



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:56 PM GMT

PDB ID : 1Z5H  
Title : Crystal structures of the Tricorn interacting Factor F3 from *Thermoplasma acidophilum*  
Authors : Kyrieleis, O.J.P.; Goettig, P.; Kiefersauer, R.; Huber, R.; Brandstetter, H.  
Deposited on : 2005-03-18  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

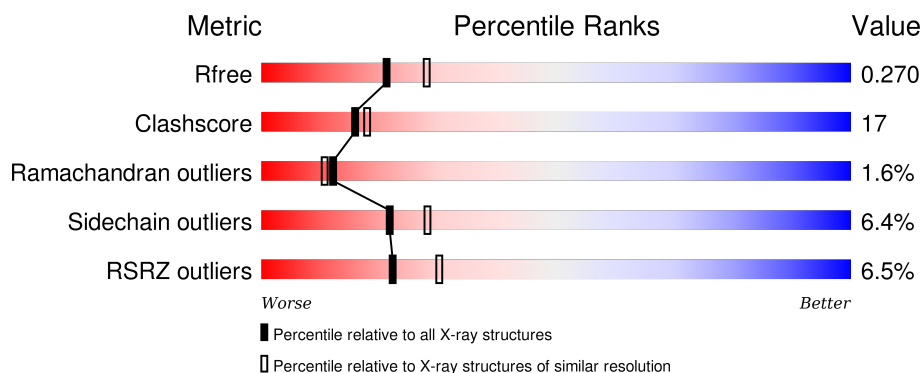
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	780	<div> <div>6%</div> <div>68%</div> <div>29%</div> <div>.</div> </div>
1	B	780	<div> <div>7%</div> <div>64%</div> <div>32%</div> <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	A	1010	-	-	-	X
2	SO4	B	1004	-	-	-	X
2	SO4	B	1011	-	-	-	X
2	SO4	B	1012	-	-	-	X
3	ZN	A	2001	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13456 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 Tricorn protease interacting factor F3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	780	Total	C	N	O	S	2	0	0
			6295	4008	1066	1190	31			
1	B	780	Total	C	N	O	S	8	0	0
			6295	4008	1066	1190	31			

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



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

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	442	Total	O	0	0
			442	442		
4	B	337	Total	O	0	0
			337	337		

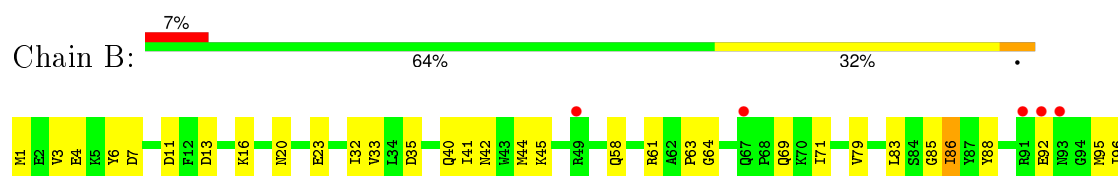
### 3 Residue-property plots

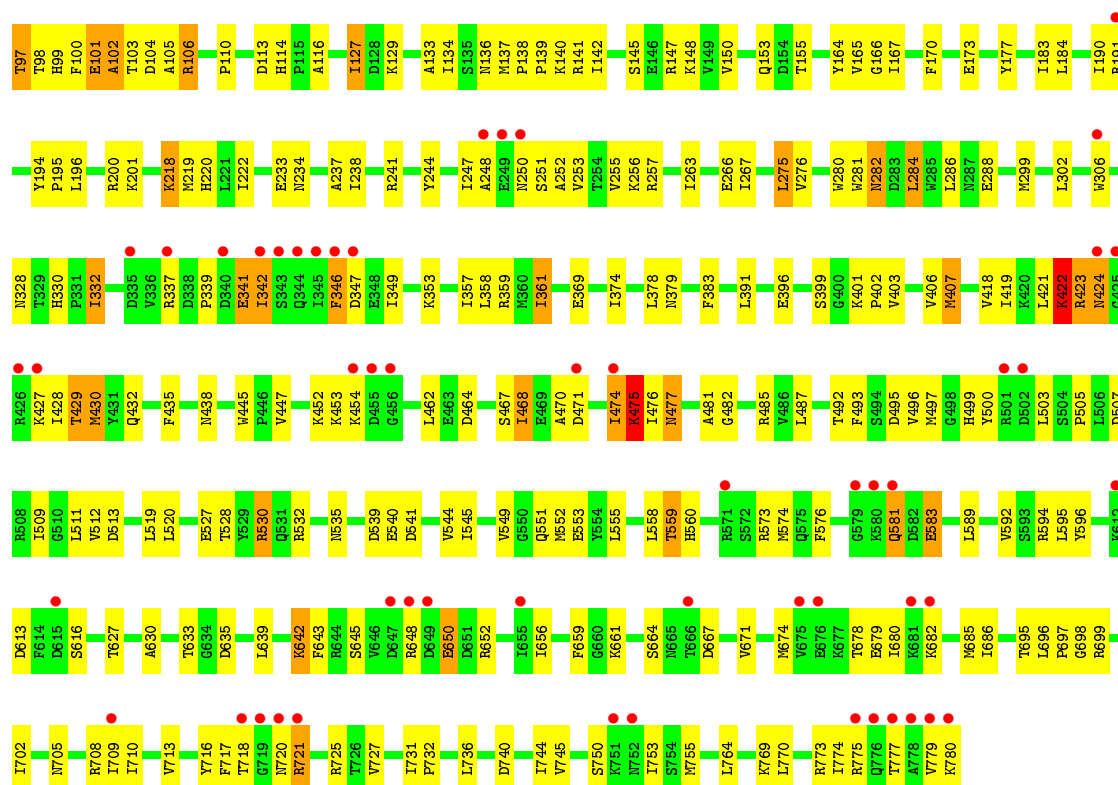
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: Tricorn protease interacting factor F3



#### • Molecule 1: Tricorn protease interacting factor F3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.20 Å   183.30 Å   105.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.48 – 2.30 19.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.48-2.30) 99.9 (19.48-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.30 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.225   ,   0.270 0.225   ,   0.270	Depositor DCC
$R_{free}$ test set	5029 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 99537 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13456	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.41	1/6429 (0.0%)	0.60	2/8677 (0.0%)
1	B	0.39	1/6429 (0.0%)	0.59	0/8677
All	All	0.40	2/12858 (0.0%)	0.60	2/17354 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4	GLU	CD-OE2	7.18	1.33	1.25
1	A	4	GLU	CD-OE2	6.78	1.33	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	PRO	N-CA-C	-5.57	97.62	112.10
1	A	485	ARG	NE-CZ-NH1	-5.33	117.63	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	6295	0	6206	193	0
1	B	6295	0	6206	233	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	65	0	0	3	0
2	B	20	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	442	0	0	23	0
4	B	337	0	0	9	0
All	All	13456	0	12412	426	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 17.

All (426) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:HD13	4:B:2040:HOH:O	1.50	1.09
1:B:332:ILE:HD11	1:B:353:LYS:HD3	1.34	1.09
1:A:106:ARG:HH21	1:A:113:ASP:HB3	1.20	1.02
1:A:233:GLU:HA	1:A:238:ILE:HD12	1.37	1.01
1:B:142:ILE:HD12	1:B:150:VAL:HG22	1.36	1.01
1:A:477:ASN:HD21	1:A:482:GLY:H	1.09	0.96
1:B:133:ALA:C	1:B:134:ILE:HD12	1.84	0.96
1:A:391:LEU:O	1:A:395:ILE:HD13	1.67	0.95
1:A:451:ILE:HD13	1:A:468:ILE:HD13	1.50	0.93
1:A:705:ASN:O	1:A:709:ILE:HD13	1.68	0.93
1:B:40:GLN:HE21	1:B:42:ASN:HD21	1.15	0.92
1:B:477:ASN:HD21	1:B:482:GLY:H	1.19	0.90
1:A:357:ILE:HD12	1:A:358:LEU:N	1.88	0.89
1:A:545:ILE:HD12	1:A:573:ARG:HG3	1.56	0.87
1:B:686:ILE:HG21	1:B:725:ARG:HH12	1.40	0.85
1:B:114:HIS:HD2	1:B:116:ALA:H	1.25	0.85
1:B:134:ILE:HD13	1:B:170:PHE:CE2	2.14	0.82
1:A:357:ILE:HD13	1:A:407:MET:CE	2.08	0.82
1:A:238:ILE:HD11	1:A:270:GLN:NE2	1.95	0.80
1:A:539:ASP:O	1:A:545:ILE:HD11	1.81	0.80
1:A:14:ILE:H	1:A:14:ILE:HD12	1.45	0.80
1:B:423:ARG:HG2	1:B:428:ILE:HG12	1.65	0.79
1:B:432:GLN:HE22	1:B:445:TRP:H	1.31	0.78
1:A:121:PHE:HB3	1:A:123:ILE:HD11	1.66	0.78
1:B:474:ILE:HD13	1:B:474:ILE:O	1.82	0.77
1:B:103:THR:O	1:B:106:ARG:HD3	1.84	0.77
1:A:234:ASN:HB2	1:A:237:ALA:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:GLU:HG3	1:B:401:LYS:O	1.85	0.77
1:A:537:PHE:O	1:A:573:ARG:HD3	1.85	0.76
1:A:432:GLN:HE22	1:A:445:TRP:H	1.33	0.75
1:A:357:ILE:HD13	1:A:407:MET:HE1	1.68	0.74
1:A:106:ARG:NH2	1:A:113:ASP:HB3	2.00	0.74
1:A:249:GLU:HA	1:A:256:LYS:HD3	1.69	0.74
1:B:361:ILE:O	1:B:361:ILE:HD13	1.88	0.74
1:A:396:GLU:HG3	1:A:401:LYS:O	1.89	0.73
1:B:627:THR:HG23	1:B:661:LYS:HG2	1.71	0.73
1:A:567:ARG:HD3	4:A:2331:HOH:O	1.89	0.72
1:A:177:TYR:HB2	1:A:200:ARG:HG3	1.72	0.72
1:B:447:VAL:HG13	1:B:462:LEU:HB3	1.72	0.72
1:A:114:HIS:HD2	1:A:116:ALA:H	1.37	0.71
1:A:195:PRO:HD3	1:A:247:ILE:HD11	1.72	0.71
1:B:23:GLU:OE1	1:B:110:PRO:HG2	1.90	0.71
1:A:238:ILE:HD11	1:A:270:GLN:HE22	1.54	0.71
1:B:69:GLN:HG3	1:B:71:ILE:HD11	1.73	0.70
1:A:573:ARG:N	1:A:573:ARG:HD2	2.05	0.70
1:B:32:ILE:HD11	1:B:64:GLY:CA	2.23	0.69
1:A:218:LYS:NZ	1:A:220:HIS:HD2	1.90	0.69
1:B:705:ASN:HD22	1:B:708:ARG:HD2	1.57	0.69
1:B:191:ARG:HH21	1:B:248:ALA:HB2	1.58	0.69
1:A:772:GLU:HG3	1:A:776:GLN:HE21	1.58	0.69
1:B:674:MET:HB3	1:B:680:ILE:HD13	1.75	0.68
1:A:627:THR:HG23	1:A:661:LYS:HG3	1.74	0.68
1:B:263:ILE:O	1:B:267:ILE:HG12	1.94	0.68
1:B:219:MET:SD	1:B:267:ILE:HD12	2.33	0.68
1:B:252:ALA:O	1:B:255:VAL:HG22	1.93	0.68
1:A:93:ASN:HB3	4:A:2318:HOH:O	1.94	0.67
1:A:754:SER:HB2	4:A:2214:HOH:O	1.92	0.67
1:B:32:ILE:HD11	1:B:64:GLY:HA3	1.76	0.67
1:B:238:ILE:HD12	1:B:238:ILE:H	1.59	0.67
1:A:374:ILE:HD13	1:A:391:LEU:HD11	1.75	0.67
1:A:630:ALA:HB2	1:A:639:LEU:HD11	1.76	0.67
1:B:40:GLN:HE21	1:B:42:ASN:ND2	1.91	0.66
1:B:559:THR:HG21	1:B:774:ILE:HD13	1.76	0.66
1:B:359:ARG:NH2	1:B:481:ALA:HA	2.10	0.66
1:A:247:ILE:H	1:A:247:ILE:HD13	1.60	0.66
1:A:341:GLU:HB2	1:A:345:ILE:HG22	1.78	0.66
1:A:450:ASN:HD21	1:A:478:ALA:HB3	1.60	0.66
1:B:452:LYS:HE3	1:B:474:ILE:HD12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PRO:HB2	1:A:142:ILE:HD11	1.78	0.65
1:A:452:LYS:HE3	1:A:478:ALA:HB1	1.76	0.65
1:A:485:ARG:NH1	1:A:513:ASP:OD1	2.29	0.65
1:B:705:ASN:O	1:B:709:ILE:HD13	1.97	0.65
1:B:342:ILE:HD11	1:B:721:ARG:HH12	1.61	0.65
1:B:136:ASN:HD21	1:B:164:TYR:H	1.43	0.65
1:B:552:MET:HB2	1:B:595:LEU:HD11	1.78	0.64
1:B:133:ALA:O	1:B:134:ILE:HD12	1.97	0.64
1:B:141:ARG:O	1:B:142:ILE:HD13	1.98	0.63
1:B:633:THR:CG2	1:B:635:ASP:HB2	2.28	0.63
1:B:184:LEU:HD22	1:B:190:ILE:CD1	2.28	0.63
1:B:142:ILE:CD1	1:B:150:VAL:HG13	2.29	0.63
1:B:432:GLN:NE2	1:B:445:TRP:H	1.96	0.63
1:B:541:ASP:O	1:B:545:ILE:HG12	1.99	0.62
1:B:88:TYR:HD1	1:B:96:ILE:HD13	1.64	0.62
1:B:731:ILE:HD11	1:B:745:VAL:HG21	1.82	0.62
1:A:419:ILE:HD13	1:A:484:TYR:CD1	2.35	0.62
1:A:369:GLU:HG2	4:A:2367:HOH:O	2.00	0.62
1:B:184:LEU:HD22	1:B:190:ILE:HD13	1.82	0.61
1:A:342:ILE:HD13	1:A:342:ILE:O	2.00	0.61
1:B:422:LYS:HG3	1:B:429:THR:HG23	1.81	0.61
1:B:328:ASN:HB3	1:B:755:MET:HE2	1.81	0.61
1:B:633:THR:HG22	1:B:635:ASP:HB2	1.82	0.61
1:A:299:MET:HE1	1:A:302:LEU:HD12	1.81	0.61
1:B:428:ILE:HD12	1:B:470:ALA:HA	1.83	0.61
1:A:509:ILE:HB	4:A:2267:HOH:O	2.01	0.61
1:A:447:VAL:HG13	1:A:462:LEU:HB3	1.83	0.61
1:A:451:ILE:CD1	1:A:468:ILE:HD13	2.28	0.60
1:B:539:ASP:O	1:B:545:ILE:HD11	2.00	0.60
1:A:773:ARG:O	1:A:777:THR:HG22	2.01	0.60
1:A:253:VAL:HG23	4:A:2158:HOH:O	2.02	0.60
1:B:114:HIS:CD2	1:B:116:ALA:H	2.15	0.60
1:A:139:PRO:CB	1:A:142:ILE:HD11	2.32	0.60
1:B:674:MET:CB	1:B:680:ILE:HD13	2.32	0.59
1:A:601:GLU:O	1:A:605:GLU:HG3	2.02	0.59
1:A:549:VAL:O	1:A:553:GLU:HG3	2.02	0.59
1:A:341:GLU:HB2	1:A:345:ILE:H	1.67	0.59
1:A:708:ARG:HB3	4:A:2213:HOH:O	2.02	0.59
1:B:139:PRO:HB3	1:B:142:ILE:HD11	1.85	0.59
1:A:357:ILE:HD13	1:A:407:MET:HE2	1.85	0.59
1:B:137:MET:HG2	1:B:155:THR:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASN:O	1:A:238:ILE:HD13	2.03	0.58
1:B:369:GLU:OE2	1:B:399:SER:HA	2.03	0.58
1:B:106:ARG:HD2	1:B:113:ASP:OD2	2.03	0.58
1:B:528:THR:O	1:B:532:ARG:HG3	2.03	0.58
1:A:101:GLU:O	1:A:102:ALA:CB	2.52	0.58
1:A:196:LEU:HD23	1:A:221:LEU:HD12	1.86	0.58
1:B:253:VAL:O	1:B:257:ARG:HG2	2.04	0.57
1:A:23:GLU:OE1	1:A:110:PRO:HG2	2.04	0.57
1:A:157:ARG:HD3	4:A:2189:HOH:O	2.03	0.57
1:A:432:GLN:NE2	1:A:445:TRP:H	2.01	0.57
1:A:69:GLN:CD	1:A:71:ILE:HD11	2.24	0.57
1:A:672:TYR:CZ	1:A:709:ILE:HD12	2.39	0.57
1:B:257:ARG:HG3	1:B:306:TRP:CZ2	2.39	0.57
1:A:643:PHE:CZ	1:A:680:ILE:HD13	2.38	0.57
1:B:779:VAL:O	1:B:780:LYS:HG3	2.04	0.57
1:A:614:PHE:HB3	1:A:642:LYS:HE2	1.86	0.57
1:A:312:PHE:O	1:A:316:ARG:HB2	2.04	0.57
1:B:710:ILE:CD1	1:B:745:VAL:HG22	2.35	0.56
1:A:613:ASP:HB3	1:A:616:SER:HB3	1.88	0.56
1:B:581:GLN:H	1:B:581:GLN:CD	2.08	0.56
1:B:251:SER:O	1:B:256:LYS:HE3	2.06	0.56
1:B:652:ARG:O	1:B:656:ILE:HG12	2.06	0.56
1:B:452:LYS:CE	1:B:474:ILE:HD12	2.35	0.56
1:B:238:ILE:HD12	1:B:238:ILE:N	2.21	0.55
1:A:686:ILE:HB	4:A:2249:HOH:O	2.05	0.55
1:A:755:MET:HB2	4:A:2392:HOH:O	2.06	0.55
1:B:101:GLU:O	1:B:102:ALA:CB	2.53	0.55
1:B:177:TYR:HB2	1:B:200:ARG:HG3	1.89	0.55
1:B:454:LYS:HE3	1:B:499:HIS:CD2	2.41	0.55
1:B:497:MET:CE	1:B:535:ASN:HB3	2.36	0.55
1:B:432:GLN:HE22	1:B:445:TRP:HB2	1.72	0.55
1:B:512:VAL:HG13	1:B:551:GLN:HE22	1.72	0.55
1:A:357:ILE:C	1:A:357:ILE:HD12	2.27	0.55
1:A:361:ILE:CD1	1:A:403:VAL:HG13	2.36	0.55
1:B:779:VAL:HA	4:B:2252:HOH:O	2.06	0.55
1:B:474:ILE:CD1	1:B:474:ILE:O	2.54	0.54
1:B:682:LYS:HD2	1:B:716:TYR:O	2.08	0.54
1:A:570:CYS:O	1:A:574:MET:HB2	2.08	0.54
1:A:341:GLU:HB3	1:A:344:GLN:HB3	1.89	0.54
1:B:505:PRO:HG2	4:B:2014:HOH:O	2.07	0.54
1:A:141:ARG:C	1:A:142:ILE:HD12	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ILE:CD1	1:B:64:GLY:CA	2.85	0.54
1:B:452:LYS:CD	1:B:474:ILE:HD12	2.38	0.53
1:A:183:ILE:N	1:A:183:ILE:HD12	2.23	0.53
1:A:333:GLU:HB2	1:A:411:ILE:HG22	1.89	0.53
1:B:419:ILE:HD12	1:B:462:LEU:HD13	1.90	0.53
1:B:32:ILE:N	1:B:32:ILE:HD12	2.22	0.53
1:B:244:TYR:O	1:B:247:ILE:HD11	2.08	0.53
1:B:358:LEU:O	1:B:361:ILE:HG22	2.08	0.53
1:B:507:ASP:O	1:B:511:LEU:HG	2.09	0.53
1:B:685:MET:CE	1:B:713:VAL:HG22	2.39	0.53
1:A:333:GLU:OE2	1:A:412:LYS:HG2	2.09	0.53
1:A:560:HIS:HB2	2:A:1005:SO4:O1	2.08	0.53
1:B:485:ARG:NH1	1:B:513:ASP:OD1	2.42	0.53
1:A:651:ASP:HA	1:A:654:ARG:HD2	1.91	0.53
1:B:100:PHE:O	1:B:101:GLU:C	2.46	0.53
1:A:379:ASN:O	1:A:382:LYS:HG2	2.09	0.53
1:A:606:GLU:O	1:A:609:LYS:HG2	2.09	0.53
1:B:418:VAL:HB	1:B:435:PHE:HB2	1.90	0.53
1:A:527:GLU:HG2	1:A:531:GLN:HE22	1.73	0.53
1:A:233:GLU:CA	1:A:238:ILE:HD12	2.24	0.53
1:A:395:ILE:CD1	1:A:395:ILE:N	2.72	0.53
1:B:183:ILE:N	1:B:183:ILE:HD12	2.23	0.53
1:B:103:THR:HB	1:B:106:ARG:NH1	2.24	0.53
1:A:194:TYR:N	1:A:195:PRO:HD2	2.23	0.53
1:A:195:PRO:HD3	1:A:247:ILE:CD1	2.38	0.53
1:A:361:ILE:HG13	1:A:407:MET:SD	2.48	0.52
1:B:520:LEU:HD23	1:B:770:LEU:HD22	1.91	0.52
1:B:136:ASN:ND2	1:B:164:TYR:H	2.08	0.52
1:B:630:ALA:HB2	1:B:639:LEU:HD11	1.90	0.52
1:A:338:ASP:O	1:A:340:ASP:N	2.42	0.52
1:B:101:GLU:O	1:B:102:ALA:HB3	2.10	0.52
1:B:234:ASN:HB2	1:B:237:ALA:O	2.09	0.52
1:B:453:LYS:HA	1:B:474:ILE:HG22	1.92	0.52
1:B:492:THR:O	1:B:496:VAL:HG23	2.09	0.52
1:A:672:TYR:OH	1:A:709:ILE:HD12	2.09	0.52
1:B:474:ILE:HD13	1:B:474:ILE:C	2.29	0.52
1:A:643:PHE:HB2	1:A:655:ILE:HG21	1.90	0.52
1:B:686:ILE:HG21	1:B:725:ARG:NH1	2.17	0.52
1:B:497:MET:HE2	1:B:535:ASN:HB3	1.91	0.52
1:A:136:ASN:HD21	1:A:164:TYR:H	1.57	0.52
1:B:328:ASN:HB3	1:B:755:MET:CE	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:THR:HG22	1:A:467:SER:OG	2.10	0.52
1:B:696:LEU:N	1:B:697:PRO:HD2	2.25	0.52
1:A:709:ILE:CD1	1:A:709:ILE:N	2.72	0.52
1:B:134:ILE:N	1:B:134:ILE:HD12	2.25	0.52
1:B:166:GLY:C	1:B:167:ILE:HD12	2.31	0.52
1:B:374:ILE:HD13	1:B:391:LEU:HD11	1.91	0.52
1:A:364:TYR:CD1	1:A:448:PRO:HB3	2.45	0.51
1:B:613:ASP:HB3	1:B:616:SER:OG	2.11	0.51
1:B:145:SER:HB2	4:B:2065:HOH:O	2.10	0.51
1:A:114:HIS:CD2	1:A:116:ALA:H	2.25	0.51
1:A:17:ARG:HB3	1:A:79:VAL:HB	1.91	0.51
1:A:69:GLN:NE2	1:A:71:ILE:HD11	2.26	0.51
1:B:142:ILE:HD11	1:B:150:VAL:HG13	1.92	0.51
1:A:361:ILE:HD12	1:A:403:VAL:HG13	1.92	0.51
1:A:252:ALA:HB3	1:A:255:VAL:HG23	1.93	0.51
1:A:341:GLU:CB	1:A:344:GLN:HB3	2.41	0.51
1:A:777:THR:HG23	4:A:2359:HOH:O	2.09	0.51
1:A:721:ARG:O	1:A:725:ARG:HG3	2.11	0.50
1:A:30:GLY:O	1:A:64:GLY:HA3	2.12	0.50
1:B:736:LEU:HD23	4:B:2218:HOH:O	2.11	0.50
1:B:421:LEU:HD23	1:B:430:MET:HB3	1.93	0.50
1:A:650:GLU:HB2	2:A:1017:SO4:O3	2.12	0.50
1:B:695:THR:O	1:B:699:ARG:HG3	2.11	0.50
1:B:218:LYS:HD2	1:B:218:LYS:C	2.33	0.50
1:A:706:LEU:HD11	1:A:710:ILE:HD11	1.94	0.50
1:A:136:ASN:HD21	1:A:163:LEU:HA	1.77	0.50
1:B:129:LYS:HA	1:B:148:LYS:HB2	1.94	0.50
1:B:233:GLU:O	1:B:234:ASN:C	2.50	0.49
1:A:432:GLN:HE22	1:A:445:TRP:HB2	1.76	0.49
1:A:218:LYS:HZ2	1:A:220:HIS:HD2	1.60	0.49
1:B:13:ASP:OD1	1:B:16:LYS:HD2	2.13	0.49
1:A:99:HIS:CE1	1:A:232:MET:HG2	2.47	0.49
1:B:493:PHE:CD2	1:B:532:ARG:HD2	2.47	0.49
1:A:465:GLU:HG3	4:A:2074:HOH:O	2.13	0.49
1:A:66:SER:O	1:A:67:GLN:HB2	2.13	0.49
1:B:341:GLU:O	1:B:342:ILE:HB	2.13	0.49
1:B:346:PHE:CE2	1:B:721:ARG:HD3	2.47	0.49
1:B:452:LYS:HG2	1:B:474:ILE:HG23	1.94	0.49
1:A:394:ALA:O	1:A:398:VAL:HG23	2.12	0.49
1:A:60:VAL:HG13	1:A:60:VAL:O	2.12	0.49
1:B:497:MET:HE3	1:B:500:TYR:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:VAL:O	1:B:553:GLU:HG3	2.13	0.49
1:B:750:SER:O	1:B:753:ILE:HG13	2.13	0.49
1:B:664:SER:HB3	1:B:667:ASP:OD2	2.12	0.49
1:B:32:ILE:O	1:B:61:ARG:HA	2.12	0.48
1:A:477:ASN:ND2	1:A:482:GLY:H	1.93	0.48
1:A:35:ASP:O	1:A:110:PRO:HA	2.14	0.48
1:A:613:ASP:HB2	4:A:2435:HOH:O	2.13	0.48
1:B:191:ARG:HD3	1:B:248:ALA:HB2	1.95	0.48
1:B:477:ASN:ND2	1:B:482:GLY:H	1.98	0.48
1:A:123:ILE:HD12	1:A:123:ILE:N	2.28	0.48
1:B:643:PHE:CE1	1:B:656:ILE:HD11	2.48	0.48
1:B:475:LYS:HZ2	1:B:507:ASP:HB3	1.79	0.48
1:B:452:LYS:HD3	1:B:474:ILE:CD1	2.44	0.48
1:B:357:ILE:HG22	1:B:407:MET:CE	2.44	0.48
1:A:521:SER:OG	1:A:523:HIS:HD2	1.97	0.48
1:B:667:ASP:O	1:B:671:VAL:HG23	2.14	0.48
1:A:7:ASP:O	1:A:23:GLU:HA	2.14	0.48
1:A:700:GLU:HG2	4:A:2385:HOH:O	2.13	0.47
1:A:450:ASN:HB3	4:A:2337:HOH:O	2.14	0.47
1:B:633:THR:HG21	1:B:635:ASP:HB2	1.96	0.47
1:B:218:LYS:NZ	1:B:220:HIS:HD2	2.12	0.47
1:B:740:ASP:O	1:B:744:ILE:HG12	2.14	0.47
1:B:685:MET:HE1	1:B:713:VAL:HG22	1.95	0.47
1:B:173:GLU:HG2	1:B:190:ILE:HD12	1.96	0.47
1:B:20:ASN:ND2	4:B:2246:HOH:O	2.47	0.47
1:A:370:PHE:O	1:A:374:ILE:HG12	2.15	0.47
1:B:432:GLN:HE22	1:B:445:TRP:N	2.07	0.47
1:B:32:ILE:CD1	1:B:64:GLY:HA3	2.45	0.47
1:A:198:MET:HA	1:A:198:MET:HE3	1.95	0.47
1:B:574:MET:HE3	1:B:592:VAL:CG1	2.45	0.47
1:A:14:ILE:H	1:A:14:ILE:CD1	2.19	0.47
1:B:241:ARG:HG3	4:B:2193:HOH:O	2.15	0.47
1:B:332:ILE:HD11	1:B:353:LYS:CD	2.25	0.47
1:A:421:LEU:HD23	1:A:430:MET:HB3	1.97	0.47
1:A:290:PHE:CE1	1:A:374:ILE:HD12	2.49	0.46
1:A:663:LYS:HD2	1:A:697:PRO:HG3	1.97	0.46
1:B:402:PRO:O	1:B:406:VAL:HG23	2.15	0.46
1:B:332:ILE:CD1	1:B:332:ILE:N	2.78	0.46
1:B:253:VAL:CG2	1:B:583:GLU:HG2	2.45	0.46
1:B:574:MET:CE	1:B:589:LEU:HD12	2.45	0.46
1:B:452:LYS:HD3	1:B:474:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ILE:HD13	1:B:63:PRO:O	2.15	0.46
1:B:731:ILE:N	1:B:732:PRO:HD2	2.31	0.46
1:B:509:ILE:HD13	1:B:544:VAL:HA	1.97	0.46
1:B:475:LYS:NZ	1:B:507:ASP:HB3	2.30	0.46
1:B:3:VAL:HG11	1:B:6:TYR:CE2	2.51	0.46
1:B:573:ARG:NE	1:B:573:ARG:HA	2.30	0.46
1:B:642:LYS:HA	1:B:645:SER:HB3	1.98	0.46
1:B:33:VAL:O	1:B:33:VAL:HG13	2.16	0.46
1:B:142:ILE:HD12	1:B:150:VAL:CG2	2.26	0.45
1:B:422:LYS:HG3	1:B:422:LYS:O	2.16	0.45
1:A:146:GLU:HG2	4:A:2113:HOH:O	2.16	0.45
1:B:421:LEU:HD11	1:B:476:ILE:HD12	1.97	0.45
1:A:751:LYS:HA	1:A:754:SER:OG	2.17	0.45
1:A:86:ILE:HD11	1:A:96:ILE:CG2	2.46	0.45
1:B:698:GLY:O	1:B:702:ILE:HG12	2.17	0.45
1:B:95:MET:HE3	1:B:97:THR:HG23	1.97	0.45
1:B:282:ASN:HD22	1:B:282:ASN:H	1.64	0.45
1:A:505:PRO:HD3	2:A:1007:SO4:O1	2.17	0.45
1:B:248:ALA:HB3	1:B:251:SER:OG	2.17	0.45
1:A:509:ILE:O	1:A:509:ILE:HD13	2.17	0.45
1:B:41:ILE:N	1:B:41:ILE:HD12	2.31	0.45
1:B:474:ILE:HD11	1:B:503:LEU:HD23	1.99	0.45
1:A:100:PHE:O	1:A:101:GLU:C	2.55	0.45
1:A:574:MET:HE1	1:A:589:LEU:CD1	2.47	0.45
1:B:247:ILE:HD12	1:B:247:ILE:N	2.32	0.45
1:B:540:GLU:HB3	1:B:576:PHE:CE2	2.52	0.45
1:B:276:VAL:HG21	1:B:378:LEU:HA	1.99	0.45
1:B:493:PHE:CE2	1:B:532:ARG:HB3	2.51	0.45
1:B:194:TYR:N	1:B:195:PRO:HD2	2.31	0.45
1:A:416:TYR:HE2	1:A:485:ARG:HG3	1.82	0.45
1:B:299:MET:CE	1:B:302:LEU:HD12	2.47	0.45
1:B:682:LYS:HE3	1:B:717:PHE:CE1	2.52	0.45
1:A:15:GLN:H	1:A:15:GLN:CD	2.20	0.45
1:B:167:ILE:N	1:B:167:ILE:HD12	2.32	0.45
1:A:724:SER:O	1:A:727:VAL:HG22	2.16	0.45
1:A:708:ARG:HG3	4:A:2122:HOH:O	2.18	0.44
1:A:32:ILE:O	1:A:61:ARG:HA	2.17	0.44
1:B:330:HIS:NE2	1:B:349:ILE:HD12	2.32	0.44
1:A:709:ILE:O	1:A:713:VAL:HG23	2.18	0.44
1:B:35:ASP:O	1:B:110:PRO:HA	2.18	0.44
1:A:184:LEU:HB2	1:A:196:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ARG:HH22	1:B:481:ALA:HA	1.80	0.44
1:B:574:MET:HE2	1:B:589:LEU:HD12	1.99	0.44
1:A:505:PRO:HG2	4:A:2060:HOH:O	2.17	0.44
1:B:7:ASP:O	1:B:23:GLU:HA	2.17	0.44
1:A:54:THR:O	1:A:60:VAL:HA	2.16	0.44
1:B:140:LYS:HB2	1:B:153:GLN:HG3	1.99	0.44
1:B:134:ILE:CD1	1:B:134:ILE:N	2.80	0.44
1:B:361:ILE:HD11	1:B:403:VAL:HG13	2.00	0.44
1:B:86:ILE:O	1:B:86:ILE:HG23	2.17	0.44
1:A:556:ARG:HD2	1:A:599:VAL:CG1	2.48	0.44
1:A:705:ASN:HB3	1:A:709:ILE:CD1	2.48	0.44
1:B:164:TYR:CE2	1:B:222:ILE:HD13	2.53	0.44
1:A:464:ASP:O	1:A:465:GLU:C	2.56	0.44
1:A:114:HIS:CD2	1:A:116:ALA:HB3	2.53	0.44
1:B:505:PRO:O	1:B:509:ILE:HG12	2.18	0.44
1:B:44:MET:HG2	1:B:45:LYS:N	2.32	0.44
1:A:83:LEU:O	1:A:84:SER:HB2	2.17	0.44
1:A:83:LEU:HG	1:A:87:TYR:CZ	2.53	0.43
1:A:190:ILE:N	1:A:190:ILE:HD12	2.32	0.43
1:B:427:LYS:HG2	1:B:467:SER:OG	2.18	0.43
1:B:428:ILE:HG13	1:B:470:ALA:HB2	1.99	0.43
1:A:570:CYS:SG	1:A:595:LEU:HD13	2.58	0.43
1:B:153:GLN:HG2	4:B:2294:HOH:O	2.18	0.43
1:A:129:LYS:HG2	1:A:144:VAL:HG13	2.00	0.43
1:A:720:ASN:HA	4:A:2106:HOH:O	2.17	0.43
1:A:681:LYS:HB3	1:A:683:GLN:HG2	2.01	0.43
1:B:284:LEU:O	1:B:284:LEU:HD22	2.18	0.43
1:A:712:LEU:C	1:A:712:LEU:HD23	2.39	0.43
1:B:545:ILE:HD12	1:B:573:ARG:CD	2.48	0.43
1:B:727:VAL:O	1:B:731:ILE:HG12	2.18	0.43
1:A:85:GLY:O	1:A:98:THR:HA	2.18	0.43
1:A:696:LEU:N	1:A:697:PRO:HD2	2.34	0.43
1:A:20:ASN:ND2	4:A:2434:HOH:O	2.52	0.43
1:B:421:LEU:HD21	1:B:476:ILE:CD1	2.49	0.43
1:B:86:ILE:HD13	1:B:86:ILE:C	2.38	0.43
1:A:136:ASN:ND2	1:A:164:TYR:H	2.17	0.43
1:B:775:ARG:HG2	1:B:775:ARG:HH21	1.83	0.43
1:B:85:GLY:O	1:B:98:THR:HA	2.19	0.43
1:A:675:VAL:HG22	1:A:680:ILE:HB	2.00	0.43
1:B:275:LEU:HD22	1:B:383:PHE:H	1.84	0.43
1:B:99:HIS:NE2	1:B:101:GLU:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:ALA:HB2	4:A:2285:HOH:O	2.17	0.43
1:A:341:GLU:CD	1:A:341:GLU:H	2.21	0.42
1:B:281:TRP:O	1:B:284:LEU:HB2	2.19	0.42
1:A:137:MET:HG2	1:A:155:THR:HG22	2.01	0.42
1:B:656:ILE:O	1:B:659:PHE:HB2	2.19	0.42
1:A:173:GLU:HG3	1:A:190:ILE:HG21	2.00	0.42
1:B:769:LYS:O	1:B:773:ARG:HG3	2.19	0.42
1:B:725:ARG:HH21	1:B:725:ARG:HG3	1.84	0.42
1:A:527:GLU:CG	1:A:531:GLN:HE22	2.33	0.42
1:B:95:MET:HE2	1:B:97:THR:HG21	2.01	0.42
1:A:369:GLU:OE1	1:A:399:SER:HA	2.19	0.42
1:B:100:PHE:CD2	1:B:105:ALA:HA	2.55	0.42
1:B:753:ILE:HD12	1:B:753:ILE:C	2.40	0.42
1:B:527:GLU:OE2	1:B:530:ARG:NH1	2.53	0.42
1:A:286:LEU:O	1:A:286:LEU:HD22	2.20	0.42
1:A:453:LYS:HB2	1:A:456:GLY:O	2.20	0.42
1:A:719:GLY:O	1:A:752:ASN:HB3	2.19	0.42
1:A:101:GLU:O	1:A:102:ALA:HB3	2.20	0.42
1:B:497:MET:HE2	1:B:535:ASN:CB	2.49	0.42
1:A:332:ILE:HD12	1:A:411:ILE:HA	2.01	0.42
1:A:86:ILE:HG23	1:A:86:ILE:O	2.19	0.42
1:A:18:THR:HA	1:A:78:LYS:HA	2.02	0.42
1:B:648:ARG:HG2	1:B:650:GLU:H	1.84	0.42
1:A:473:LEU:C	1:A:473:LEU:HD23	2.41	0.42
1:A:177:TYR:OH	1:A:204:GLU:HG3	2.20	0.41
1:A:452:LYS:HE3	1:A:478:ALA:CB	2.45	0.41
1:B:97:THR:CG2	1:B:164:TYR:OH	2.68	0.41
1:A:276:VAL:HG21	1:A:378:LEU:HA	2.02	0.41
1:B:201:LYS:NZ	4:B:2317:HOH:O	2.42	0.41
1:B:559:THR:OG1	1:B:560:HIS:N	2.54	0.41
1:A:59:THR:HG22	1:A:60:VAL:N	2.35	0.41
1:B:280:TRP:HB3	1:B:282:ASN:ND2	2.35	0.41
1:B:643:PHE:CZ	1:B:656:ILE:HD11	2.54	0.41
1:B:79:VAL:HG22	1:B:86:ILE:HD12	2.03	0.41
1:B:97:THR:HG22	1:B:164:TYR:CE1	2.55	0.41
1:A:313:PHE:CD2	1:A:509:ILE:HD12	2.56	0.41
1:B:509:ILE:HD11	1:B:544:VAL:N	2.35	0.41
1:B:558:LEU:HG	1:B:736:LEU:HD21	2.02	0.41
1:B:69:GLN:HG3	1:B:71:ILE:CD1	2.45	0.41
1:B:165:VAL:HG12	1:B:167:ILE:CD1	2.50	0.41
1:A:127:ILE:HD12	1:A:131:TYR:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ILE:N	1:A:395:ILE:HD12	2.36	0.41
1:B:528:THR:O	1:B:532:ARG:CG	2.68	0.41
1:B:476:ILE:HG22	1:B:477:ASN:N	2.35	0.41
1:A:530:ARG:O	1:A:534:ARG:HG3	2.21	0.41
1:B:349:ILE:O	1:B:353:LYS:HB3	2.20	0.41
1:B:134:ILE:HD13	1:B:170:PHE:HE2	1.77	0.41
1:B:428:ILE:O	1:B:468:ILE:HD13	2.21	0.41
1:A:218:LYS:HZ3	1:A:220:HIS:HD2	1.68	0.41
1:B:184:LEU:HD22	1:B:190:ILE:HD11	2.01	0.41
1:B:422:LYS:CD	1:B:429:THR:HG23	2.51	0.41
1:A:649:ASP:OD1	1:A:652:ARG:NH2	2.54	0.41
1:A:327:LYS:HD3	4:A:2058:HOH:O	2.20	0.41
1:A:424:ASN:OD1	1:A:427:LYS:HB3	2.20	0.41
1:B:332:ILE:HD12	1:B:349:ILE:CG2	2.51	0.41
1:A:233:GLU:HA	1:A:238:ILE:CD1	2.27	0.41
1:B:196:LEU:HA	1:B:196:LEU:HD23	1.91	0.41
1:B:332:ILE:HD12	1:B:332:ILE:N	2.36	0.40
1:B:137:MET:HB3	1:B:138:PRO:CD	2.51	0.40
1:A:697:PRO:O	1:A:700:GLU:HB2	2.21	0.40
1:A:671:VAL:HG13	1:A:674:MET:HE3	2.02	0.40
1:A:361:ILE:HG13	1:A:407:MET:CG	2.51	0.40
1:A:577:LEU:HD13	1:A:589:LEU:HA	2.03	0.40
1:B:492:THR:HA	1:B:495:ASP:OD1	2.21	0.40
1:A:583:GLU:HB3	4:A:2252:HOH:O	2.21	0.40
1:B:11:ASP:OD1	1:B:147:ARG:NH1	2.54	0.40
1:B:656:ILE:HD12	1:B:680:ILE:HG13	2.04	0.40
1:B:86:ILE:HD11	1:B:96:ILE:CG2	2.51	0.40
1:A:262:VAL:O	1:A:265:HIS:HB3	2.21	0.40
1:A:43:TRP:CZ3	1:A:45:LYS:HE3	2.56	0.40
1:B:127:ILE:H	1:B:127:ILE:HD13	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	778/780 (100%)	729 (94%)	41 (5%)	8 (1%)	19	21
1	B	778/780 (100%)	716 (92%)	45 (6%)	17 (2%)	8	6
All	All	1556/1560 (100%)	1445 (93%)	86 (6%)	25 (2%)	12	11

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ALA
1	B	102	ALA
1	B	341	GLU
1	B	342	ILE
1	B	347	ASP
1	B	423	ARG
1	B	83	LEU
1	B	346	PHE
1	B	422	LYS
1	B	475	LYS
1	A	91	ARG
1	A	778	ALA
1	B	101	GLU
1	B	464	ASP
1	B	718	THR
1	A	84	SER
1	A	101	GLU
1	A	339	PRO
1	A	718	THR
1	B	678	THR
1	B	721	ARG
1	B	720	ASN
1	A	648	ARG
1	B	424	ASN
1	B	339	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	677/677 (100%)	635 (94%)	42 (6%)	23	30
1	B	677/677 (100%)	632 (93%)	45 (7%)	21	27
All	All	1354/1354 (100%)	1267 (94%)	87 (6%)	22	28

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	58	GLN
1	A	81	ASP
1	A	86	ILE
1	A	141	ARG
1	A	187	LEU
1	A	198	MET
1	A	218	LYS
1	A	232	MET
1	A	235	TRP
1	A	247	ILE
1	A	258	ASN
1	A	261	ASN
1	A	275	LEU
1	A	282	ASN
1	A	284	LEU
1	A	286	LEU
1	A	341	GLU
1	A	342	ILE
1	A	361	ILE
1	A	395	ILE
1	A	417	PRO
1	A	447	VAL
1	A	462	LEU
1	A	471	ASP
1	A	477	ASN
1	A	487	LEU
1	A	509	ILE
1	A	531	GLN
1	A	539	ASP
1	A	555	LEU
1	A	595	LEU
1	A	596	TYR
1	A	607	MET

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Mol	Chain	Res	Type
1	A	636	LEU
1	A	647	ASP
1	A	686	ILE
1	A	696	LEU
1	A	709	ILE
1	A	720	ASN
1	A	764	LEU
1	A	770	LEU
1	B	1	MET
1	B	58	GLN
1	B	86	ILE
1	B	92	GLU
1	B	97	THR
1	B	104	ASP
1	B	106	ARG
1	B	127	ILE
1	B	218	LYS
1	B	250	ASN
1	B	266	GLU
1	B	275	LEU
1	B	282	ASN
1	B	284	LEU
1	B	286	LEU
1	B	288	GLU
1	B	332	ILE
1	B	337	ARG
1	B	361	ILE
1	B	379	ASN
1	B	407	MET
1	B	422	LYS
1	B	424	ASN
1	B	429	THR
1	B	430	MET
1	B	438	ASN
1	B	468	ILE
1	B	471	ASP
1	B	474	ILE
1	B	475	LYS
1	B	477	ASN
1	B	487	LEU
1	B	519	LEU
1	B	530	ARG

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Mol	Chain	Res	Type
1	B	555	LEU
1	B	559	THR
1	B	581	GLN
1	B	583	GLU
1	B	594	ARG
1	B	596	TYR
1	B	642	LYS
1	B	650	GLU
1	B	679	GLU
1	B	764	LEU
1	B	777	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	40	GLN
1	A	42	ASN
1	A	58	GLN
1	A	69	GLN
1	A	99	HIS
1	A	114	HIS
1	A	136	ASN
1	A	220	HIS
1	A	258	ASN
1	A	261	ASN
1	A	287	ASN
1	A	379	ASN
1	A	432	GLN
1	A	477	ASN
1	A	499	HIS
1	A	523	HIS
1	A	531	GLN
1	A	581	GLN
1	A	720	ASN
1	A	776	GLN
1	B	20	ASN
1	B	42	ASN
1	B	58	GLN
1	B	114	HIS
1	B	136	ASN
1	B	220	HIS

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Mol	Chain	Res	Type
1	B	234	ASN
1	B	258	ASN
1	B	282	ASN
1	B	287	ASN
1	B	344	GLN
1	B	432	GLN
1	B	438	ASN
1	B	477	ASN
1	B	535	ASN
1	B	551	GLN
1	B	581	GLN
1	B	705	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	1001	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	A	1002	-	4,4,4	0.34	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	1003	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	A	1005	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	A	1006	-	4,4,4	0.20	0	6,6,6	0.09	0
2	SO4	A	1007	-	4,4,4	0.30	0	6,6,6	0.07	0
2	SO4	A	1008	-	4,4,4	0.29	0	6,6,6	0.08	0
2	SO4	A	1009	-	4,4,4	0.29	0	6,6,6	0.07	0
2	SO4	A	1010	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	A	1014	-	4,4,4	0.30	0	6,6,6	0.10	0
2	SO4	A	1015	-	4,4,4	0.29	0	6,6,6	0.10	0
2	SO4	A	1016	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	A	1017	-	4,4,4	0.30	0	6,6,6	0.09	0
2	SO4	B	1004	-	4,4,4	0.34	0	6,6,6	0.09	0
2	SO4	B	1011	-	4,4,4	0.39	0	6,6,6	0.07	0
2	SO4	B	1012	-	4,4,4	0.31	0	6,6,6	0.09	0
2	SO4	B	1013	-	4,4,4	0.26	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	A	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1006	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1007	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1008	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1009	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1010	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1014	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1015	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1016	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1017	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1004	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1011	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1012	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1013	-	-	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1005	SO4	1	0
2	A	1007	SO4	1	0
2	A	1017	SO4	1	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	780/780 (100%)	0.17	44 (5%)	28 36	18, 34, 58, 67	1 (0%)
1	B	780/780 (100%)	0.30	58 (7%)	17 25	19, 38, 60, 68	4 (0%)
All	All	1560/1560 (100%)	0.24	102 (6%)	22 30	18, 37, 59, 68	5 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	779	VAL	13.0
1	B	779	VAL	11.2
1	B	778	ALA	9.2
1	B	720	ASN	7.8
1	B	345	ILE	7.3
1	A	346	PHE	7.3
1	A	778	ALA	6.7
1	B	425	GLY	6.6
1	B	248	ALA	6.1
1	A	780	LYS	5.7
1	B	780	LYS	5.3
1	B	424	ASN	5.0
1	A	720	ASN	4.9
1	B	777	THR	4.9
1	B	718	THR	4.9
1	A	249	GLU	4.8
1	B	344	GLN	4.8
1	A	343	SER	4.8
1	B	649	ASP	4.7
1	B	454	LYS	4.7
1	B	426	ARG	4.7
1	B	455	ASP	4.6
1	A	337	ARG	4.3
1	B	647	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	250	ASN	4.2
1	A	191	ARG	4.2
1	B	93	ASN	4.1
1	B	721	ARG	4.0
1	B	250	ASN	4.0
1	B	581	GLN	4.0
1	A	721	ARG	3.7
1	B	471	ASP	3.7
1	A	344	GLN	3.7
1	A	345	ILE	3.5
1	B	342	ILE	3.5
1	A	248	ALA	3.5
1	A	342	ILE	3.5
1	B	249	GLU	3.5
1	A	57	GLY	3.4
1	B	346	PHE	3.4
1	B	427	LYS	3.4
1	A	65	ASP	3.4
1	B	501	ARG	3.4
1	B	456	GLY	3.3
1	B	49	ARG	3.3
1	B	579	GLY	3.2
1	A	91	ARG	3.2
1	A	718	THR	3.2
1	B	343	SER	3.1
1	A	340	ASP	3.1
1	A	709	ILE	3.1
1	A	49	ARG	3.0
1	A	501	ARG	3.0
1	B	91	ARG	2.9
1	B	648	ARG	2.9
1	B	191	ARG	2.9
1	B	719	GLY	2.9
1	A	335	ASP	2.9
1	B	337	ARG	2.8
1	A	338	ASP	2.8
1	A	752	ASN	2.8
1	A	349	ILE	2.7
1	B	67	GLN	2.7
1	A	92	GLU	2.7
1	A	251	SER	2.7
1	A	66	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	92	GLU	2.6
1	A	93	ASN	2.6
1	B	306	TRP	2.6
1	B	676	GLU	2.6
1	A	82	SER	2.6
1	B	675	VAL	2.6
1	B	655	ILE	2.6
1	B	752	ASN	2.5
1	B	681	LYS	2.5
1	A	260	ALA	2.5
1	B	347	ASP	2.5
1	B	571	ARG	2.5
1	B	335	ASP	2.4
1	B	612	LYS	2.4
1	B	502	ASP	2.4
1	B	709	ILE	2.3
1	A	348	GLU	2.3
1	B	580	LYS	2.3
1	B	751	LYS	2.3
1	A	725	ARG	2.3
1	A	67	GLN	2.3
1	A	747	ASN	2.3
1	B	776	GLN	2.3
1	A	647	ASP	2.2
1	B	340	ASP	2.2
1	B	682	LYS	2.2
1	B	474	ILE	2.2
1	A	253	VAL	2.2
1	B	775	ARG	2.2
1	A	775	ARG	2.1
1	B	666	THR	2.1
1	A	751	LYS	2.1
1	A	48	GLY	2.0
1	A	755	MET	2.0
1	A	68	PRO	2.0
1	B	615	ASP	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	1011	5/5	0.73	0.46	25.40	78,78,79,82	0
2	SO4	B	1012	5/5	0.72	0.44	24.74	85,85,87,87	0
2	SO4	B	1004	5/5	0.87	0.25	5.39	76,78,78,79	0
2	SO4	A	1010	5/5	0.85	0.33	4.89	71,72,74,74	0
3	ZN	A	2001	1/1	0.99	0.11	2.79	33,33,33,33	0
2	SO4	A	1003	5/5	0.89	0.21	1.64	74,75,75,77	0
3	ZN	B	2002	1/1	0.99	0.06	-1.77	30,30,30,30	0
2	SO4	A	1009	5/5	0.91	0.33	-	76,76,78,78	0
2	SO4	A	1008	5/5	0.88	0.29	-	78,80,80,80	0
2	SO4	A	1005	5/5	0.97	0.11	-	66,66,68,68	0
2	SO4	A	1016	5/5	0.80	0.30	-	73,74,76,77	0
2	SO4	A	1014	5/5	0.87	0.34	-	78,79,79,80	0
2	SO4	A	1015	5/5	0.92	0.27	-	73,73,74,74	0
2	SO4	A	1001	5/5	0.95	0.13	-	58,59,60,60	0
2	SO4	A	1006	5/5	0.98	0.13	-	61,62,63,63	0
2	SO4	A	1017	5/5	0.82	0.44	-	89,89,90,91	0
2	SO4	A	1002	5/5	0.89	0.35	-	80,81,81,83	0
2	SO4	B	1013	5/5	0.94	0.16	-	76,76,77,77	0
2	SO4	A	1007	5/5	0.81	0.40	-	82,82,83,83	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.