



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:40 PM GMT

PDB ID : 1Q2V
Title : Crystal structure of the chaperonin from Thermococcus strain KS-1
(nucleotide-free form)
Authors : Shomura, Y.; Yoshida, T.; Iizuka, R.; Yohda, M.; Maruyama, T.; Miki, K.
Deposited on : 2003-07-26
Resolution : 2.40 Å(reported)

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

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

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

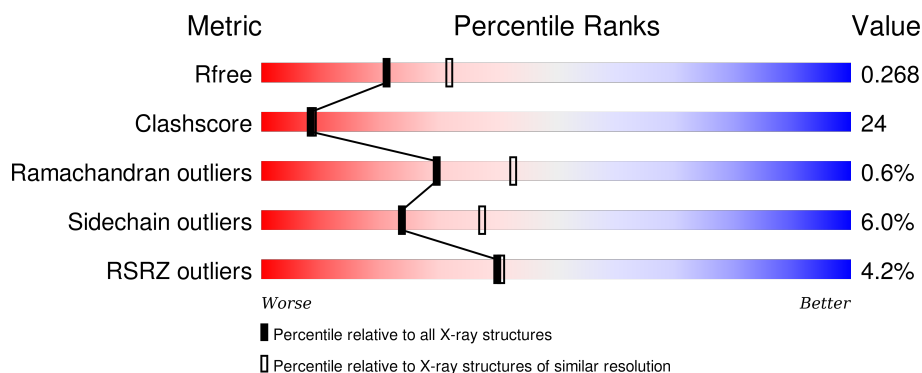
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	548	<div> <div>5%</div> <div> <div>56%</div> <div>36%</div> <div>• 5%</div> </div> </div>
1	B	548	<div> <div>4%</div> <div> <div>57%</div> <div>33%</div> <div>• 5%</div> </div> </div>
1	C	548	<div> <div>3%</div> <div> <div>57%</div> <div>35%</div> <div>• 5%</div> </div> </div>
1	D	548	<div> <div>4%</div> <div> <div>58%</div> <div>32%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15963 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 Thermosome alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			3947	2485	673	772	17			
1	B	518	Total	C	N	O	S	0	0	0
			3947	2485	673	772	17			
1	C	518	Total	C	N	O	S	0	0	0
			3947	2485	673	772	17			
1	D	518	Total	C	N	O	S	0	0	0
			3947	2485	673	772	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	CYS	GLY	ENGINEERED	UNP O24729
A	125	THR	ILE	ENGINEERED	UNP O24729
B	65	CYS	GLY	ENGINEERED	UNP O24729
B	125	THR	ILE	ENGINEERED	UNP O24729
C	65	CYS	GLY	ENGINEERED	UNP O24729
C	125	THR	ILE	ENGINEERED	UNP O24729
D	65	CYS	GLY	ENGINEERED	UNP O24729
D	125	THR	ILE	ENGINEERED	UNP O24729

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



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

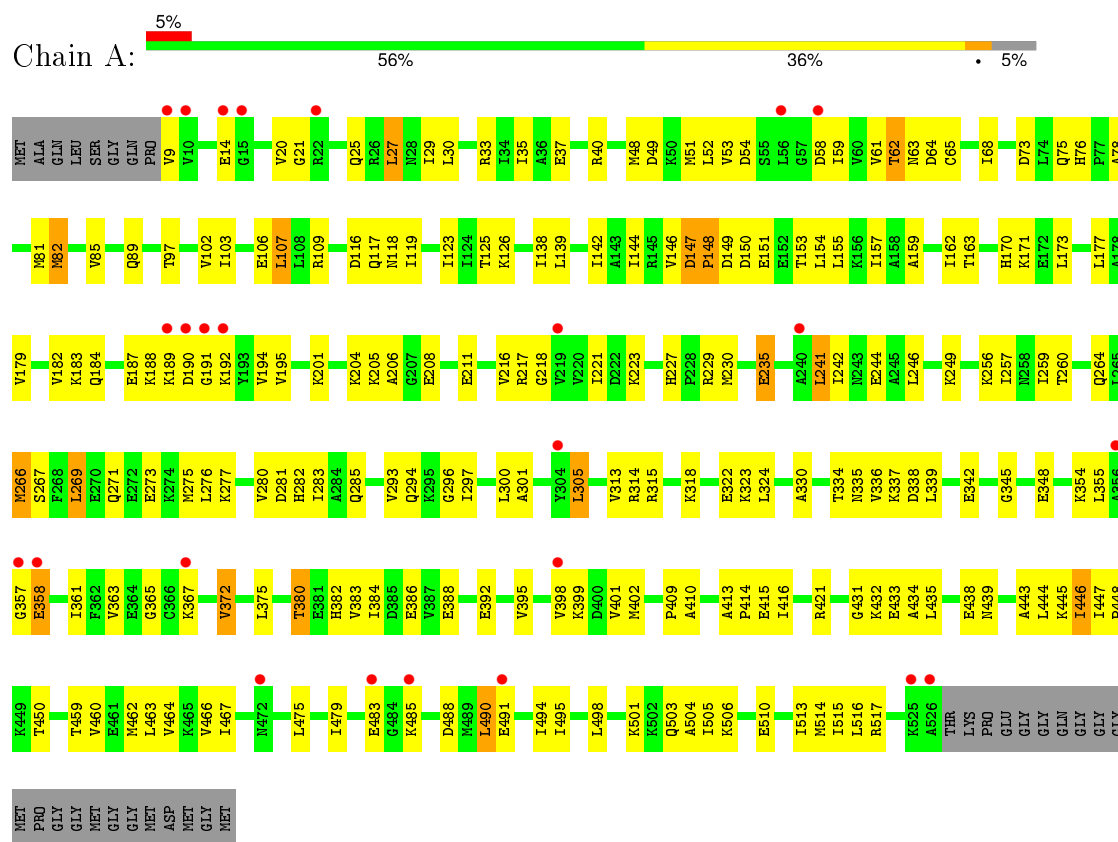
- Molecule 3 is water.

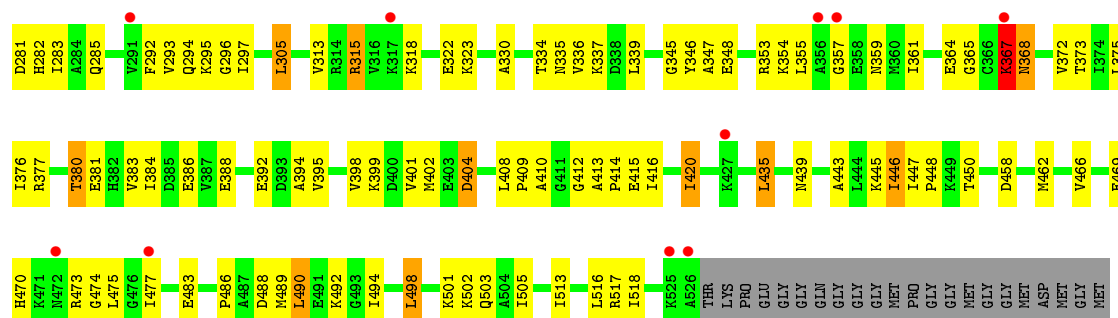
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total	O	0	0
			43	43		
3	B	40	Total	O	0	0
			40	40		
3	C	36	Total	O	0	0
			36	36		
3	D	36	Total	O	0	0
			36	36		

3 Residue-property plots

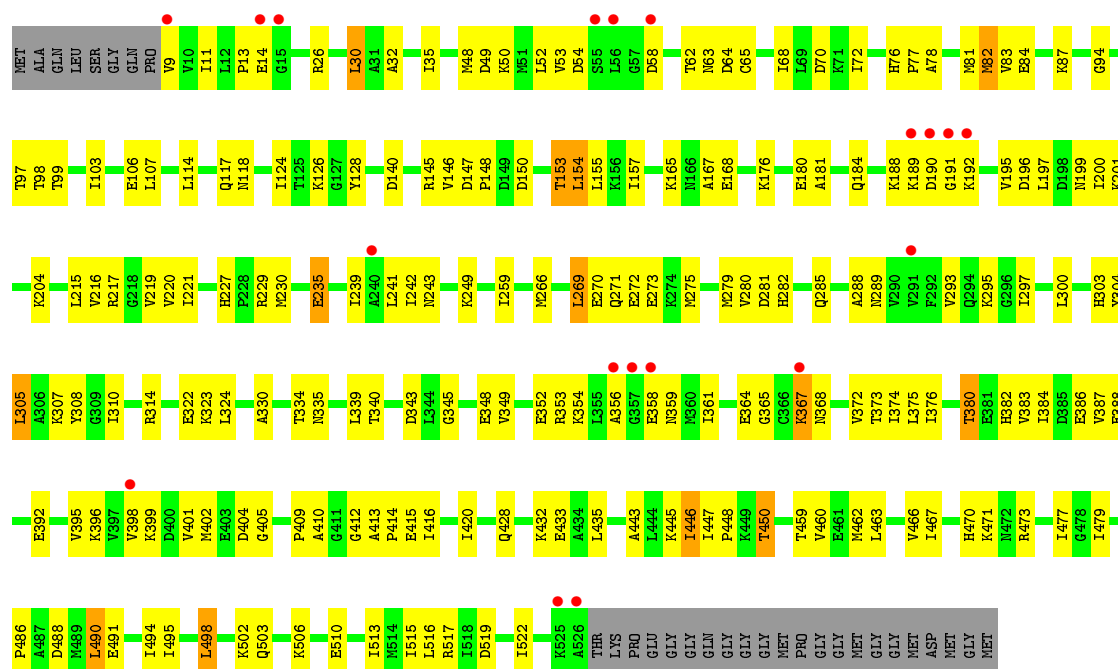
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Thermosome alpha subunit

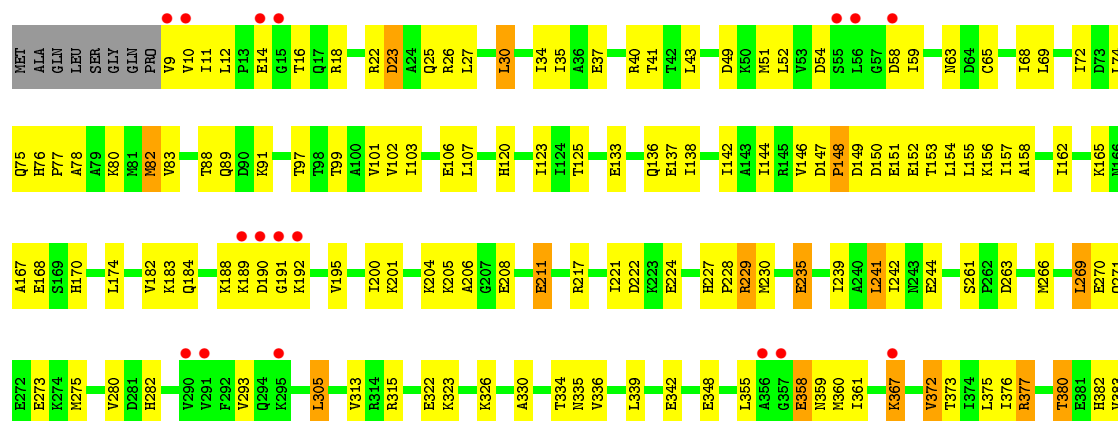


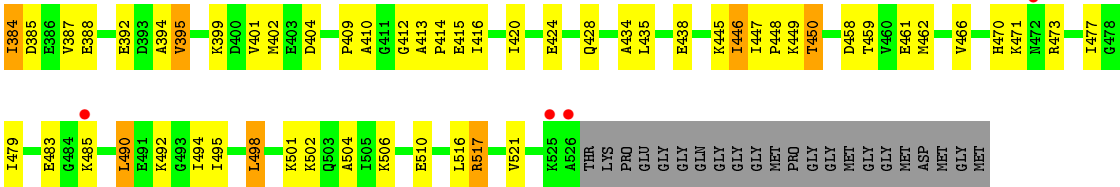


• Molecule 1: Thermosome alpha subunit



• Molecule 1: Thermosome alpha subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	209.27Å 209.27Å 156.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.40 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.99-2.40) 99.3 (19.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.269 0.245 , 0.268	Depositor DCC
R_{free} test set	6736 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 134056 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15963	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.36	0/3982	0.63	0/5367
1	B	0.38	1/3982 (0.0%)	0.64	2/5367 (0.0%)
1	C	0.37	0/3982	0.64	0/5367
1	D	0.37	1/3982 (0.0%)	0.62	0/5367
All	All	0.37	2/15928 (0.0%)	0.63	2/21468 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	11	ILE	C-N	-6.78	1.18	1.34
1	D	158	ALA	C-N	-6.17	1.19	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	ASP	N-CA-C	-5.11	97.19	111.00
1	B	236	ASN	N-CA-C	-5.09	97.24	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3947	0	4127	213	0
1	B	3947	0	4126	219	0
1	C	3947	0	4127	189	0
1	D	3947	0	4126	193	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	43	0	0	3	0
3	B	40	0	0	4	0
3	C	36	0	0	1	0
3	D	36	0	0	1	0
All	All	15963	0	16506	782	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 24.

All (782) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:VAL:HG22	1:A:59:ILE:HD13	1.22	1.14
1:B:120:HIS:HB3	1:B:123:ILE:HD13	1.23	1.13
1:D:120:HIS:HB3	1:D:123:ILE:HD13	1.32	1.10
1:D:52:LEU:HD22	1:D:72:ILE:HD11	1.33	1.09
1:B:473:ARG:HB2	1:B:477:ILE:HD11	1.35	1.07
1:C:289:ASN:HA	1:C:310:ILE:HD12	1.38	1.06
1:A:416:ILE:HG23	1:A:467:ILE:HD13	1.42	1.02
1:A:462:MET:O	1:A:466:VAL:HG23	1.64	0.97
1:B:293:VAL:HG21	1:B:297:ILE:HD11	1.48	0.96
1:D:462:MET:O	1:D:466:VAL:HG23	1.65	0.96
1:A:61:VAL:HG13	1:B:518:ILE:HD11	1.46	0.95
1:D:103:ILE:HA	1:D:446:ILE:HD11	1.49	0.92
1:C:446:ILE:O	1:C:450:THR:HG23	1.67	0.92
1:A:52:LEU:HD11	1:A:68:ILE:HD13	1.49	0.92
1:D:446:ILE:O	1:D:450:THR:HG23	1.70	0.92
1:B:29:ILE:HD12	1:B:108:LEU:HB3	1.52	0.91
1:A:206:ALA:HA	1:A:384:ILE:HD11	1.51	0.90
1:B:446:ILE:O	1:B:450:THR:HG23	1.72	0.90
1:C:189:LYS:HG3	1:C:190:ASP:H	1.35	0.89
1:D:189:LYS:HG3	1:D:190:ASP:H	1.35	0.89
1:B:462:MET:O	1:B:466:VAL:HG23	1.71	0.89
1:D:380:THR:HG22	1:D:383:VAL:H	1.34	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:VAL:HG21	1:A:297:ILE:HD11	1.53	0.88
1:A:246:LEU:HD22	1:A:297:ILE:HD12	1.53	0.88
1:C:410:ALA:HB3	1:C:494:ILE:HG22	1.56	0.88
1:D:380:THR:HG21	3:D:4541:HOH:O	1.75	0.87
1:B:473:ARG:CB	1:B:477:ILE:HD11	2.04	0.87
1:C:201:LYS:HB2	1:C:323:LYS:HE2	1.56	0.86
1:C:128:TYR:CB	1:C:513:ILE:HD11	2.06	0.86
1:B:52:LEU:HD22	1:B:72:ILE:HD11	1.56	0.86
1:C:272:GLU:HA	1:C:275:MET:HE2	1.56	0.85
1:C:52:LEU:HD22	1:C:72:ILE:HD11	1.58	0.85
1:B:246:LEU:HD22	1:B:297:ILE:HD12	1.59	0.85
1:B:416:ILE:O	1:B:420:ILE:HD13	1.76	0.84
1:A:25:GLN:O	1:A:29:ILE:HD13	1.77	0.84
1:B:29:ILE:CD1	1:B:108:LEU:HD22	2.05	0.84
1:B:409:PRO:HB3	1:B:490:LEU:HD13	1.60	0.84
1:D:492:LYS:HB2	1:D:494:ILE:HD13	1.59	0.84
1:C:52:LEU:HD11	1:C:68:ILE:HD13	1.57	0.84
1:C:463:LEU:O	1:C:467:ILE:HD13	1.76	0.84
1:D:517:ARG:HB3	1:D:517:ARG:HH11	1.43	0.83
1:A:155:LEU:HD12	1:A:179:VAL:HG21	1.58	0.83
1:A:260:THR:H	1:A:264:GLN:NE2	1.77	0.82
1:C:462:MET:O	1:C:466:VAL:HG23	1.78	0.82
1:C:280:VAL:HG13	1:C:305:LEU:HD13	1.61	0.82
1:A:409:PRO:HB3	1:A:490:LEU:HD13	1.61	0.82
1:A:283:ILE:HD11	1:A:336:VAL:HG13	1.61	0.82
1:B:473:ARG:HB2	1:B:477:ILE:CD1	2.10	0.82
1:A:271:GLN:HG3	1:A:275:MET:CE	2.10	0.82
1:D:409:PRO:HB3	1:D:490:LEU:HD13	1.61	0.81
1:D:170:HIS:CD2	1:D:211:GLU:HG2	2.15	0.81
1:A:61:VAL:CG1	1:B:518:ILE:HD11	2.11	0.80
1:B:52:LEU:HD11	1:B:68:ILE:HD13	1.64	0.80
1:A:54:ASP:OD2	1:A:58:ASP:HB3	1.82	0.79
1:A:446:ILE:O	1:A:450:THR:HG23	1.82	0.79
1:B:120:HIS:HB3	1:B:123:ILE:CD1	2.10	0.79
1:A:446:ILE:HD12	1:A:447:ILE:HD12	1.62	0.79
1:C:128:TYR:HB2	1:C:513:ILE:HD11	1.65	0.79
1:B:470:HIS:HA	1:B:477:ILE:HD13	1.62	0.78
1:B:447:ILE:HB	1:B:448:PRO:HD3	1.66	0.78
1:A:49:ASP:OD1	1:A:63:ASN:HB2	1.84	0.78
1:B:159:ALA:O	1:B:163:THR:HG22	1.84	0.77
1:C:181:ALA:HB1	1:C:200:ILE:HD12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:MET:O	1:C:270:GLU:HG3	1.83	0.77
1:A:355:LEU:O	1:A:358:GLU:HG2	1.84	0.77
1:D:76:HIS:HD2	1:D:78:ALA:H	1.33	0.77
1:B:162:ILE:HD13	3:B:2543:HOH:O	1.85	0.77
1:D:76:HIS:CD2	1:D:78:ALA:H	2.03	0.77
1:A:204:LYS:HB2	1:A:384:ILE:HG21	1.65	0.76
1:B:380:THR:HG22	1:B:383:VAL:H	1.49	0.76
1:D:447:ILE:HB	1:D:448:PRO:HD3	1.67	0.76
1:C:380:THR:HG22	1:C:383:VAL:H	1.50	0.76
1:B:139:LEU:HD11	1:B:505:ILE:HD12	1.68	0.76
1:C:62:THR:HG22	1:C:64:ASP:H	1.48	0.76
1:B:204:LYS:HB3	1:B:384:ILE:HG21	1.67	0.76
1:B:470:HIS:HA	1:B:477:ILE:CD1	2.14	0.76
1:A:227:HIS:HB3	1:A:230:MET:HG3	1.67	0.76
1:C:189:LYS:HG3	1:C:190:ASP:N	2.01	0.76
1:D:227:HIS:HD2	1:D:229:ARG:H	1.31	0.76
1:A:506:LYS:O	1:A:510:GLU:HG3	1.86	0.76
1:D:189:LYS:HG3	1:D:190:ASP:N	2.01	0.75
1:D:157:ILE:HG12	1:D:495:ILE:CD1	2.16	0.75
1:A:271:GLN:HG3	1:A:275:MET:HE3	1.68	0.75
1:D:495:ILE:HD12	1:D:495:ILE:O	1.86	0.75
1:B:283:ILE:HD11	1:B:336:VAL:HG13	1.69	0.74
1:A:188:LYS:HE3	1:A:191:GLY:HA2	1.69	0.74
1:D:334:THR:HG22	1:D:335:ASN:ND2	2.02	0.74
1:C:443:ALA:O	1:C:446:ILE:HG13	1.87	0.74
1:B:76:HIS:CD2	1:B:78:ALA:H	2.06	0.74
1:C:271:GLN:O	1:C:275:MET:HG3	1.87	0.73
1:A:483:GLU:CG	1:A:485:LYS:HE2	2.17	0.73
1:A:53:VAL:CG2	1:A:59:ILE:HD13	2.11	0.73
1:A:59:ILE:HD12	1:B:77:PRO:HB3	1.70	0.73
1:B:188:LYS:HE3	1:B:191:GLY:HA2	1.69	0.73
1:C:62:THR:HG23	1:C:386:GLU:OE2	1.87	0.73
1:B:246:LEU:HB2	1:B:297:ILE:HD12	1.71	0.73
1:A:380:THR:HG22	1:A:383:VAL:H	1.53	0.72
1:A:260:THR:H	1:A:264:GLN:HE22	1.36	0.72
1:B:266:MET:O	1:B:270:GLU:HG3	1.88	0.72
1:B:211:GLU:HB2	3:B:2533:HOH:O	1.89	0.72
1:B:446:ILE:HD12	1:B:447:ILE:HD12	1.71	0.72
1:C:432:LYS:HA	1:C:435:LEU:HD23	1.72	0.72
1:D:49:ASP:OD1	1:D:63:ASN:HB2	1.90	0.72
1:B:354:LYS:HE2	1:B:357:GLY:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLU:HA	1:B:275:MET:CE	2.20	0.71
1:C:466:VAL:HG21	1:C:479:ILE:HG12	1.72	0.71
1:D:492:LYS:CB	1:D:494:ILE:HD13	2.18	0.71
1:A:415:GLU:HG3	1:A:447:ILE:HB	1.72	0.71
1:D:205:LYS:C	1:D:384:ILE:HD11	2.11	0.71
1:B:498:LEU:HD11	1:B:502:LYS:HD2	1.71	0.71
1:C:49:ASP:OD1	1:C:63:ASN:HB2	1.91	0.71
1:A:227:HIS:HD2	1:A:229:ARG:H	1.37	0.70
1:A:432:LYS:HA	1:A:435:LEU:HD13	1.73	0.70
1:B:206:ALA:HA	1:B:384:ILE:HD11	1.73	0.70
1:B:413:ALA:HB3	1:B:414:PRO:HD3	1.73	0.70
1:D:313:VAL:HG21	1:D:361:ILE:HD13	1.74	0.70
1:C:272:GLU:HA	1:C:275:MET:CE	2.21	0.70
1:D:410:ALA:HB3	1:D:494:ILE:HG22	1.72	0.70
1:A:283:ILE:HD12	1:A:339:LEU:CD2	2.21	0.70
1:A:81:MET:SD	1:A:515:ILE:HD11	2.32	0.70
1:B:76:HIS:HD2	1:B:78:ALA:H	1.38	0.70
1:C:200:ILE:HD13	1:C:372:VAL:HG12	1.72	0.70
1:A:204:LYS:HB2	1:A:384:ILE:CG2	2.21	0.70
1:C:81:MET:SD	1:C:515:ILE:HD11	2.32	0.70
1:A:447:ILE:HB	1:A:448:PRO:HD3	1.72	0.69
1:B:376:ILE:HG22	1:B:384:ILE:HG23	1.74	0.69
1:A:296:GLY:O	1:A:297:ILE:HD13	1.92	0.69
1:C:140:ASP:OD1	1:C:502:LYS:HE3	1.92	0.69
1:B:443:ALA:O	1:B:446:ILE:HG13	1.92	0.69
1:C:401:VAL:O	1:C:404:ASP:O	2.10	0.69
1:B:49:ASP:OD1	1:B:63:ASN:HB2	1.92	0.69
1:B:103:ILE:CG1	1:B:447:ILE:HD11	2.22	0.69
1:A:246:LEU:HB2	1:A:297:ILE:HD12	1.74	0.69
1:B:259:ILE:HD13	1:B:265:LEU:HD23	1.75	0.69
1:C:447:ILE:HB	1:C:448:PRO:HD3	1.74	0.69
1:C:352:GLU:HA	1:C:361:ILE:HD13	1.74	0.69
1:B:227:HIS:HB3	1:B:230:MET:HG3	1.73	0.69
1:C:204:LYS:HB3	1:C:384:ILE:HG21	1.72	0.69
1:D:102:VAL:HG12	1:D:446:ILE:HD12	1.74	0.68
1:D:266:MET:O	1:D:270:GLU:HG3	1.94	0.68
1:B:293:VAL:CG2	1:B:297:ILE:HD11	2.22	0.68
1:A:159:ALA:O	1:A:163:THR:HG23	1.94	0.68
1:C:114:LEU:CD1	1:C:124:ILE:HD12	2.24	0.68
1:A:283:ILE:HD12	1:A:339:LEU:HD22	1.75	0.68
1:D:52:LEU:HD22	1:D:72:ILE:CD1	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ILE:HG12	1:D:495:ILE:HD11	1.76	0.68
1:B:170:HIS:CD2	1:B:211:GLU:HG2	2.28	0.68
1:D:409:PRO:HB3	1:D:490:LEU:CD1	2.23	0.67
1:B:146:VAL:HG21	1:B:153:THR:HG21	1.76	0.67
1:B:246:LEU:HB2	1:B:297:ILE:CD1	2.25	0.67
1:C:128:TYR:HB3	1:C:513:ILE:HD11	1.73	0.67
1:D:201:LYS:HB2	1:D:323:LYS:HE2	1.75	0.66
1:D:498:LEU:HD22	1:D:502:LYS:HG3	1.76	0.66
1:B:215:LEU:HD11	1:B:372:VAL:HG21	1.77	0.66
1:A:139:LEU:HD11	1:A:505:ILE:HD12	1.78	0.66
1:A:227:HIS:CD2	1:A:229:ARG:H	2.12	0.66
1:A:246:LEU:HB2	1:A:297:ILE:CD1	2.26	0.66
1:D:204:LYS:HD2	1:D:384:ILE:HG23	1.77	0.66
1:B:313:VAL:HG21	1:B:361:ILE:HD13	1.77	0.66
1:A:162:ILE:HD13	3:A:1533:HOH:O	1.96	0.66
1:B:474:GLY:O	1:B:477:ILE:HD12	1.96	0.66
1:A:483:GLU:HG2	1:A:485:LYS:HE2	1.78	0.66
1:A:53:VAL:HG22	1:A:59:ILE:CD1	2.14	0.65
1:A:483:GLU:HG3	1:A:485:LYS:HE2	1.78	0.65
1:D:235:GLU:O	1:D:348:GLU:O	2.14	0.65
1:B:29:ILE:HD11	1:B:108:LEU:HD22	1.79	0.65
1:C:463:LEU:HD13	1:C:467:ILE:HD11	1.79	0.65
1:A:410:ALA:HB3	1:A:494:ILE:HG22	1.77	0.65
1:B:170:HIS:HD2	1:B:211:GLU:HG2	1.62	0.65
1:C:409:PRO:HB3	1:C:490:LEU:HD13	1.79	0.65
1:C:201:LYS:HB2	1:C:323:LYS:CE	2.27	0.65
1:D:227:HIS:HB3	1:D:230:MET:HG3	1.78	0.65
1:C:380:THR:O	1:C:384:ILE:HG12	1.97	0.65
1:C:415:GLU:HG3	1:C:447:ILE:HB	1.78	0.65
1:A:182:VAL:CG2	1:A:395:VAL:HG13	2.27	0.65
1:A:76:HIS:HD2	1:A:78:ALA:H	1.45	0.65
1:B:151:GLU:O	1:B:155:LEU:HD22	1.97	0.64
1:C:62:THR:HG22	1:C:63:ASN:H	1.63	0.64
1:D:106:GLU:HG2	1:D:446:ILE:HG12	1.79	0.64
1:D:420:ILE:HD12	1:D:471:LYS:HE3	1.80	0.64
1:C:420:ILE:HD12	1:C:471:LYS:HE3	1.80	0.64
1:D:334:THR:HG22	1:D:335:ASN:HD22	1.62	0.64
1:C:503:GLN:HE22	1:D:208:GLU:H	1.46	0.64
1:B:244:GLU:OE2	1:B:249:LYS:HD3	1.96	0.64
1:C:221:ILE:HD11	1:C:324:LEU:HD11	1.80	0.64
1:D:157:ILE:CD1	1:D:495:ILE:HD13	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LYS:HB2	1:B:323:LYS:HE2	1.78	0.63
1:A:380:THR:HG22	1:A:383:VAL:HG23	1.79	0.63
1:D:227:HIS:CD2	1:D:229:ARG:H	2.16	0.63
1:C:76:HIS:CD2	1:C:78:ALA:H	2.17	0.63
1:B:272:GLU:HA	1:B:275:MET:HE3	1.81	0.63
1:C:466:VAL:HG22	1:C:486:PRO:HG3	1.81	0.63
1:D:388:GLU:O	1:D:392:GLU:HG3	1.99	0.63
1:B:415:GLU:OE1	1:B:501:LYS:HE3	1.99	0.62
1:A:150:ASP:OD2	1:A:153:THR:HG23	1.99	0.62
1:C:114:LEU:HD12	1:C:124:ILE:HD12	1.80	0.62
1:C:76:HIS:HD2	1:C:78:ALA:H	1.47	0.62
1:A:61:VAL:HG13	1:B:518:ILE:CD1	2.27	0.62
1:C:353:ARG:HH22	1:C:364:GLU:CD	2.02	0.62
1:D:492:LYS:CB	1:D:494:ILE:CD1	2.77	0.62
1:B:296:GLY:O	1:B:297:ILE:HD13	1.99	0.62
1:B:103:ILE:HG12	1:B:447:ILE:HD11	1.81	0.62
1:B:376:ILE:CG2	1:B:384:ILE:HG23	2.30	0.62
1:A:443:ALA:O	1:A:446:ILE:HG13	1.99	0.62
1:A:246:LEU:CD2	1:A:297:ILE:HD12	2.27	0.62
1:A:52:LEU:HD11	1:A:68:ILE:CD1	2.25	0.62
1:A:380:THR:CG2	1:A:383:VAL:H	2.12	0.62
1:D:162:ILE:HD11	1:D:394:ALA:HB2	1.81	0.62
1:C:54:ASP:OD2	1:C:58:ASP:HB3	2.00	0.62
1:A:416:ILE:HG23	1:A:467:ILE:CD1	2.23	0.61
1:A:447:ILE:H	1:A:447:ILE:HD12	1.64	0.61
1:A:76:HIS:CD2	1:A:78:ALA:H	2.18	0.61
1:B:151:GLU:HG3	1:B:155:LEU:HD21	1.83	0.61
1:B:469:GLU:O	1:B:477:ILE:HD13	2.01	0.61
1:A:235:GLU:O	1:A:348:GLU:O	2.18	0.61
1:B:409:PRO:HB3	1:B:490:LEU:CD1	2.30	0.61
1:C:52:LEU:CD1	1:C:68:ILE:HD13	2.31	0.61
1:B:163:THR:HB	1:B:171:LYS:NZ	2.15	0.61
1:D:415:GLU:HG3	1:D:447:ILE:HB	1.82	0.61
1:D:102:VAL:HG12	1:D:446:ILE:CD1	2.31	0.61
1:B:408:LEU:HD11	1:B:498:LEU:HD23	1.83	0.61
1:B:182:VAL:CG2	1:B:395:VAL:HG13	2.30	0.61
1:A:59:ILE:CD1	1:B:77:PRO:HB3	2.31	0.61
1:A:182:VAL:HG22	1:A:395:VAL:HG13	1.82	0.61
1:A:335:ASN:OD1	1:A:337:LYS:HG2	1.99	0.61
1:C:77:PRO:HB2	1:D:51:MET:CE	2.31	0.60
1:A:75:GLN:NE2	1:B:13:PRO:HG3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:VAL:HG11	1:D:479:ILE:CD1	2.31	0.60
1:A:204:LYS:HD2	1:A:384:ILE:HG22	1.83	0.60
1:B:355:LEU:HD22	1:B:377:ARG:NH2	2.16	0.60
1:B:282:HIS:HE1	1:B:339:LEU:O	1.84	0.60
1:D:242:ILE:O	1:D:293:VAL:HA	2.00	0.60
1:D:492:LYS:HB3	1:D:494:ILE:CD1	2.31	0.60
1:A:173:LEU:O	1:A:177:LEU:HG	2.02	0.60
1:B:294:GLN:O	1:B:315:ARG:HA	2.00	0.60
1:D:76:HIS:HD2	1:D:78:ALA:N	1.99	0.60
1:A:189:LYS:HG3	1:A:190:ASP:H	1.67	0.60
1:D:495:ILE:HD12	1:D:495:ILE:C	2.23	0.60
1:C:13:PRO:HG3	1:D:75:GLN:NE2	2.17	0.60
1:D:146:VAL:HG22	1:D:147:ASP:N	2.15	0.60
1:B:106:GLU:HB2	1:B:446:ILE:HG12	1.83	0.59
1:C:52:LEU:HD11	1:C:68:ILE:CD1	2.31	0.59
1:B:206:ALA:CA	1:B:384:ILE:HD11	2.32	0.59
1:C:249:LYS:HB2	1:D:269:LEU:HD21	1.82	0.59
1:A:273:GLU:OE2	1:B:337:LYS:HE2	2.02	0.59
1:A:313:VAL:HG21	1:A:361:ILE:HD13	1.84	0.59
1:A:293:VAL:CG2	1:A:297:ILE:HD11	2.29	0.59
1:B:247:GLU:HA	1:B:276:LEU:HD11	1.84	0.59
1:C:106:GLU:CB	1:C:446:ILE:HG12	2.33	0.59
1:B:189:LYS:HG3	1:B:190:ASP:H	1.67	0.59
1:C:188:LYS:HE2	1:C:191:GLY:HA2	1.84	0.59
1:A:142:ILE:HD12	1:A:475:LEU:HD11	1.84	0.59
1:D:188:LYS:HE2	1:D:191:GLY:HA2	1.84	0.59
1:C:297:ILE:HD12	1:C:314:ARG:HB3	1.85	0.59
1:C:498:LEU:HD22	1:C:502:LYS:HG3	1.83	0.59
1:C:242:ILE:O	1:C:293:VAL:HA	2.03	0.59
1:C:432:LYS:HA	1:C:435:LEU:CD2	2.33	0.59
1:D:157:ILE:HG12	1:D:495:ILE:HD13	1.85	0.58
1:D:434:ALA:O	1:D:438:GLU:HG3	2.01	0.58
1:C:503:GLN:HE22	1:D:208:GLU:N	2.01	0.58
1:B:235:GLU:O	1:B:348:GLU:O	2.21	0.58
1:A:138:ILE:HD12	1:A:421:ARG:HD2	1.84	0.58
1:A:246:LEU:HD22	1:A:297:ILE:CD1	2.32	0.58
1:D:157:ILE:HD12	1:D:401:VAL:HG21	1.85	0.58
1:A:106:GLU:HB2	1:A:446:ILE:HG12	1.84	0.58
1:C:289:ASN:HA	1:C:310:ILE:CD1	2.24	0.58
1:B:139:LEU:HD11	1:B:505:ILE:CD1	2.33	0.58
1:B:293:VAL:HG11	1:B:297:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ILE:HD13	1:C:495:ILE:HG13	1.84	0.58
1:D:242:ILE:HD13	1:D:336:VAL:HG22	1.85	0.58
1:C:348:GLU:HG2	1:C:349:VAL:HG23	1.85	0.58
1:C:380:THR:CG2	1:C:383:VAL:H	2.17	0.58
1:B:243:ASN:O	1:B:295:LYS:HG2	2.04	0.58
1:B:415:GLU:HG3	1:B:447:ILE:HB	1.86	0.58
1:A:354:LYS:HE2	1:A:357:GLY:O	2.04	0.57
1:B:293:VAL:HG21	1:B:297:ILE:CD1	2.29	0.57
1:D:170:HIS:NE2	1:D:211:GLU:HG2	2.18	0.57
1:D:37:GLU:O	1:D:40:ARG:HG2	2.04	0.57
1:A:146:VAL:HG22	1:A:147:ASP:H	1.69	0.57
1:A:283:ILE:CD1	1:A:339:LEU:CD2	2.82	0.57
1:B:367:LYS:HD2	1:B:368:ASN:HB2	1.85	0.57
1:B:381:GLU:HA	1:B:384:ILE:HD12	1.85	0.57
1:B:155:LEU:HD13	1:B:179:VAL:HG21	1.86	0.57
1:B:182:VAL:HG22	1:B:395:VAL:HG13	1.85	0.57
1:D:54:ASP:OD2	1:D:58:ASP:HB3	2.04	0.57
1:A:445:LYS:O	1:A:448:PRO:HD2	2.05	0.57
1:A:416:ILE:CG2	1:A:467:ILE:HD13	2.24	0.57
1:D:103:ILE:HA	1:D:446:ILE:CD1	2.29	0.57
1:B:103:ILE:HD11	1:B:447:ILE:HD11	1.86	0.57
1:C:70:ASP:HB2	1:C:87:LYS:HE2	1.87	0.57
1:A:48:MET:HA	1:A:48:MET:HE2	1.87	0.57
1:B:224:GLU:HG2	1:B:359:ASN:HB2	1.86	0.57
1:C:416:ILE:HD11	1:C:448:PRO:HG2	1.86	0.57
1:A:386:GLU:OE2	1:A:386:GLU:HA	2.05	0.57
1:D:375:LEU:C	1:D:375:LEU:HD23	2.24	0.57
1:C:83:VAL:O	1:C:87:LYS:HG2	2.05	0.56
1:C:157:ILE:HG13	1:C:401:VAL:HG21	1.86	0.56
1:A:189:LYS:HG3	1:A:190:ASP:N	2.20	0.56
1:A:82:MET:CE	1:A:82:MET:HA	2.36	0.56
1:C:466:VAL:HG21	1:C:479:ILE:CG1	2.34	0.56
1:C:372:VAL:HG22	1:C:373:THR:N	2.21	0.56
1:B:272:GLU:HA	1:B:275:MET:HE2	1.87	0.56
1:C:388:GLU:O	1:C:392:GLU:HG3	2.04	0.56
1:A:103:ILE:CG1	1:A:447:ILE:HD11	2.35	0.56
1:A:283:ILE:CD1	1:A:336:VAL:HG13	2.35	0.56
1:A:380:THR:HG23	1:A:382:HIS:N	2.21	0.56
1:C:372:VAL:HG22	1:C:373:THR:H	1.71	0.56
1:D:82:MET:HG3	1:D:101:VAL:HG13	1.88	0.56
1:A:380:THR:HG23	1:A:382:HIS:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:VAL:HG13	1:A:305:LEU:HD13	1.88	0.56
1:B:498:LEU:CD1	1:B:502:LYS:HD2	2.37	0.55
1:A:460:VAL:HG22	3:C:3540:HOH:O	2.05	0.55
1:D:492:LYS:O	1:D:494:ILE:HD12	2.07	0.55
1:B:189:LYS:HG3	1:B:190:ASP:N	2.20	0.55
1:D:138:ILE:O	1:D:142:ILE:HG12	2.07	0.55
1:B:106:GLU:CB	1:B:446:ILE:HG12	2.36	0.55
1:D:517:ARG:NH1	1:D:517:ARG:HB3	2.19	0.55
1:B:216:VAL:O	1:B:372:VAL:HG23	2.06	0.55
1:B:470:HIS:CA	1:B:477:ILE:HD13	2.36	0.55
1:C:62:THR:HG22	1:C:63:ASN:N	2.21	0.55
1:C:197:LEU:HD22	1:C:395:VAL:HG13	1.87	0.55
1:C:348:GLU:HB3	1:C:365:GLY:HA3	1.89	0.55
1:B:162:ILE:HD11	1:B:394:ALA:HB2	1.88	0.55
1:A:48:MET:HA	1:A:48:MET:CE	2.37	0.55
1:D:184:GLN:NE2	1:D:217:ARG:HH21	2.05	0.55
1:B:353:ARG:NH2	1:B:364:GLU:OE2	2.40	0.55
1:D:449:LYS:HE2	1:D:459:THR:HG21	1.88	0.54
1:A:513:ILE:O	1:A:517:ARG:HG3	2.07	0.54
1:B:246:LEU:CD2	1:B:297:ILE:HD12	2.34	0.54
1:D:65:CYS:HB3	1:D:97:THR:OG1	2.08	0.54
1:D:413:ALA:HB3	1:D:414:PRO:HD3	1.89	0.54
1:D:282:HIS:HE1	1:D:339:LEU:O	1.90	0.54
1:A:151:GLU:O	1:A:155:LEU:HD13	2.08	0.54
1:B:498:LEU:HD22	1:B:498:LEU:O	2.08	0.54
1:A:434:ALA:O	1:A:438:GLU:HG3	2.07	0.54
1:C:227:HIS:HB3	1:C:230:MET:HG3	1.89	0.54
1:D:204:LYS:HD2	1:D:384:ILE:CG2	2.38	0.54
1:B:227:HIS:CE1	1:B:229:ARG:HB2	2.43	0.54
1:C:420:ILE:HD12	1:C:471:LYS:CE	2.36	0.54
1:B:76:HIS:HD2	1:B:78:ALA:N	2.03	0.54
1:C:184:GLN:NE2	1:C:217:ARG:NH2	2.55	0.54
1:C:488:ASP:CG	1:C:491:GLU:HG3	2.29	0.54
1:B:401:VAL:O	1:B:404:ASP:O	2.26	0.54
1:C:446:ILE:O	1:C:450:THR:CG2	2.48	0.54
1:B:215:LEU:HD11	1:B:372:VAL:CG2	2.38	0.54
1:C:48:MET:HA	1:C:48:MET:HE2	1.90	0.54
1:B:123:ILE:N	1:B:123:ILE:HD12	2.22	0.53
1:A:466:VAL:HG21	1:A:479:ILE:HG13	1.89	0.53
1:D:412:GLY:O	1:D:416:ILE:HG12	2.08	0.53
1:A:82:MET:HE2	1:A:82:MET:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLU:HB2	3:A:1539:HOH:O	2.07	0.53
1:D:144:ILE:H	1:D:144:ILE:HD12	1.72	0.53
1:D:22:ARG:HD2	1:D:25:GLN:OE1	2.09	0.53
1:C:281:ASP:O	1:C:285:GLN:HG3	2.09	0.53
1:B:318:LYS:O	1:B:322:GLU:HG3	2.08	0.53
1:C:103:ILE:HD13	1:C:446:ILE:HD11	1.90	0.53
1:B:473:ARG:CA	1:B:477:ILE:HD11	2.37	0.53
1:A:330:ALA:HB2	1:A:345:GLY:HA3	1.91	0.53
1:A:184:GLN:NE2	1:A:217:ARG:HH21	2.06	0.53
1:C:243:ASN:O	1:C:295:LYS:HG2	2.08	0.53
1:B:139:LEU:CD1	1:B:505:ILE:HD12	2.37	0.53
1:C:167:ALA:HB2	1:C:387:VAL:HG22	1.91	0.53
1:A:102:VAL:HG12	1:A:446:ILE:HD13	1.91	0.53
1:A:49:ASP:HB2	1:B:518:ILE:HD13	1.91	0.53
1:B:29:ILE:HD12	1:B:108:LEU:HD22	1.91	0.53
1:B:103:ILE:CD1	1:B:447:ILE:HD11	2.38	0.53
1:A:283:ILE:CD1	1:A:339:LEU:HD23	2.38	0.53
1:A:266:MET:HA	1:A:266:MET:CE	2.39	0.53
1:C:412:GLY:O	1:C:415:GLU:HG2	2.09	0.52
1:D:88:THR:HA	1:D:91:LYS:HE2	1.91	0.52
1:D:494:ILE:N	1:D:494:ILE:HD12	2.24	0.52
1:A:276:LEU:HD23	1:A:300:LEU:HB3	1.92	0.52
1:C:227:HIS:CD2	1:C:229:ARG:H	2.28	0.52
1:A:206:ALA:HA	1:A:384:ILE:CD1	2.33	0.52
1:C:189:LYS:HE2	1:C:192:LYS:HB2	1.92	0.52
1:C:352:GLU:CA	1:C:361:ILE:HD13	2.38	0.52
1:D:146:VAL:HG22	1:D:147:ASP:H	1.74	0.52
1:A:170:HIS:CD2	1:A:211:GLU:HG2	2.44	0.52
1:A:139:LEU:HD11	1:A:505:ILE:CD1	2.38	0.52
1:D:144:ILE:HD12	1:D:144:ILE:N	2.25	0.52
1:C:99:THR:HG23	1:C:447:ILE:HD11	1.92	0.52
1:A:189:LYS:HG3	1:A:190:ASP:OD2	2.10	0.52
1:B:473:ARG:C	1:B:477:ILE:HD11	2.29	0.52
1:D:189:LYS:HE2	1:D:192:LYS:HB2	1.92	0.52
1:D:151:GLU:O	1:D:155:LEU:HB2	2.10	0.52
1:A:144:ILE:HD12	1:A:144:ILE:N	2.25	0.52
1:B:65:CYS:HB3	1:B:97:THR:OG1	2.09	0.52
1:A:479:ILE:N	1:A:479:ILE:HD12	2.24	0.52
1:C:106:GLU:HB2	1:C:446:ILE:HG12	1.91	0.52
1:B:189:LYS:HG3	1:B:190:ASP:OD2	2.10	0.52
1:A:146:VAL:HG22	1:A:147:ASP:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:THR:HG22	1:D:41:THR:O	2.10	0.51
1:D:149:ASP:HB2	1:D:183:LYS:NZ	2.24	0.51
1:D:376:ILE:H	1:D:376:ILE:HD12	1.75	0.51
1:D:23:ASP:O	1:D:27:LEU:HG	2.10	0.51
1:B:488:ASP:O	1:B:492:LYS:HG2	2.10	0.51
1:C:498:LEU:HD13	1:C:502:LYS:HD2	1.91	0.51
1:D:420:ILE:CD1	1:D:471:LYS:HE3	2.40	0.51
1:B:280:VAL:HG13	1:B:305:LEU:HD13	1.91	0.51
1:B:283:ILE:CD1	1:B:336:VAL:HG13	2.38	0.51
1:A:182:VAL:HG11	1:A:398:VAL:HG12	1.91	0.51
1:B:244:GLU:HB3	1:B:334:THR:O	2.09	0.51
1:B:119:ILE:HD11	1:B:435:LEU:HD23	1.92	0.51
1:A:126:LYS:HD3	1:A:433:GLU:CG	2.40	0.51
1:A:123:ILE:HG21	1:A:432:LYS:HB3	1.92	0.51
1:B:151:GLU:HG3	1:B:155:LEU:CD2	2.40	0.51
1:D:167:ALA:HB1	1:D:174:LEU:CD1	2.40	0.51
1:B:335:ASN:HB3	1:B:337:LYS:HG2	1.93	0.51
1:B:221:ILE:N	1:B:221:ILE:HD12	2.26	0.51
1:A:106:GLU:CB	1:A:446:ILE:HG12	2.40	0.51
1:C:386:GLU:OE2	1:C:386:GLU:HA	2.11	0.51
1:A:155:LEU:CD1	1:A:179:VAL:HG11	2.41	0.51
1:D:412:GLY:HA2	1:D:415:GLU:OE2	2.11	0.51
1:C:197:LEU:HD22	1:C:395:VAL:CG1	2.41	0.51
1:C:154:LEU:HG	1:C:398:VAL:HG13	1.93	0.51
1:C:416:ILE:CD1	1:C:448:PRO:HG2	2.41	0.51
1:C:114:LEU:HD13	1:C:124:ILE:HD12	1.92	0.51
1:C:76:HIS:HD2	1:C:78:ALA:N	2.08	0.51
1:C:184:GLN:NE2	1:C:217:ARG:HH21	2.08	0.51
1:D:376:ILE:N	1:D:376:ILE:HD12	2.26	0.51
1:A:103:ILE:HD11	1:A:447:ILE:HD11	1.93	0.51
1:A:216:VAL:O	1:A:372:VAL:HG22	2.10	0.51
1:C:330:ALA:HB2	1:C:345:GLY:HA3	1.93	0.51
1:A:488:ASP:CG	1:A:491:GLU:HG3	2.31	0.51
1:B:293:VAL:CB	1:B:297:ILE:HD11	2.42	0.50
1:B:355:LEU:HD11	1:B:375:LEU:HD21	1.93	0.50
1:C:334:THR:HG22	1:C:335:ASN:ND2	2.26	0.50
1:A:103:ILE:HG22	1:A:107:LEU:HD22	1.93	0.50
1:A:514:MET:HG3	3:A:1554:HOH:O	2.10	0.50
1:B:372:VAL:HG22	1:B:373:THR:N	2.26	0.50
1:A:208:GLU:H	1:B:503:GLN:HE22	1.59	0.50
1:C:189:LYS:HE3	1:C:190:ASP:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ILE:CD1	1:C:324:LEU:HD11	2.40	0.50
1:C:303:HIS:O	1:C:307:LYS:HG3	2.12	0.50
1:C:420:ILE:HD11	1:C:467:ILE:HG23	1.92	0.50
1:D:271:GLN:O	1:D:275:MET:HG3	2.12	0.50
1:A:409:PRO:HB3	1:A:490:LEU:CD1	2.35	0.50
1:D:189:LYS:HE3	1:D:190:ASP:OD1	2.11	0.50
1:B:187:GLU:HB2	1:B:194:VAL:CG1	2.41	0.50
1:B:147:ASP:HB3	1:B:150:ASP:HB2	1.94	0.49
1:C:239:ILE:HD12	1:C:239:ILE:N	2.27	0.49
1:D:241:LEU:HD22	1:D:330:ALA:HB3	1.93	0.49
1:C:445:LYS:O	1:C:448:PRO:HD2	2.11	0.49
1:A:73:ASP:O	1:B:13:PRO:HD3	2.11	0.49
1:A:33:ARG:HD2	1:A:109:ARG:HB2	1.94	0.49
1:C:32:ALA:HB1	1:C:82:MET:CE	2.41	0.49
1:B:117:GLN:O	1:B:118:ASN:HB2	2.12	0.49
1:D:271:GLN:HG3	1:D:275:MET:CE	2.42	0.49
1:D:59:ILE:N	1:D:59:ILE:HD12	2.27	0.49
1:A:445:LYS:C	1:A:448:PRO:HD2	2.33	0.49
1:D:458:ASP:OD1	1:D:461:GLU:HG3	2.13	0.49
1:A:201:LYS:HB2	1:A:323:LYS:HE2	1.95	0.49
1:A:264:GLN:HA	1:A:267:SER:OG	2.11	0.49
1:B:189:LYS:NZ	1:B:192:LYS:HB2	2.28	0.49
1:B:388:GLU:O	1:B:392:GLU:HG3	2.11	0.49
1:A:27:LEU:HD12	1:A:76:HIS:HE1	1.77	0.49
1:C:374:ILE:O	1:C:376:ILE:HD12	2.12	0.49
1:D:189:LYS:CE	1:D:192:LYS:HB2	2.42	0.49
1:D:375:LEU:HD21	1:D:377:ARG:HD3	1.93	0.49
1:D:380:THR:HG23	1:D:382:HIS:H	1.78	0.49
1:A:205:LYS:HE3	1:A:358:GLU:HG3	1.95	0.49
1:B:154:LEU:HG	1:B:398:VAL:HG13	1.94	0.49
1:A:163:THR:HG22	1:A:171:LYS:NZ	2.27	0.49
1:D:148:PRO:O	1:D:402:MET:HG2	2.13	0.49
1:C:282:HIS:HE1	1:C:339:LEU:O	1.95	0.49
1:C:340:THR:O	1:C:343:ASP:HB2	2.12	0.49
1:D:239:ILE:N	1:D:239:ILE:HD12	2.27	0.49
1:C:50:LYS:HB2	1:C:68:ILE:CD1	2.43	0.49
1:A:148:PRO:O	1:A:402:MET:HG2	2.10	0.49
1:C:189:LYS:CE	1:C:192:LYS:HB2	2.42	0.49
1:C:215:LEU:HD11	1:C:372:VAL:HG21	1.94	0.48
1:D:99:THR:HG23	1:D:447:ILE:CD1	2.43	0.48
1:B:367:LYS:HD2	1:B:368:ASN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:LEU:O	1:D:358:GLU:HG2	2.13	0.48
1:A:301:ALA:O	1:A:305:LEU:HB2	2.13	0.48
1:A:208:GLU:N	1:B:503:GLN:HE22	2.10	0.48
1:A:149:ASP:HB2	1:A:183:LYS:NZ	2.27	0.48
1:C:288:ALA:O	1:C:310:ILE:HD12	2.12	0.48
1:D:483:GLU:HG3	1:D:485:LYS:HE3	1.94	0.48
1:D:157:ILE:CD1	1:D:401:VAL:HG21	2.44	0.48
1:D:157:ILE:CG1	1:D:495:ILE:HD13	2.43	0.48
1:D:136:GLN:HE22	1:D:502:LYS:HG2	1.79	0.48
1:A:189:LYS:NZ	1:A:192:LYS:HB2	2.28	0.48
1:B:513:ILE:O	1:B:517:ARG:HG3	2.14	0.48
1:B:123:ILE:CD1	1:B:123:ILE:N	2.75	0.48
1:D:445:LYS:O	1:D:448:PRO:HD2	2.13	0.48
1:C:380:THR:HG22	1:C:383:VAL:HG23	1.95	0.48
1:D:506:LYS:O	1:D:510:GLU:HG3	2.14	0.48
1:C:99:THR:HG23	1:C:447:ILE:CD1	2.43	0.48
1:B:330:ALA:HB2	1:B:345:GLY:HA3	1.95	0.48
1:D:221:ILE:HD12	1:D:221:ILE:N	2.29	0.48
1:D:189:LYS:CG	1:D:190:ASP:H	2.17	0.48
1:D:445:LYS:C	1:D:448:PRO:HD2	2.34	0.48
1:B:54:ASP:OD2	1:B:58:ASP:HB3	2.13	0.48
1:B:409:PRO:HB2	1:B:489:MET:HB2	1.96	0.48
1:D:244:GLU:HB3	1:D:334:THR:O	2.13	0.48
1:C:503:GLN:NE2	1:D:208:GLU:H	2.12	0.48
1:C:239:ILE:HG22	1:C:241:LEU:HD13	1.96	0.48
1:A:259:ILE:HD12	1:A:264:GLN:HB3	1.95	0.47
1:B:354:LYS:HG2	1:B:357:GLY:C	2.35	0.47
1:B:265:LEU:O	1:B:269:LEU:HD22	2.14	0.47
1:A:459:THR:O	1:A:463:LEU:HD23	2.14	0.47
1:C:176:LYS:O	1:C:180:GLU:HG3	2.14	0.47
1:D:123:ILE:HD12	1:D:123:ILE:N	2.29	0.47
1:C:189:LYS:CG	1:C:190:ASP:H	2.17	0.47
1:A:242:ILE:HD13	1:A:336:VAL:HG22	1.95	0.47
1:C:235:GLU:O	1:C:348:GLU:O	2.32	0.47
1:B:445:LYS:C	1:B:448:PRO:HD2	2.35	0.47
1:D:205:LYS:C	1:D:384:ILE:CD1	2.83	0.47
1:A:318:LYS:O	1:A:322:GLU:HG3	2.15	0.47
1:A:282:HIS:HE1	1:A:339:LEU:O	1.97	0.47
1:B:420:ILE:CD1	1:B:420:ILE:N	2.77	0.47
1:D:446:ILE:O	1:D:450:THR:CG2	2.52	0.47
1:B:466:VAL:HG22	1:B:486:PRO:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:HIS:HA	1:B:228:PRO:HD3	1.78	0.47
1:A:431:GLY:O	1:A:434:ALA:HB3	2.15	0.47
1:C:150:ASP:HB3	1:C:153:THR:HG23	1.97	0.47
1:B:470:HIS:HA	1:B:477:ILE:HD12	1.97	0.47
1:D:280:VAL:HG13	1:D:305:LEU:HD13	1.97	0.47
1:B:355:LEU:HD22	1:B:377:ARG:HH21	1.77	0.47
1:A:227:HIS:CD2	1:A:229:ARG:HB2	2.49	0.47
1:C:409:PRO:HB3	1:C:490:LEU:CD1	2.43	0.47
1:C:147:ASP:HB2	1:C:150:ASP:HB2	1.96	0.47
1:B:184:GLN:NE2	1:B:217:ARG:HH21	2.12	0.47
1:D:495:ILE:CD1	1:D:495:ILE:C	2.83	0.47
1:D:269:LEU:O	1:D:273:GLU:HG3	2.14	0.47
1:A:266:MET:HE3	1:A:269:LEU:HD23	1.96	0.47
1:A:273:GLU:CD	1:B:337:LYS:HE2	2.36	0.47
1:C:195:VAL:HB	1:C:399:LYS:HG3	1.98	0.47
1:C:354:LYS:HG3	1:C:359:ASN:OD1	2.14	0.47
1:A:446:ILE:HD12	1:A:447:ILE:CD1	2.40	0.46
1:C:146:VAL:HG21	1:C:153:THR:HG21	1.96	0.46
1:C:216:VAL:O	1:C:372:VAL:HG23	2.16	0.46
1:D:205:LYS:O	1:D:384:ILE:HD11	2.16	0.46
1:C:77:PRO:HB2	1:D:51:MET:HE1	1.96	0.46
1:B:280:VAL:HG13	1:B:305:LEU:CD1	2.45	0.46
1:B:346:TYR:CG	1:B:347:ALA:N	2.83	0.46
1:C:196:ASP:HB3	1:C:199:ASN:ND2	2.30	0.46
1:D:52:LEU:HD11	1:D:68:ILE:HA	1.98	0.46
1:D:230:MET:CE	1:D:305:LEU:HB3	2.45	0.46
1:C:304:TYR:O	1:C:308:TYR:HD1	1.97	0.46
1:A:20:VAL:HG12	1:A:21:GLY:N	2.30	0.46
1:B:474:GLY:N	1:B:477:ILE:CD1	2.79	0.46
1:C:380:THR:HG23	1:C:382:HIS:N	2.31	0.46
1:D:230:MET:HE1	1:D:305:LEU:HB3	1.97	0.46
1:A:117:GLN:O	1:A:118:ASN:HB2	2.16	0.46
1:A:283:ILE:CD1	1:A:339:LEU:HD22	2.42	0.46
1:A:283:ILE:HD13	1:A:339:LEU:HD23	1.97	0.46
1:C:227:HIS:CD2	1:C:229:ARG:HB2	2.50	0.46
1:B:160:THR:O	1:B:163:THR:HG23	2.16	0.46
1:D:358:GLU:H	1:D:358:GLU:HG2	1.55	0.46
1:A:51:MET:CE	1:B:77:PRO:HB2	2.46	0.46
1:C:103:ILE:HD13	1:C:446:ILE:CD1	2.46	0.46
1:A:242:ILE:O	1:A:293:VAL:HA	2.16	0.46
1:C:230:MET:CE	1:C:305:LEU:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:VAL:HB	1:A:399:LYS:HG3	1.96	0.46
1:A:157:ILE:HG13	1:A:401:VAL:HG21	1.97	0.46
1:D:466:VAL:HG11	1:D:479:ILE:HD12	1.97	0.46
1:B:269:LEU:O	1:B:273:GLU:HG3	2.16	0.46
1:D:167:ALA:HB2	1:D:387:VAL:HG22	1.97	0.46
1:C:165:LYS:O	1:C:168:GLU:HG2	2.16	0.46
1:B:348:GLU:HB3	1:B:365:GLY:HA3	1.97	0.46
1:A:241:LEU:HD22	1:A:330:ALA:HB3	1.98	0.46
1:D:492:LYS:C	1:D:494:ILE:HD12	2.36	0.46
1:D:74:LEU:O	1:D:80:LYS:HE2	2.16	0.46
1:C:26:ARG:O	1:C:30:LEU:HB2	2.16	0.46
1:C:259:ILE:HD12	1:C:259:ILE:N	2.31	0.46
1:D:466:VAL:HG11	1:D:479:ILE:HD11	1.97	0.45
1:B:106:GLU:OE2	1:B:446:ILE:HG23	2.16	0.45
1:C:420:ILE:CD1	1:C:471:LYS:HE3	2.46	0.45
1:C:412:GLY:O	1:C:416:ILE:HG12	2.16	0.45
1:B:146:VAL:HG22	1:B:147:ASP:H	1.81	0.45
1:A:189:LYS:HZ3	1:A:192:LYS:HB2	1.82	0.45
1:D:335:ASN:N	1:D:335:ASN:HD22	2.13	0.45
1:B:95:ASP:HA	3:B:2563:HOH:O	2.16	0.45
1:D:69:LEU:HB3	1:D:83:VAL:HG22	1.98	0.45
1:C:9:VAL:O	1:C:11:ILE:HD12	2.16	0.45
1:D:165:LYS:O	1:D:168:GLU:HG2	2.16	0.45
1:C:94:GLY:CA	1:C:396:LYS:HD2	2.46	0.45
1:D:473:ARG:HB2	1:D:477:ILE:HG13	1.99	0.45
1:B:224:GLU:HG2	1:B:359:ASN:CB	2.47	0.45
1:D:182:VAL:HG22	1:D:395:VAL:HG22	1.97	0.45
1:A:447:ILE:N	1:A:447:ILE:HD12	2.31	0.45
1:B:293:VAL:HG11	1:B:297:ILE:CD1	2.46	0.45
1:A:157:ILE:HD13	1:A:495:ILE:HG13	1.98	0.45
1:D:470:HIS:HA	1:D:477:ILE:HB	1.99	0.45
1:C:488:ASP:OD1	1:C:491:GLU:HG3	2.17	0.45
1:B:148:PRO:O	1:B:402:MET:HG2	2.16	0.45
1:C:269:LEU:O	1:C:273:GLU:HG3	2.17	0.45
1:A:76:HIS:HB2	1:B:10:VAL:O	2.17	0.45
1:A:82:MET:HE2	1:A:85:VAL:HG21	1.99	0.45
1:B:447:ILE:H	1:B:447:ILE:HD12	1.81	0.45
1:C:204:LYS:HB3	1:C:384:ILE:CG2	2.45	0.45
1:C:53:VAL:HA	1:C:58:ASP:O	2.16	0.45
1:A:266:MET:HE3	1:A:266:MET:HA	1.98	0.45
1:B:46:LYS:HB2	3:B:2529:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:HG12	1:A:447:ILE:HD11	1.98	0.45
1:A:448:PRO:HB3	1:A:479:ILE:HD11	1.98	0.45
1:B:386:GLU:HA	1:B:386:GLU:OE2	2.17	0.45
1:A:65:CYS:HB3	1:A:97:THR:OG1	2.17	0.45
1:B:123:ILE:CD1	1:B:123:ILE:H	2.30	0.44
1:B:394:ALA:O	1:B:398:VAL:HG23	2.17	0.44
1:A:479:ILE:H	1:A:479:ILE:HD12	1.82	0.44
1:B:445:LYS:O	1:B:448:PRO:HD2	2.16	0.44
1:C:128:TYR:HB2	1:C:513:ILE:CD1	2.43	0.44
1:D:375:LEU:CD2	1:D:377:ARG:HG2	2.47	0.44
1:C:334:THR:HG22	1:C:335:ASN:HD22	1.82	0.44
1:A:244:GLU:HB3	1:A:334:THR:O	2.17	0.44
1:D:206:ALA:N	1:D:384:ILE:CD1	2.80	0.44
1:C:519:ASP:OD2	1:D:41:THR:HG21	2.18	0.44
1:A:37:GLU:HA	1:A:40:ARG:HG2	1.98	0.44
1:A:305:LEU:HD12	1:A:305:LEU:HA	1.88	0.44
1:C:506:LYS:O	1:C:510:GLU:HG3	2.17	0.44
1:D:372:VAL:HG13	1:D:373:THR:N	2.33	0.44
1:B:189:LYS:HZ3	1:B:192:LYS:HB2	1.81	0.44
1:B:475:LEU:O	1:B:475:LEU:HD12	2.18	0.44
1:A:382:HIS:HD1	1:B:84:GLU:CD	2.20	0.44
1:A:266:MET:CE	1:A:269:LEU:HD23	2.48	0.44
1:D:167:ALA:HB1	1:D:174:LEU:HD11	1.99	0.44
1:B:458:ASP:OD2	1:B:458:ASP:C	2.56	0.44
1:B:68:ILE:O	1:B:72:ILE:HG12	2.17	0.44
1:C:204:LYS:HD2	1:C:384:ILE:HG22	2.00	0.44
1:A:335:ASN:HB3	1:A:338:ASP:OD2	2.18	0.44
1:A:64:ASP:O	1:A:68:ILE:HG12	2.18	0.44
1:A:242:ILE:HG22	1:A:244:GLU:H	1.83	0.44
1:D:384:ILE:HG22	1:D:385:ASP:N	2.32	0.44
1:A:76:HIS:HD2	1:A:78:ALA:N	2.12	0.44
1:B:119:ILE:CD1	1:B:435:LEU:HD23	2.48	0.44
1:D:43:LEU:HD23	1:D:450:THR:OG1	2.16	0.44
1:A:380:THR:CG2	1:A:383:VAL:HG23	2.45	0.44
1:B:102:VAL:HG12	1:B:446:ILE:HD13	2.00	0.44
1:B:501:LYS:O	1:B:505:ILE:HG13	2.17	0.44
1:B:334:THR:HG22	1:B:335:ASN:ND2	2.33	0.44
1:A:460:VAL:O	1:A:464:VAL:HG23	2.16	0.44
1:C:126:LYS:HD3	1:C:433:GLU:OE1	2.18	0.44
1:B:242:ILE:O	1:B:293:VAL:HA	2.18	0.43
1:D:261:SER:OG	1:D:263:ASP:OD2	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:VAL:CG2	1:D:147:ASP:N	2.80	0.43
1:C:219:VAL:HG12	1:C:220:VAL:N	2.32	0.43
1:C:356:ALA:O	1:C:358:GLU:OE1	2.36	0.43
1:A:413:ALA:HB3	1:A:414:PRO:HD3	2.01	0.43
1:B:246:LEU:HD22	1:B:297:ILE:CD1	2.40	0.43
1:D:355:LEU:HD11	1:D:375:LEU:HD11	2.00	0.43
1:D:88:THR:HA	1:D:91:LYS:CE	2.48	0.43
1:A:218:GLY:HA3	1:A:363:VAL:O	2.18	0.43
1:C:522:ILE:HG21	1:D:72:ILE:HD12	2.00	0.43
1:C:215:LEU:HD11	1:C:372:VAL:CG2	2.48	0.43
1:B:150:ASP:OD1	1:B:153:THR:HG23	2.18	0.43
1:B:243:ASN:OD1	1:B:334:THR:HA	2.18	0.43
1:D:271:GLN:HG3	1:D:275:MET:HE1	2.01	0.43
1:B:76:HIS:HA	1:B:77:PRO:HD3	1.85	0.43
1:C:148:PRO:O	1:C:402:MET:HG2	2.19	0.43
1:A:257:ILE:HB	1:B:255:ALA:CB	2.48	0.43
1:A:294:GLN:O	1:A:315:ARG:HA	2.18	0.43
1:A:221:ILE:HD11	1:A:324:LEU:HD11	1.99	0.43
1:C:52:LEU:HD22	1:C:72:ILE:CD1	2.39	0.43
1:B:488:ASP:OD1	1:B:490:LEU:HB2	2.18	0.43
1:B:184:GLN:NE2	1:B:217:ARG:NH2	2.66	0.43
1:C:117:GLN:O	1:C:118:ASN:HB2	2.19	0.43
1:B:190:ASP:C	1:B:192:LYS:H	2.22	0.43
1:C:413:ALA:HB3	1:C:414:PRO:HD3	2.00	0.43
1:B:76:HIS:CD2	1:B:78:ALA:HB3	2.53	0.43
1:A:29:ILE:N	1:A:29:ILE:CD1	2.81	0.43
1:A:380:THR:O	1:A:384:ILE:HD12	2.18	0.43
1:A:293:VAL:HG21	1:A:297:ILE:CD1	2.37	0.43
1:B:52:LEU:HD22	1:B:72:ILE:CD1	2.39	0.43
1:D:133:GLU:O	1:D:137:GLU:HG3	2.19	0.43
1:A:89:GLN:HE22	1:A:504:ALA:N	2.17	0.43
1:D:200:ILE:HD13	1:D:395:VAL:HG21	2.00	0.42
1:D:424:GLU:O	1:D:428:GLN:HG3	2.19	0.42
1:C:470:HIS:HA	1:C:477:ILE:HB	2.01	0.42
1:B:293:VAL:CG1	1:B:297:ILE:HD11	2.48	0.42
1:D:466:VAL:HG21	1:D:479:ILE:CG1	2.49	0.42
1:B:412:GLY:O	1:B:415:GLU:HG2	2.18	0.42
1:C:50:LYS:HB2	1:C:68:ILE:HD12	2.00	0.42
1:D:334:THR:C	1:D:335:ASN:HD22	2.23	0.42
1:C:498:LEU:CD1	1:C:502:LYS:HD2	2.49	0.42
1:C:76:HIS:HA	1:C:77:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASP:C	1:A:192:LYS:H	2.22	0.42
1:C:376:ILE:HD12	1:C:376:ILE:N	2.34	0.42
1:A:388:GLU:O	1:A:392:GLU:HG3	2.19	0.42
1:D:76:HIS:HA	1:D:77:PRO:HD3	1.81	0.42
1:B:197:LEU:HD22	1:B:395:VAL:HG12	2.01	0.42
1:D:188:LYS:CE	1:D:191:GLY:HA2	2.49	0.42
1:D:449:LYS:HG3	1:D:459:THR:HG23	2.02	0.42
1:C:84:GLU:OE1	1:D:382:HIS:ND1	2.47	0.42
1:A:348:GLU:HB3	1:A:365:GLY:HA3	2.00	0.42
1:B:59:ILE:N	1:B:59:ILE:HD12	2.35	0.42
1:B:205:LYS:HD3	1:B:205:LYS:HA	1.85	0.42
1:B:35:ILE:HD11	1:B:74:LEU:CD2	2.50	0.42
1:B:420:ILE:CD1	1:B:420:ILE:H	2.33	0.42
1:D:415:GLU:HG3	1:D:448:PRO:HD3	2.00	0.42
1:C:503:GLN:HE22	1:D:208:GLU:CA	2.32	0.42
1:D:146:VAL:HG21	1:D:153:THR:HG21	2.02	0.42
1:B:9:VAL:HG13	1:B:9:VAL:O	2.20	0.42
1:A:9:VAL:HG13	1:A:9:VAL:O	2.20	0.42
1:A:52:LEU:CD1	1:A:68:ILE:HD13	2.36	0.42
1:C:145:ARG:HA	1:C:405:GLY:O	2.20	0.42
1:C:380:THR:HG23	1:C:382:HIS:H	1.83	0.42
1:B:261:SER:HA	1:B:262:PRO:HD3	1.91	0.42
1:B:121:PRO:O	1:B:125:THR:HB	2.20	0.42
1:C:65:CYS:HB2	1:C:98:THR:OG1	2.19	0.42
1:A:227:HIS:HB3	1:A:230:MET:CG	2.43	0.42
1:D:150:ASP:OD1	1:D:153:THR:HG23	2.20	0.42
1:C:473:ARG:HB2	1:C:477:ILE:HG13	2.00	0.42
1:A:256:LYS:HE2	1:B:256:LYS:HB2	2.00	0.42
1:B:173:LEU:O	1:B:177:LEU:HG	2.19	0.42
1:C:9:VAL:HG23	1:C:11:ILE:HD11	2.01	0.42
1:D:26:ARG:O	1:D:30:LEU:HB2	2.20	0.42
1:A:206:ALA:CA	1:A:384:ILE:HD11	2.37	0.42
1:A:246:LEU:HB2	1:A:297:ILE:HD13	2.01	0.42
1:C:322:GLU:HG2	1:D:228:PRO:HG2	2.02	0.42
1:A:103:ILE:CD1	1:A:447:ILE:HD11	2.50	0.41
1:A:444:LEU:O	1:A:447:ILE:HD13	2.20	0.41
1:C:188:LYS:CE	1:C:191:GLY:HA2	2.49	0.41
1:C:176:LYS:HG2	1:C:180:GLU:OE1	2.20	0.41
1:B:462:MET:HE3	1:B:466:VAL:CG2	2.50	0.41
1:C:275:MET:O	1:C:279:MET:HG3	2.20	0.41
1:D:99:THR:HG23	1:D:447:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LYS:HE3	1:A:315:ARG:O	2.20	0.41
1:A:277:LYS:HG2	1:A:281:ASP:OD2	2.19	0.41
1:D:224:GLU:HG2	1:D:359:ASN:HB2	2.02	0.41
1:D:9:VAL:O	1:D:11:ILE:HG13	2.20	0.41
1:A:217:ARG:HA	1:A:372:VAL:CG2	2.50	0.41
1:C:146:VAL:CG2	1:C:153:THR:HG21	2.50	0.41
1:A:416:ILE:HD13	1:A:466:VAL:HG12	2.02	0.41
1:D:157:ILE:HD12	1:D:401:VAL:CG2	2.49	0.41
1:D:182:VAL:CG2	1:D:395:VAL:HG22	2.49	0.41
1:A:342:GLU:N	1:A:342:GLU:OE2	2.52	0.41
1:A:244:GLU:OE2	1:A:249:LYS:HD3	2.20	0.41
1:B:283:ILE:HD13	1:B:339:LEU:CD2	2.50	0.41
1:A:62:THR:CG2	1:A:386:GLU:OE2	2.69	0.41
1:A:184:GLN:HE22	1:A:217:ARG:HH21	1.68	0.41
1:D:322:GLU:O	1:D:326:LYS:HG3	2.20	0.41
1:D:146:VAL:CG2	1:D:147:ASP:H	2.34	0.41
1:D:89:GLN:HE22	1:D:504:ALA:N	2.19	0.41
1:B:246:LEU:HB2	1:B:297:ILE:HD13	2.03	0.41
1:D:227:HIS:HA	1:D:228:PRO:HD3	1.89	0.41
1:D:153:THR:O	1:D:156:LYS:HB2	2.21	0.41
1:D:12:LEU:HD13	1:D:16:THR:HG21	2.03	0.41
1:B:410:ALA:HB3	1:B:494:ILE:HG22	2.01	0.41
1:D:498:LEU:HD22	1:D:498:LEU:O	2.19	0.41
1:C:76:HIS:CD2	1:C:78:ALA:HB3	2.56	0.41
1:D:106:GLU:CG	1:D:446:ILE:HG12	2.49	0.41
1:A:297:ILE:HG12	1:A:314:ARG:HB3	2.02	0.41
1:B:490:LEU:HD12	1:B:490:LEU:HA	1.87	0.41
1:B:146:VAL:HG22	1:B:147:ASP:N	2.36	0.41
1:C:300:LEU:HG	1:C:304:TYR:CE2	2.56	0.41
1:B:35:ILE:HD11	1:B:74:LEU:HD22	2.02	0.41
1:B:195:VAL:HB	1:B:399:LYS:HG3	2.03	0.41
1:A:119:ILE:HD13	1:C:460:VAL:HG21	2.02	0.41
1:D:157:ILE:CG1	1:D:495:ILE:CD1	2.92	0.41
1:C:32:ALA:HB1	1:C:82:MET:HE1	2.03	0.41
1:B:43:LEU:HB2	1:B:98:THR:HG21	2.03	0.41
1:B:241:LEU:HD12	1:B:292:PHE:HB2	2.01	0.41
1:C:367:LYS:HD2	1:C:368:ASN:HB2	2.02	0.41
1:B:163:THR:HB	1:B:171:LYS:HZ1	1.85	0.40
1:A:189:LYS:CG	1:A:190:ASP:H	2.31	0.40
1:A:126:LYS:HD3	1:A:433:GLU:HG3	2.03	0.40
1:D:222:ASP:HA	1:D:360:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:LEU:CD2	1:D:72:ILE:HD11	2.24	0.40
1:C:11:ILE:HD13	1:D:34:ILE:HG21	2.03	0.40
1:C:65:CYS:HB3	1:C:97:THR:OG1	2.22	0.40
1:B:239:ILE:HG22	1:B:241:LEU:HD13	2.03	0.40
1:B:281:ASP:O	1:B:285:GLN:HG3	2.21	0.40
1:D:195:VAL:HB	1:D:399:LYS:HG3	2.01	0.40
1:C:517:ARG:HH11	1:D:49:ASP:CG	2.25	0.40
1:D:201:LYS:HB2	1:D:323:LYS:CE	2.46	0.40
1:D:420:ILE:HD12	1:D:471:LYS:CE	2.48	0.40
1:B:189:LYS:CG	1:B:190:ASP:N	2.85	0.40
1:A:89:GLN:HE22	1:A:503:GLN:C	2.25	0.40
1:A:281:ASP:O	1:A:285:GLN:HG3	2.22	0.40
1:A:29:ILE:N	1:A:29:ILE:HD12	2.36	0.40
1:D:271:GLN:HG3	1:D:275:MET:HE2	2.04	0.40
1:A:187:GLU:O	1:A:194:VAL:HG12	2.21	0.40
1:D:18:ARG:HA	1:D:521:VAL:O	2.22	0.40
1:C:467:ILE:N	1:C:467:ILE:HD12	2.36	0.40
1:C:266:MET:HE2	1:C:266:MET:HA	2.02	0.40
1:B:158:ALA:O	1:B:162:ILE:HG12	2.21	0.40
1:B:206:ALA:CB	1:B:384:ILE:HD11	2.52	0.40
1:D:136:GLN:NE2	1:D:136:GLN:HA	2.37	0.40
1:D:149:ASP:HB2	1:D:183:LYS:HZ1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	516/548 (94%)	495 (96%)	18 (4%)	3 (1%)	30	43
1	B	516/548 (94%)	499 (97%)	14 (3%)	3 (1%)	30	43
1	C	516/548 (94%)	501 (97%)	13 (2%)	2 (0%)	39	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	516/548 (94%)	500 (97%)	12 (2%)	4 (1%)	24	35
All	All	2064/2192 (94%)	1995 (97%)	57 (3%)	12 (1%)	30	43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	LYS
1	C	235	GLU
1	A	235	GLU
1	B	235	GLU
1	B	367	LYS
1	D	235	GLU
1	D	367	LYS
1	C	367	LYS
1	A	148	PRO
1	B	148	PRO
1	D	10	VAL
1	D	148	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	423/441 (96%)	398 (94%)	25 (6%)	24	38
1	B	423/441 (96%)	398 (94%)	25 (6%)	24	38
1	C	423/441 (96%)	404 (96%)	19 (4%)	34	52
1	D	423/441 (96%)	391 (92%)	32 (8%)	16	25
All	All	1692/1764 (96%)	1591 (94%)	101 (6%)	24	37

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	27	LEU

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Mol	Chain	Res	Type
1	A	30	LEU
1	A	35	ILE
1	A	62	THR
1	A	82	MET
1	A	107	LEU
1	A	116	ASP
1	A	125	THR
1	A	147	ASP
1	A	154	LEU
1	A	241	LEU
1	A	266	MET
1	A	269	LEU
1	A	305	LEU
1	A	358	GLU
1	A	372	VAL
1	A	375	LEU
1	A	380	THR
1	A	439	ASN
1	A	446	ILE
1	A	490	LEU
1	A	498	LEU
1	A	501	LYS
1	A	516	LEU
1	B	27	LEU
1	B	30	LEU
1	B	107	LEU
1	B	123	ILE
1	B	125	THR
1	B	147	ASP
1	B	154	LEU
1	B	163	THR
1	B	211	GLU
1	B	229	ARG
1	B	241	LEU
1	B	269	LEU
1	B	305	LEU
1	B	315	ARG
1	B	367	LYS
1	B	368	ASN
1	B	380	THR
1	B	420	ILE
1	B	435	LEU

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Mol	Chain	Res	Type
1	B	439	ASN
1	B	446	ILE
1	B	483	GLU
1	B	490	LEU
1	B	498	LEU
1	B	516	LEU
1	C	14	GLU
1	C	30	LEU
1	C	35	ILE
1	C	82	MET
1	C	107	LEU
1	C	153	THR
1	C	154	LEU
1	C	155	LEU
1	C	269	LEU
1	C	305	LEU
1	C	375	LEU
1	C	380	THR
1	C	428	GLN
1	C	446	ILE
1	C	450	THR
1	C	459	THR
1	C	490	LEU
1	C	498	LEU
1	C	516	LEU
1	D	14	GLU
1	D	23	ASP
1	D	30	LEU
1	D	35	ILE
1	D	82	MET
1	D	107	LEU
1	D	125	THR
1	D	152	GLU
1	D	154	LEU
1	D	211	GLU
1	D	229	ARG
1	D	241	LEU
1	D	269	LEU
1	D	305	LEU
1	D	315	ARG
1	D	342	GLU
1	D	358	GLU

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Mol	Chain	Res	Type
1	D	367	LYS
1	D	372	VAL
1	D	377	ARG
1	D	380	THR
1	D	384	ILE
1	D	395	VAL
1	D	404	ASP
1	D	435	LEU
1	D	446	ILE
1	D	450	THR
1	D	490	LEU
1	D	498	LEU
1	D	501	LYS
1	D	516	LEU
1	D	517	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	75	GLN
1	A	76	HIS
1	A	89	GLN
1	A	170	HIS
1	A	184	GLN
1	A	227	HIS
1	A	264	GLN
1	A	271	GLN
1	A	282	HIS
1	A	285	GLN
1	A	368	ASN
1	A	439	ASN
1	B	28	ASN
1	B	76	HIS
1	B	89	GLN
1	B	117	GLN
1	B	118	ASN
1	B	170	HIS
1	B	184	GLN
1	B	258	ASN
1	B	282	HIS
1	B	285	GLN

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Mol	Chain	Res	Type
1	B	335	ASN
1	B	368	ASN
1	B	439	ASN
1	B	503	GLN
1	C	28	ASN
1	C	76	HIS
1	C	89	GLN
1	C	117	GLN
1	C	170	HIS
1	C	184	GLN
1	C	227	HIS
1	C	282	HIS
1	C	285	GLN
1	C	303	HIS
1	C	335	ASN
1	C	368	ASN
1	C	428	GLN
1	C	503	GLN
1	D	28	ASN
1	D	75	GLN
1	D	76	HIS
1	D	89	GLN
1	D	117	GLN
1	D	136	GLN
1	D	184	GLN
1	D	227	HIS
1	D	282	HIS
1	D	285	GLN
1	D	335	ASN
1	D	368	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1527	-	4,4,4	0.23	0	6,6,6	0.19	0
2	SO4	B	2527	-	4,4,4	0.18	0	6,6,6	0.10	0
2	SO4	C	3527	-	4,4,4	0.23	0	6,6,6	0.16	0
2	SO4	D	4527	-	4,4,4	0.30	0	6,6,6	0.20	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	1527	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2527	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3527	-	-	0/0/0/0	0/0/0/0
2	SO4	D	4527	-	-	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	518/548 (94%)	-0.09	25 (4%) 34 35	23, 37, 58, 93	0
1	B	518/548 (94%)	-0.04	22 (4%) 40 41	22, 39, 58, 93	0
1	C	518/548 (94%)	-0.10	19 (3%) 45 46	20, 35, 55, 96	0
1	D	518/548 (94%)	-0.09	21 (4%) 41 42	24, 38, 58, 96	0
All	All	2072/2192 (94%)	-0.08	87 (4%) 40 41	20, 37, 57, 96	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	56	LEU	5.6
1	C	189	LYS	5.4
1	B	357	GLY	5.1
1	A	526	ALA	5.0
1	B	9	VAL	4.8
1	B	189	LYS	4.8
1	A	56	LEU	4.7
1	C	191	GLY	4.7
1	C	357	GLY	4.7
1	B	192	LYS	4.6
1	D	191	GLY	4.4
1	A	190	ASP	4.4
1	B	14	GLU	4.4
1	D	190	ASP	4.3
1	A	357	GLY	4.3
1	C	526	ALA	4.2
1	C	56	LEU	4.1
1	D	367	LYS	3.9
1	C	58	ASP	3.8
1	B	526	ALA	3.8
1	D	14	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	190	ASP	3.8
1	A	192	LYS	3.7
1	C	190	ASP	3.7
1	C	9	VAL	3.6
1	C	14	GLU	3.4
1	D	9	VAL	3.4
1	A	189	LYS	3.4
1	B	525	LYS	3.3
1	B	10	VAL	3.3
1	D	15	GLY	3.3
1	A	191	GLY	3.3
1	C	356	ALA	3.2
1	B	367	LYS	3.1
1	A	483	GLU	3.1
1	D	192	LYS	3.1
1	B	188	LYS	3.0
1	B	56	LEU	3.0
1	A	9	VAL	3.0
1	B	15	GLY	2.9
1	C	358	GLU	2.9
1	A	14	GLU	2.9
1	D	189	LYS	2.9
1	D	357	GLY	2.9
1	B	191	GLY	2.9
1	A	525	LYS	2.8
1	C	525	LYS	2.8
1	B	240	ALA	2.7
1	B	356	ALA	2.7
1	C	367	LYS	2.6
1	C	192	LYS	2.6
1	D	356	ALA	2.6
1	C	240	ALA	2.5
1	A	472	ASN	2.5
1	A	491	GLU	2.4
1	C	15	GLY	2.4
1	C	398	VAL	2.4
1	C	291	VAL	2.4
1	D	55	SER	2.4
1	A	358	GLU	2.4
1	A	367	LYS	2.3
1	B	472	ASN	2.3
1	C	55	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	291	VAL	2.3
1	A	356	ALA	2.3
1	D	525	LYS	2.3
1	D	10	VAL	2.3
1	A	240	ALA	2.2
1	A	22	ARG	2.2
1	B	427	LYS	2.2
1	D	485	LYS	2.2
1	B	477	ILE	2.2
1	D	295	LYS	2.2
1	A	58	ASP	2.1
1	A	10	VAL	2.1
1	D	290	VAL	2.1
1	B	317	LYS	2.1
1	A	304	TYR	2.1
1	A	15	GLY	2.1
1	A	398	VAL	2.1
1	B	22	ARG	2.1
1	A	485	LYS	2.1
1	D	526	ALA	2.1
1	D	58	ASP	2.1
1	B	291	VAL	2.1
1	A	219	VAL	2.0
1	D	472	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	D	4527	5/5	0.97	0.10	-1.17	34,35,36,37	0
2	SO4	C	3527	5/5	0.99	0.08	-1.29	33,33,35,35	0
2	SO4	B	2527	5/5	0.99	0.09	-1.70	36,37,38,40	0
2	SO4	A	1527	5/5	0.99	0.07	-1.77	31,32,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.