
1:B:195:LEU:HD12	1:B:195:LEU:N	2.32	0.45
1:B:297:VAL:CG2	1:B:298:THR:N	2.79	0.45
1:B:215:ARG:HH11	1:B:354:LEU:HD11	1.81	0.45
1:B:356:VAL:HG23	1:B:393:PHE:HE1	1.82	0.45
1:C:459:GLN:HE22	1:C:465:ARG:HG2	1.82	0.45
1:D:199:ARG:NH1	1:D:203:ARG:NH2	2.65	0.45
1:D:199:ARG:HD2	1:D:203:ARG:NE	2.32	0.45
1:D:492:LEU:HD12	1:D:492:LEU:HA	1.85	0.45
1:A:205:ILE:CG2	1:A:206:VAL:N	2.79	0.45
1:C:294:ARG:O	1:C:294:ARG:HD3	2.17	0.45
1:D:171:ILE:HD11	1:D:197:VAL:HG13	1.98	0.45
1:A:420:ILE:O	1:A:420:ILE:HG13	2.16	0.44
1:B:310:ALA:HA	1:B:404:MET:HE1	1.99	0.44
1:C:229:VAL:HG22	1:C:280:SER:O	2.16	0.44
1:D:358:HIS:HB2	1:D:393:PHE:CD1	2.51	0.44
1:D:458:TRP:CG	1:D:464:LEU:HD12	2.52	0.44
1:C:244:ARG:NH1	1:C:244:ARG:HG2	2.32	0.44
1:E:420:ILE:O	1:E:420:ILE:HG13	2.16	0.44
1:A:224:TRP:CH2	1:A:225:ARG:HD2	2.53	0.44
1:B:432:VAL:HA	1:B:433:PRO:HD3	1.83	0.44
1:C:498:GLN:O	1:C:499:GLU:CG	2.64	0.44
1:D:195:LEU:HD12	1:D:195:LEU:N	2.31	0.44
1:D:459:GLN:NE2	1:D:459:GLN:HA	2.33	0.44
1:E:297:VAL:CG2	1:E:298:THR:N	2.80	0.44
1:A:371:HIS:O	1:A:373:VAL:HG13	2.18	0.44
1:C:204:THR:HG22	1:C:224:TRP:NE1	2.31	0.44
1:C:298:THR:CG2	1:C:299:VAL:N	2.79	0.44
1:C:365:ILE:CG2	1:C:366:ASP:H	2.30	0.44
1:E:308:SER:OG	1:E:347:CYS:HB2	2.16	0.44
1:E:331:HIS:O	1:E:332:ARG:HB2	2.17	0.44
1:E:425:GLN:HB3	1:E:429:TYR:CD2	2.52	0.44
1:A:468:ALA:O	1:A:472:ARG:HG3	2.18	0.44
1:A:489:LYS:O	1:A:493:SER:HB2	2.18	0.44
1:B:215:ARG:NH1	1:B:354:LEU:HD11	2.32	0.44
1:B:458:TRP:CG	1:B:464:LEU:HD12	2.52	0.44
1:E:294:ARG:O	1:E:294:ARG:HD3	2.18	0.44
1:A:285:HIS:HB2	1:A:341:VAL:O	2.17	0.44
1:A:294:ARG:O	1:A:294:ARG:HD3	2.17	0.44
1:B:199:ARG:HD2	1:B:203:ARG:NE	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:TRP:HB2	1:C:471:MET:CE	2.48	0.44
1:D:298:THR:CG2	1:D:299:VAL:N	2.81	0.44
1:E:428:TYR:O	1:E:432:VAL:HG12	2.18	0.44
1:A:458:TRP:CG	1:A:464:LEU:HD12	2.53	0.44
1:B:462:GLU:O	1:B:466:VAL:HG23	2.17	0.44
1:C:459:GLN:NE2	1:C:465:ARG:CG	2.81	0.44
1:C:287:SER:HA	1:C:340:LEU:HD23	2.00	0.44
1:D:317:HIS:HD2	1:D:329:ILE:O	2.01	0.44
1:E:458:TRP:CG	1:E:464:LEU:HD12	2.52	0.43
1:E:199:ARG:HD2	1:E:203:ARG:NE	2.32	0.43
1:E:205:ILE:HG22	1:E:206:VAL:N	2.33	0.43
1:A:366:ASP:O	1:A:366:ASP:OD2	2.36	0.43
1:A:454:ILE:HG23	1:A:458:TRP:CE3	2.54	0.43
1:B:459:GLN:NE2	1:B:459:GLN:HA	2.34	0.43
1:A:240:ARG:NH1	1:A:240:ARG:HB2	2.34	0.43
1:D:331:HIS:HD2	1:D:333:ASP:N	2.16	0.43
1:A:195:LEU:N	1:A:195:LEU:HD12	2.33	0.43
1:B:409:TRP:HB2	1:B:471:MET:CE	2.47	0.43
1:B:489:LYS:O	1:B:493:SER:HB2	2.18	0.43
1:C:467:MET:O	1:C:471:MET:HG3	2.17	0.43
1:C:306:ALA:HB1	1:C:492:LEU:HD21	2.00	0.43
1:D:459:GLN:HE22	1:D:465:ARG:HG2	1.84	0.43
1:E:310:ALA:HA	1:E:404:MET:CE	2.49	0.43
1:A:199:ARG:NH1	1:A:203:ARG:NH2	2.66	0.43
1:A:323:THR:OG1	1:A:324:GLN:N	2.50	0.43
1:B:428:TYR:O	1:B:432:VAL:HG12	2.18	0.43
1:C:291:TYR:CG	1:C:341:VAL:HG11	2.52	0.43
1:A:204:THR:HG21	1:A:224:TRP:HE1	1.78	0.43
1:D:414:ARG:HD2	1:D:424:TYR:HB2	2.01	0.43
1:B:211:ILE:O	1:B:211:ILE:HG22	2.19	0.43
1:B:331:HIS:CD2	1:B:333:ASP:H	2.34	0.43
1:B:362:THR:HG22	1:B:364:THR:CG2	2.49	0.43
1:C:458:TRP:CG	1:C:464:LEU:HD12	2.53	0.43
1:C:459:GLN:HA	1:C:459:GLN:NE2	2.34	0.43
1:D:237:ARG:HG2	1:D:237:ARG:O	2.19	0.43
1:D:331:HIS:O	1:D:332:ARG:HB2	2.19	0.43
1:E:195:LEU:HD12	1:E:195:LEU:N	2.33	0.43
1:E:459:GLN:NE2	1:E:459:GLN:HA	2.34	0.43
1:A:428:TYR:O	1:A:432:VAL:HG12	2.19	0.43
1:C:457:ARG:C	1:C:459:GLN:H	2.22	0.43
1:D:211:ILE:HG22	1:D:211:ILE:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:457:ARG:C	1:E:459:GLN:H	2.21	0.43
1:A:204:THR:HG22	1:A:224:TRP:NE1	2.32	0.43
1:C:190:GLY:CA	1:C:324:GLN:HE22	2.27	0.43
1:C:428:TYR:O	1:C:432:VAL:HG12	2.19	0.43
1:B:307:LEU:HA	1:B:492:LEU:HD23	2.01	0.42
1:C:297:VAL:CG2	1:C:301:GLY:HA3	2.48	0.42
1:E:365:ILE:N	1:E:365:ILE:HD12	2.34	0.42
1:C:195:LEU:N	1:C:195:LEU:HD12	2.34	0.42
1:C:253:MET:O	1:C:254:LEU:C	2.57	0.42
1:C:473:GLU:HB2	1:C:483:LEU:CD1	2.49	0.42
1:D:468:ALA:O	1:D:472:ARG:HG3	2.19	0.42
1:E:211:ILE:O	1:E:211:ILE:HG22	2.18	0.42
1:E:237:ARG:HG2	1:E:237:ARG:O	2.19	0.42
1:E:362:THR:HG22	1:E:364:THR:CG2	2.50	0.42
1:A:470:ILE:HD13	1:A:488:ILE:HG23	2.01	0.42
1:B:495:LEU:O	1:B:499:GLU:HG2	2.19	0.42
1:C:368:ALA:CB	1:C:369:PRO:CD	2.95	0.42
1:C:372:ARG:HD2	1:C:383:VAL:O	2.19	0.42
1:C:433:PRO:O	1:C:436:PRO:HG3	2.19	0.42
1:D:457:ARG:C	1:D:459:GLN:H	2.23	0.42
1:B:457:ARG:C	1:B:459:GLN:H	2.23	0.42
1:B:385:ASP:OD1	1:B:387:SER:N	2.51	0.42
1:D:252:VAL:O	1:D:253:MET:CG	2.58	0.42
1:D:459:GLN:NE2	1:D:465:ARG:CG	2.82	0.42
1:E:204:THR:HG22	1:E:224:TRP:NE1	2.28	0.42
1:B:252:VAL:C	1:B:253:MET:HG3	2.40	0.42
1:B:254:LEU:C	1:B:254:LEU:CD2	2.88	0.42
1:B:294:ARG:O	1:B:294:ARG:HD3	2.20	0.42
1:B:433:PRO:O	1:B:436:PRO:HG3	2.19	0.42
1:C:490:LYS:HE3	1:C:490:LYS:HB2	1.85	0.42
1:E:409:TRP:HB2	1:E:471:MET:CE	2.49	0.42
1:C:432:VAL:HA	1:C:433:PRO:HD3	1.82	0.42
1:A:251:THR:HG21	1:A:357:ARG:NH1	2.34	0.42
1:B:308:SER:HB2	1:B:346:THR:HG22	2.02	0.42
1:B:467:MET:O	1:B:471:MET:HG3	2.19	0.42
1:D:242:TRP:CD1	1:D:278:LEU:HD13	2.54	0.42
1:D:368:ALA:O	1:D:370:ASN:N	2.52	0.42
1:D:432:VAL:HA	1:D:433:PRO:HD3	1.80	0.42
1:B:490:LYS:HB2	1:B:490:LYS:HE3	1.86	0.42
1:D:470:ILE:HD13	1:D:488:ILE:HG23	2.01	0.42
1:A:197:VAL:O	1:A:201:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:ILE:HD13	1:C:488:ILE:HG23	2.02	0.41
1:D:357:ARG:H	1:D:366:ASP:CB	2.33	0.41
1:E:367:ILE:HG21	1:E:370:ASN:OD1	2.20	0.41
1:C:193:LEU:HA	1:C:194:PRO:HD3	1.93	0.41
1:D:240:ARG:HB2	1:D:240:ARG:NH1	2.35	0.41
1:B:184:MET:O	1:B:188:GLY:HA3	2.20	0.41
1:B:434:SER:O	1:B:435:ASP:HB3	2.21	0.41
1:B:469:LYS:O	1:B:473:GLU:HG3	2.19	0.41
1:C:443:LYS:O	1:C:447:GLU:HB2	2.19	0.41
1:D:229:VAL:HG22	1:D:280:SER:O	2.21	0.41
1:E:368:ALA:CB	1:E:369:PRO:CD	2.75	0.41
1:C:246:ALA:HB2	1:C:278:LEU:HD11	2.02	0.41
1:C:468:ALA:O	1:C:472:ARG:HG3	2.21	0.41
1:D:252:VAL:CG1	1:D:326:LYS:HB2	2.41	0.41
1:E:190:GLY:O	1:E:191:SER:C	2.59	0.41
1:E:358:HIS:HB2	1:E:393:PHE:CD1	2.55	0.41
1:A:183:ASP:O	1:A:187:SER:HB2	2.21	0.41
1:A:443:LYS:O	1:A:447:GLU:HB2	2.20	0.41
1:D:443:LYS:O	1:D:447:GLU:HB2	2.21	0.41
1:E:285:HIS:HB3	1:E:341:VAL:HG13	2.02	0.41
1:A:323:THR:C	1:A:325:GLY:N	2.73	0.41
1:B:193:LEU:HA	1:B:194:PRO:HD3	1.90	0.41
1:B:270:ASN:O	1:B:271:GLY:C	2.58	0.41
1:B:343:LYS:HB2	2:B:6:SO4:O4	2.20	0.41
1:D:310:ALA:HA	1:D:404:MET:HE1	2.03	0.41
1:A:492:LEU:HA	1:A:492:LEU:HD12	1.87	0.41
1:D:326:LYS:CB	1:D:327:PRO:HD2	2.51	0.41
1:E:278:LEU:HD12	1:E:278:LEU:HA	1.95	0.41
1:E:331:HIS:CD2	1:E:333:ASP:H	2.35	0.41
1:B:358:HIS:HB2	1:B:393:PHE:CD1	2.55	0.41
1:E:187:SER:O	1:E:188:GLY:C	2.59	0.41
1:E:444:VAL:HG13	1:E:450:LEU:HD12	2.03	0.41
1:A:414:ARG:HD2	1:A:424:TYR:HB2	2.03	0.41
1:B:237:ARG:HG2	1:B:237:ARG:O	2.21	0.41
1:D:432:VAL:CG2	1:D:433:PRO:HD2	2.51	0.41
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.90	0.41
1:A:331:HIS:O	1:A:332:ARG:HB2	2.21	0.41
1:A:490:LYS:HE3	1:A:490:LYS:HB2	1.87	0.41
1:B:331:HIS:O	1:B:332:ARG:HB2	2.21	0.41
1:B:443:LYS:O	1:B:447:GLU:HB2	2.21	0.41
1:B:459:GLN:NE2	1:B:465:ARG:CG	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ILE:HG22	1:D:206:VAL:N	2.35	0.41
1:E:331:HIS:HE1	1:E:350:ALA:O	2.04	0.41
1:E:414:ARG:HD2	1:E:424:TYR:HB2	2.03	0.41
1:C:357:ARG:HB2	1:C:366:ASP:CG	2.42	0.41
1:D:433:PRO:O	1:D:436:PRO:HG3	2.21	0.41
1:E:240:ARG:NH1	1:E:240:ARG:HB2	2.36	0.41
1:A:407:VAL:O	1:A:411:ILE:HG13	2.22	0.40
1:B:308:SER:OG	1:B:347:CYS:HB2	2.21	0.40
1:B:302:MET:HG3	1:B:411:ILE:HG22	2.02	0.40
1:B:473:GLU:HB2	1:B:483:LEU:CD1	2.52	0.40
1:C:190:GLY:HA3	1:C:324:GLN:NE2	2.31	0.40
1:C:258:ASN:O	1:C:348:CYS:HA	2.20	0.40
1:C:362:THR:HG22	1:C:364:THR:CG2	2.50	0.40
1:D:372:ARG:HG2	1:D:379:MET:HE2	2.02	0.40
1:D:376:LYS:N	1:D:376:LYS:HD2	2.36	0.40
1:B:414:ARG:HD2	1:B:424:TYR:HB2	2.03	0.40
1:C:224:TRP:CH2	1:C:225:ARG:HD2	2.57	0.40
1:A:433:PRO:O	1:A:436:PRO:HG3	2.22	0.40
1:A:365:ILE:CD1	1:A:365:ILE:N	2.80	0.40
1:A:372:ARG:CG	1:A:379:MET:HE2	2.52	0.40
1:B:459:GLN:HE22	1:B:465:ARG:HG2	1.86	0.40
1:C:237:ARG:HG2	1:C:237:ARG:O	2.21	0.40
1:C:331:HIS:O	1:C:332:ARG:HB2	2.22	0.40
1:C:434:SER:O	1:C:435:ASP:HB3	2.21	0.40
1:D:171:ILE:HG22	1:D:171:ILE:O	2.20	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:E:453:ASN:ND2	1:E:453:ASN:ND2[4_566]	2.19	0.01

## 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	328/342 (96%)	291 (89%)	29 (9%)	8 (2%)	7	27
1	B	318/342 (93%)	284 (89%)	26 (8%)	8 (2%)	6	25
1	C	328/342 (96%)	287 (88%)	33 (10%)	8 (2%)	7	27
1	D	328/342 (96%)	291 (89%)	31 (10%)	6 (2%)	10	34
1	E	328/342 (96%)	291 (89%)	28 (8%)	9 (3%)	6	23
All	All	1630/1710 (95%)	1444 (89%)	147 (9%)	39 (2%)	7	27

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	PRO
1	B	188	GLY
1	D	370	ASN
1	A	323	THR
1	A	324	GLN
1	B	271	GLY
1	C	190	GLY
1	C	254	LEU
1	E	188	GLY
1	E	191	SER
1	A	271	GLY
1	A	447	GLU
1	A	460	SER
1	B	366	ASP
1	B	460	SER
1	C	271	GLY
1	C	460	SER
1	D	460	SER
1	E	271	GLY
1	E	368	ALA
1	E	460	SER
1	B	447	GLU
1	C	447	GLU
1	C	458	TRP
1	D	271	GLY
1	D	447	GLU
1	E	447	GLU
1	B	458	TRP

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Mol	Chain	Res	Type
1	C	448	GLN
1	D	369	PRO
1	D	458	TRP
1	A	448	GLN
1	A	458	TRP
1	B	448	GLN
1	E	458	TRP
1	C	455	PRO
1	E	369	PRO
1	E	455	PRO
1	B	455	PRO

### 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	282/294 (96%)	266 (94%)	16 (6%)	24	56
1	B	278/294 (95%)	261 (94%)	17 (6%)	22	53
1	C	282/294 (96%)	265 (94%)	17 (6%)	22	54
1	D	282/294 (96%)	264 (94%)	18 (6%)	20	50
1	E	282/294 (96%)	265 (94%)	17 (6%)	22	54
All	All	1406/1470 (96%)	1321 (94%)	85 (6%)	22	54

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	THR
1	A	209	GLU
1	A	229	VAL
1	A	244	ARG
1	A	267	ASN
1	A	269	ASP
1	A	278	LEU
1	A	292	LEU

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Mol	Chain	Res	Type
1	A	307	LEU
1	A	326	LYS
1	A	341	VAL
1	A	365	ILE
1	A	367	ILE
1	A	422	GLU
1	A	486	LEU
1	A	491	THR
1	B	204	THR
1	B	209	GLU
1	B	229	VAL
1	B	244	ARG
1	B	251	THR
1	B	254	LEU
1	B	267	ASN
1	B	269	ASP
1	B	278	LEU
1	B	292	LEU
1	B	307	LEU
1	B	326	LYS
1	B	341	VAL
1	B	372	ARG
1	B	422	GLU
1	B	486	LEU
1	B	491	THR
1	C	204	THR
1	C	209	GLU
1	C	229	VAL
1	C	244	ARG
1	C	253	MET
1	C	255	ARG
1	C	267	ASN
1	C	269	ASP
1	C	278	LEU
1	C	292	LEU
1	C	307	LEU
1	C	324	GLN
1	C	341	VAL
1	C	366	ASP
1	C	370	ASN
1	C	486	LEU
1	C	491	THR

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Mol	Chain	Res	Type
1	D	187	SER
1	D	204	THR
1	D	209	GLU
1	D	229	VAL
1	D	244	ARG
1	D	267	ASN
1	D	269	ASP
1	D	278	LEU
1	D	292	LEU
1	D	307	LEU
1	D	321	VAL
1	D	326	LYS
1	D	341	VAL
1	D	422	GLU
1	D	486	LEU
1	D	491	THR
1	D	497	GLN
1	D	499	GLU
1	E	204	THR
1	E	209	GLU
1	E	229	VAL
1	E	244	ARG
1	E	267	ASN
1	E	269	ASP
1	E	278	LEU
1	E	292	LEU
1	E	307	LEU
1	E	321	VAL
1	E	326	LYS
1	E	341	VAL
1	E	366	ASP
1	E	367	ILE
1	E	376	LYS
1	E	486	LEU
1	E	491	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	256	HIS
1	A	258	ASN

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Mol	Chain	Res	Type
1	A	267	ASN
1	A	315	HIS
1	A	331	HIS
1	A	389	ASN
1	A	448	GLN
1	A	459	GLN
1	B	250	GLN
1	B	256	HIS
1	B	258	ASN
1	B	267	ASN
1	B	315	HIS
1	B	331	HIS
1	B	389	ASN
1	B	448	GLN
1	B	459	GLN
1	C	250	GLN
1	C	256	HIS
1	C	258	ASN
1	C	267	ASN
1	C	285	HIS
1	C	315	HIS
1	C	324	GLN
1	C	331	HIS
1	C	389	ASN
1	C	448	GLN
1	C	459	GLN
1	C	497	GLN
1	D	250	GLN
1	D	256	HIS
1	D	258	ASN
1	D	267	ASN
1	D	315	HIS
1	D	331	HIS
1	D	370	ASN
1	D	389	ASN
1	D	448	GLN
1	D	459	GLN
1	D	497	GLN
1	E	250	GLN
1	E	256	HIS
1	E	258	ASN
1	E	267	ASN

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Mol	Chain	Res	Type
1	E	315	HIS
1	E	331	HIS
1	E	370	ASN
1	E	389	ASN
1	E	448	GLN
1	E	459	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

15 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	18	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SO4	A	21	-	4,4,4	0.39	0	6,6,6	0.05	0
2	SO4	A	9	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SO4	B	11	-	4,4,4	0.35	0	6,6,6	0.17	0
2	SO4	B	12	-	4,4,4	0.42	0	6,6,6	0.19	0
2	SO4	B	6	-	4,4,4	0.36	0	6,6,6	0.21	0
2	SO4	C	10	-	4,4,4	0.39	0	6,6,6	0.13	0
2	SO4	C	4	-	4,4,4	0.42	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	C	5	-	4,4,4	0.38	0	6,6,6	0.10	0
2	SO4	D	13	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	D	14	-	4,4,4	0.34	0	6,6,6	0.17	0
2	SO4	D	15	-	4,4,4	0.41	0	6,6,6	0.12	0
2	SO4	E	1	-	4,4,4	0.35	0	6,6,6	0.36	0
2	SO4	E	2	-	4,4,4	0.36	0	6,6,6	0.14	0
2	SO4	E	20	-	4,4,4	0.39	0	6,6,6	0.13	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	18	-	-	0/0/0/0	0/0/0/0
2	SO4	A	21	-	-	0/0/0/0	0/0/0/0
2	SO4	A	9	-	-	0/0/0/0	0/0/0/0
2	SO4	B	11	-	-	0/0/0/0	0/0/0/0
2	SO4	B	12	-	-	0/0/0/0	0/0/0/0
2	SO4	B	6	-	-	0/0/0/0	0/0/0/0
2	SO4	C	10	-	-	0/0/0/0	0/0/0/0
2	SO4	C	4	-	-	0/0/0/0	0/0/0/0
2	SO4	C	5	-	-	0/0/0/0	0/0/0/0
2	SO4	D	13	-	-	0/0/0/0	0/0/0/0
2	SO4	D	14	-	-	0/0/0/0	0/0/0/0
2	SO4	D	15	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1	-	-	0/0/0/0	0/0/0/0
2	SO4	E	2	-	-	0/0/0/0	0/0/0/0
2	SO4	E	20	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9	SO4	1	0
2	B	6	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	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, 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	330/342 (96%)	0.45	12 (3%) 43 37	38, 78, 104, 120	0
1	B	324/342 (94%)	0.67	19 (5%) 23 18	34, 60, 93, 108	0
1	C	330/342 (96%)	0.93	46 (13%) 3 2	34, 77, 103, 124	0
1	D	330/342 (96%)	0.54	8 (2%) 59 55	30, 65, 98, 109	0
1	E	330/342 (96%)	0.37	4 (1%) 79 77	30, 57, 94, 107	0
All	All	1644/1710 (96%)	0.59	89 (5%) 26 22	30, 67, 101, 124	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	368	ALA	6.0
1	C	369	PRO	5.6
1	D	458	TRP	4.7
1	C	481	ALA	4.6
1	C	295	TYR	4.4
1	C	323	THR	4.4
1	C	426	LEU	4.3
1	A	417	ILE	4.3
1	C	472	ARG	4.2
1	C	463	ALA	4.0
1	C	476	TYR	3.9
1	D	417	ILE	3.8
1	C	349	ILE	3.7
1	B	190	GLY	3.5
1	C	254	LEU	3.5
1	B	388	ILE	3.4
1	D	420	ILE	3.3
1	C	409	TRP	3.2
1	B	325	GLY	3.1
1	D	438	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	427	PRO	3.0
1	B	251	THR	3.0
1	C	474	CYS	2.9
1	C	188	GLY	2.9
1	C	443	LYS	2.7
1	C	406	LEU	2.7
1	C	324	GLN	2.7
1	B	443	LYS	2.7
1	C	485	ALA	2.7
1	A	428	TYR	2.7
1	B	187	SER	2.6
1	C	482	ARG	2.6
1	E	432	VAL	2.6
1	A	431	LEU	2.6
1	C	190	GLY	2.6
1	A	371	HIS	2.6
1	B	383	VAL	2.6
1	B	253	MET	2.6
1	E	431	LEU	2.6
1	C	475	TRP	2.6
1	C	450	LEU	2.5
1	C	296	THR	2.5
1	B	365	ILE	2.5
1	B	254	LEU	2.5
1	B	431	LEU	2.5
1	D	439	GLU	2.5
1	B	396	PHE	2.5
1	C	420	ILE	2.5
1	A	237	ARG	2.4
1	C	433	PRO	2.4
1	C	496	SER	2.4
1	C	376	LYS	2.4
1	C	215	ARG	2.4
1	C	252	VAL	2.4
1	C	411	ILE	2.4
1	A	442	ARG	2.4
1	C	379	MET	2.4
1	C	318	MET	2.4
1	B	438	VAL	2.3
1	D	236	SER	2.3
1	B	444	VAL	2.3
1	A	369	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	432	VAL	2.3
1	C	187	SER	2.3
1	B	393	PHE	2.2
1	D	431	LEU	2.2
1	D	253	MET	2.2
1	B	213	LYS	2.2
1	C	479	GLY	2.2
1	B	450	LEU	2.2
1	C	483	LEU	2.2
1	C	383	VAL	2.2
1	C	458	TRP	2.2
1	C	189	SER	2.2
1	A	427	PRO	2.1
1	C	294	ARG	2.1
1	E	450	LEU	2.1
1	C	365	ILE	2.1
1	A	292	LEU	2.1
1	A	384	LEU	2.1
1	B	392	HIS	2.1
1	A	302	MET	2.1
1	B	216	PHE	2.1
1	E	368	ALA	2.0
1	C	491	THR	2.0
1	C	487	ARG	2.0
1	C	417	ILE	2.0
1	C	452	PRO	2.0
1	C	464	LEU	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, 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
2	SO4	A	9	5/5	0.89	0.25	1.33	111,112,112,112	0
2	SO4	C	5	5/5	0.88	0.29	-0.45	118,119,119,120	0
2	SO4	D	14	5/5	0.88	0.18	-0.59	109,109,109,110	0
2	SO4	D	13	5/5	0.95	0.19	-1.07	93,93,94,94	0
2	SO4	E	2	5/5	0.86	0.17	-1.18	111,111,113,113	0
2	SO4	C	10	5/5	0.92	0.18	-1.21	98,99,100,100	0
2	SO4	E	1	5/5	0.86	0.18	-1.26	93,94,94,95	0
2	SO4	B	12	5/5	0.92	0.19	-1.31	98,99,100,100	0
2	SO4	A	21	5/5	0.91	0.13	-1.46	123,123,123,123	0
2	SO4	B	6	5/5	0.87	0.16	-1.89	99,99,100,100	0
2	SO4	B	11	5/5	0.95	0.12	-	99,100,100,101	0
2	SO4	D	15	5/5	0.84	0.23	-	111,111,112,112	0
2	SO4	A	18	5/5	0.89	0.15	-	104,104,105,105	0
2	SO4	C	4	5/5	0.88	0.13	-	100,101,102,102	0
2	SO4	E	20	5/5	0.91	0.14	-	109,109,110,110	0

## 6.5 Other polymers

There are no such residues in this entry.