Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2021 – 02:41 PM EST

PDB ID	:	3D8K
Title	:	Crystal structure of a phosphatase from a toxoplasma gondii
Authors	:	Damodharan, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-05-23
Resolution	:	2.71 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
https://www.wwpdb.org/validation/2017/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:

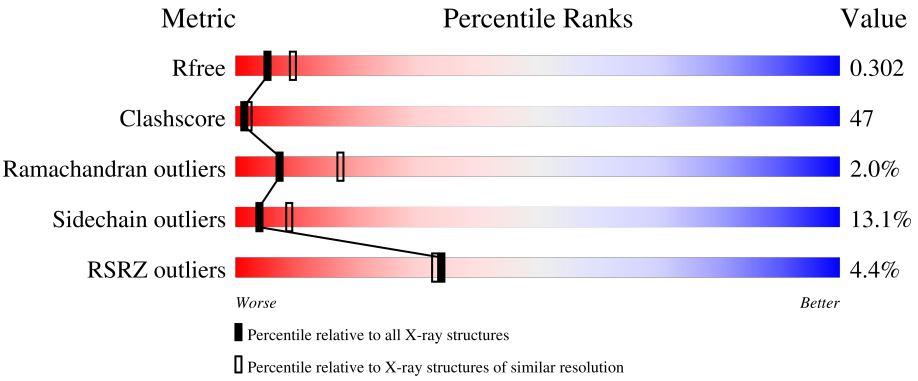
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	377	3% 42% 42% 8% 8%
1	B	377	3% 44% 42% 7% 7%
1	C	377	5% 40% 42% 10% • 7%
1	D	377	4% 40% 44% 8% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10892 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 Protein phosphatase 2C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	Se	0	0	0
			2664	1656	498	497	2	11			
1	B	350	Total	C	N	O	S	Se	0	0	0
			2679	1662	499	505	2	11			
1	C	351	Total	C	N	O	S	Se	0	0	0
			2696	1674	503	507	2	10			
1	D	346	Total	C	N	O	S	Se	0	0	0
			2652	1645	496	499	2	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MSE	-	expression tag	UNP A4GX63
A	77	SER	-	expression tag	UNP A4GX63
A	78	LEU	-	expression tag	UNP A4GX63
A	445	GLU	-	expression tag	UNP A4GX63
A	446	GLY	-	expression tag	UNP A4GX63
A	447	HIS	-	expression tag	UNP A4GX63
A	448	HIS	-	expression tag	UNP A4GX63
A	449	HIS	-	expression tag	UNP A4GX63
A	450	HIS	-	expression tag	UNP A4GX63
A	451	HIS	-	expression tag	UNP A4GX63
A	452	HIS	-	expression tag	UNP A4GX63
B	76	MSE	-	expression tag	UNP A4GX63
B	77	SER	-	expression tag	UNP A4GX63
B	78	LEU	-	expression tag	UNP A4GX63
B	445	GLU	-	expression tag	UNP A4GX63
B	446	GLY	-	expression tag	UNP A4GX63
B	447	HIS	-	expression tag	UNP A4GX63
B	448	HIS	-	expression tag	UNP A4GX63
B	449	HIS	-	expression tag	UNP A4GX63
B	450	HIS	-	expression tag	UNP A4GX63
B	451	HIS	-	expression tag	UNP A4GX63

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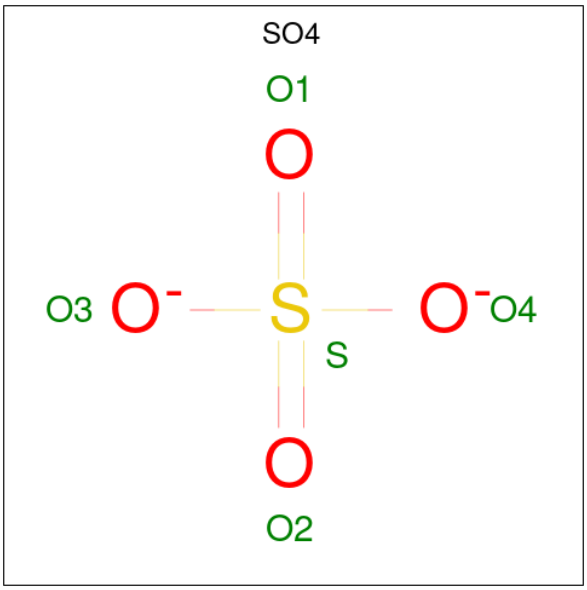
Chain	Residue	Modelled	Actual	Comment	Reference
B	452	HIS	-	expression tag	UNP A4GX63
C	76	MSE	-	expression tag	UNP A4GX63
C	77	SER	-	expression tag	UNP A4GX63
C	78	LEU	-	expression tag	UNP A4GX63
C	445	GLU	-	expression tag	UNP A4GX63
C	446	GLY	-	expression tag	UNP A4GX63
C	447	HIS	-	expression tag	UNP A4GX63
C	448	HIS	-	expression tag	UNP A4GX63
C	449	HIS	-	expression tag	UNP A4GX63
C	450	HIS	-	expression tag	UNP A4GX63
C	451	HIS	-	expression tag	UNP A4GX63
C	452	HIS	-	expression tag	UNP A4GX63
D	76	MSE	-	expression tag	UNP A4GX63
D	77	SER	-	expression tag	UNP A4GX63
D	78	LEU	-	expression tag	UNP A4GX63
D	445	GLU	-	expression tag	UNP A4GX63
D	446	GLY	-	expression tag	UNP A4GX63
D	447	HIS	-	expression tag	UNP A4GX63
D	448	HIS	-	expression tag	UNP A4GX63
D	449	HIS	-	expression tag	UNP A4GX63
D	450	HIS	-	expression tag	UNP A4GX63
D	451	HIS	-	expression tag	UNP A4GX63
D	452	HIS	-	expression tag	UNP A4GX63

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

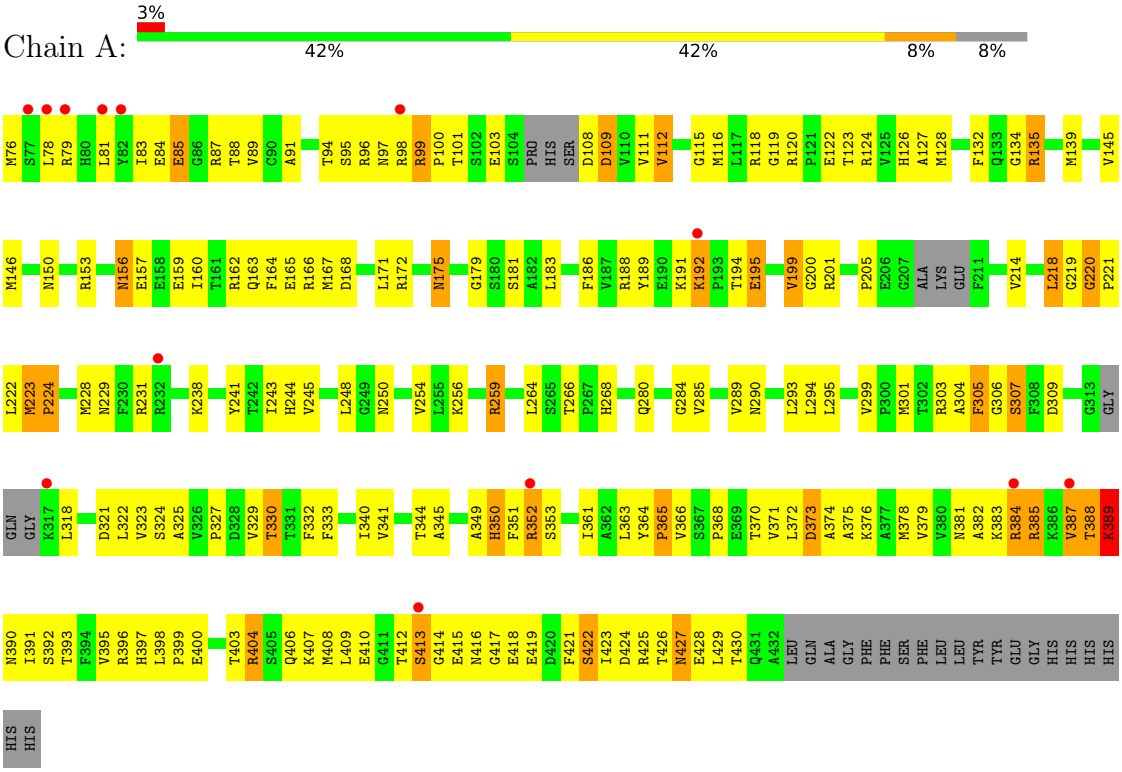
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	50	Total O 50 50	0	0
3	B	42	Total O 42 42	0	0
3	C	50	Total O 50 50	0	0
3	D	39	Total O 39 39	0	0

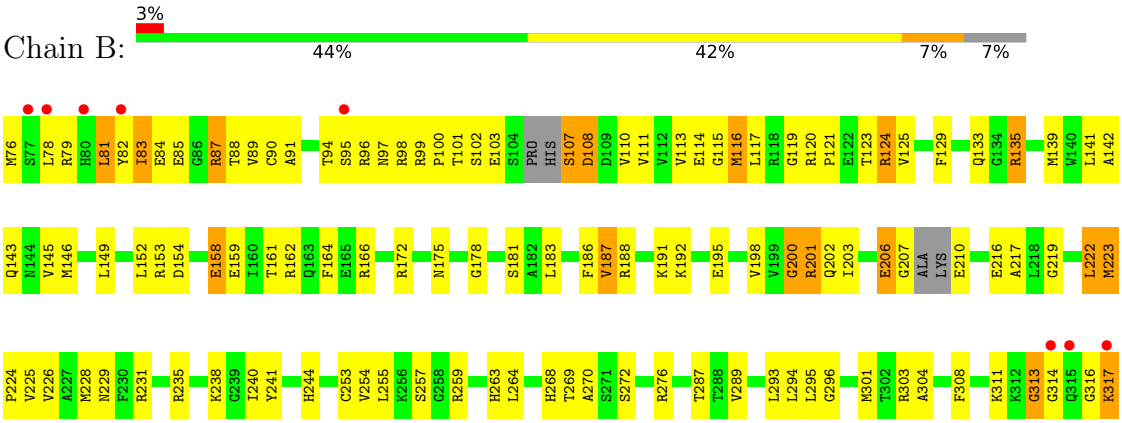
3 Residue-property plots (i)

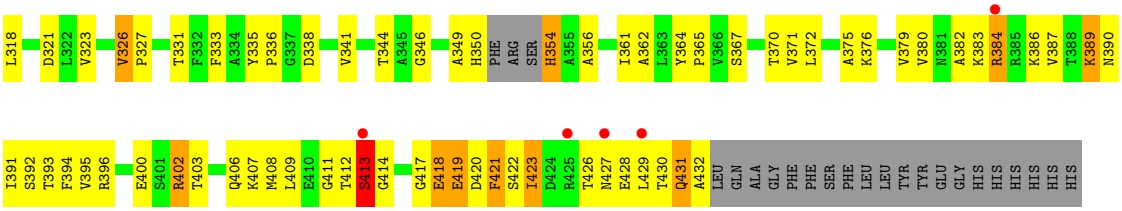
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Protein phosphatase 2C



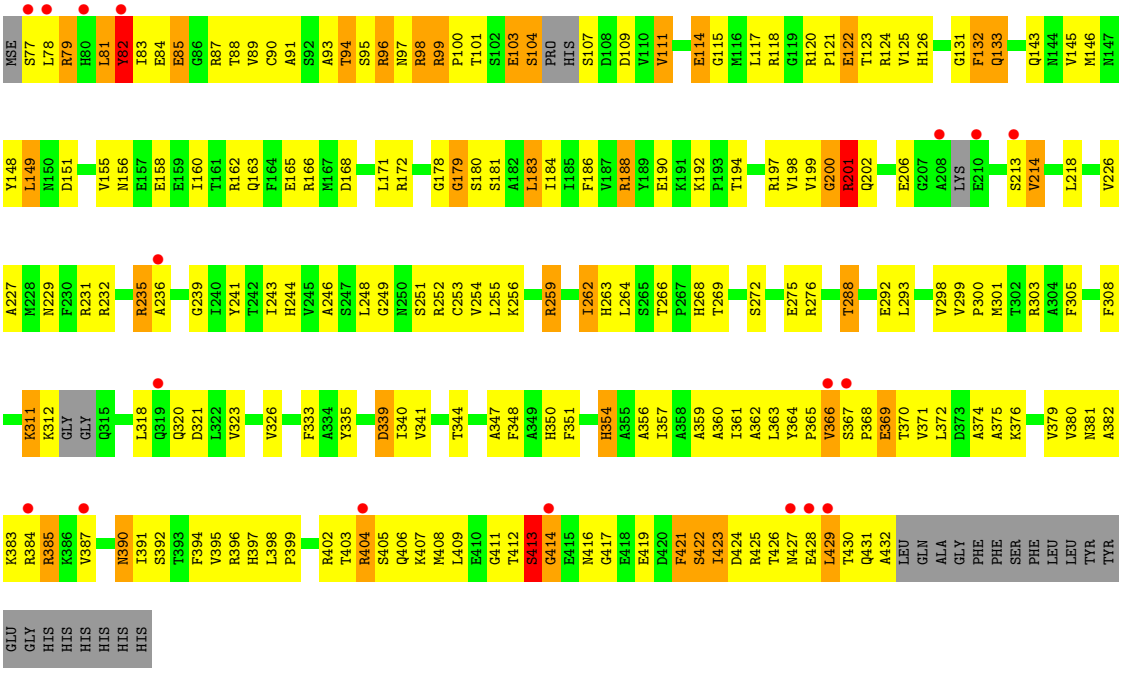
• Molecule 1: Protein phosphatase 2C





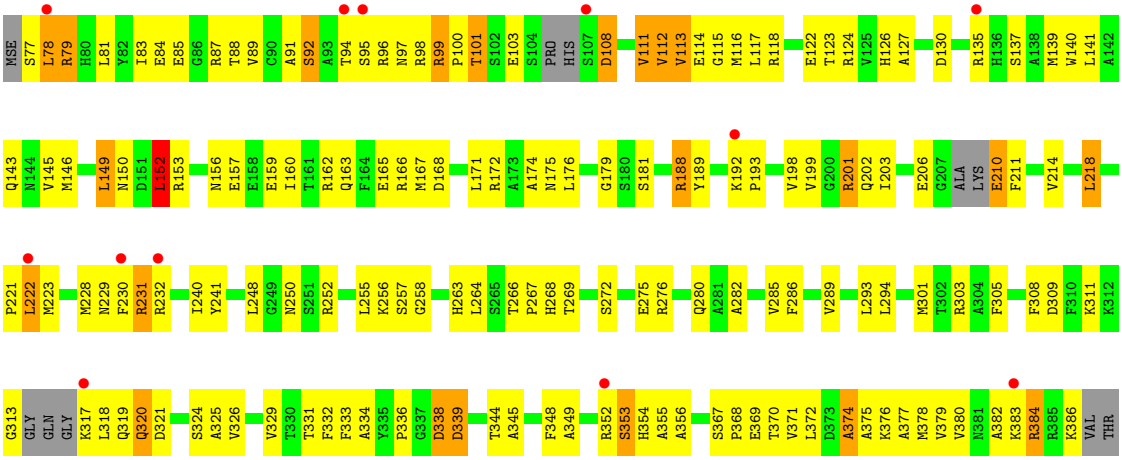
• Molecule 1: Protein phosphatase 2C

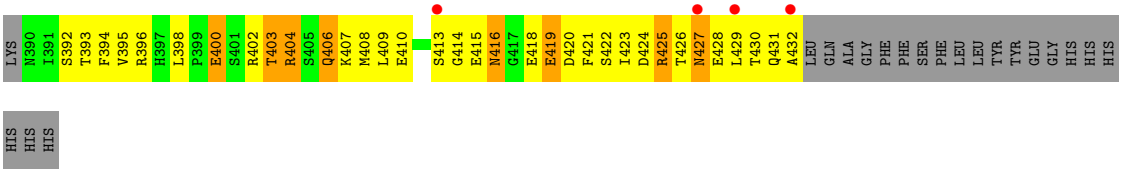
Chain C:



• Molecule 1: Protein phosphatase 2C

Chain D:




LYS N390 I391 S392 T393 F394 V395 R396 H397 L398 P399 E400 S401 R402 T403 R404 S405 Q406 K407 M408 L409 E410 S413 G414 E415 N416 G417 E418 E419 D420 F421 S422 I423 D424 R425 T426 M427 E428 L429 T430 Q431 A432 LEU GLN ALA GLY PHE PHE SER PHE LEU LEU TYR TYR GLU GLY HIS HIS HIS
HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.88Å 169.05Å 87.01Å 90.00° 104.47° 90.00°	Depositor
Resolution (Å)	46.71 – 2.71 46.84 – 2.59	Depositor EDS
% Data completeness (in resolution range)	94.6 (46.71-2.71) 91.8 (46.84-2.59)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.96 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.304 0.250 , 0.302	Depositor DCC
R_{free} test set	1052 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	10892	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.48	0/2700	0.84	6/3628 (0.2%)
1	B	0.44	0/2714	0.74	2/3646 (0.1%)
1	C	0.45	0/2732	0.80	6/3671 (0.2%)
1	D	0.43	0/2686	0.80	5/3607 (0.1%)
All	All	0.45	0/10832	0.79	19/14552 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	414	GLY	N-CA-C	-10.70	86.35	113.10
1	A	389	LYS	N-CA-C	-10.67	82.19	111.00
1	D	414	GLY	N-CA-C	-10.16	87.70	113.10
1	A	385	ARG	N-CA-C	-8.97	86.77	111.00
1	B	414	GLY	N-CA-C	-8.52	91.80	113.10
1	C	414	GLY	N-CA-C	-7.88	93.39	113.10
1	D	353	SER	N-CA-C	-7.46	90.86	111.00
1	C	413	SER	N-CA-C	-6.47	93.54	111.00
1	D	404	ARG	N-CA-C	-6.25	94.13	111.00
1	C	81	LEU	CA-CB-CG	6.05	129.21	115.30
1	B	413	SER	N-CA-C	-5.88	95.12	111.00
1	D	152	LEU	CA-CB-CG	5.46	127.86	115.30
1	C	385	ARG	N-CA-C	-5.44	96.31	111.00
1	A	388	THR	N-CA-C	-5.40	96.43	111.00
1	C	366	VAL	N-CA-C	-5.39	96.44	111.00
1	D	384	ARG	N-CA-C	-5.38	96.49	111.00
1	A	388	THR	OG1-CB-CG2	-5.17	98.11	110.00
1	A	387	VAL	CB-CA-C	-5.12	101.68	111.40
1	C	82	TYR	CA-CB-CG	5.04	122.98	113.40

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	2664	0	2646	280	0
1	B	2679	0	2663	239	0
1	C	2696	0	2680	270	0
1	D	2652	0	2630	240	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	1	0
3	A	50	0	0	2	0
3	B	42	0	0	6	0
3	C	50	0	0	7	0
3	D	39	0	0	4	0
All	All	10892	0	10619	999	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 47.

All (999) 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:C:87:ARG:HH11	1:D:84:GLU:HG2	1.05	1.16
1:D:222:LEU:O	1:D:223:MSE:HE2	1.45	1.15
1:D:371:VAL:HG23	1:D:427:ASN:HD22	0.96	1.13
1:B:98:ARG:HG2	1:B:146:MSE:HG3	1.26	1.12
1:D:221:PRO:HB2	1:D:223:MSE:HE3	1.31	1.12
1:A:248:LEU:HG	1:A:303:ARG:HG3	1.30	1.12
1:C:88:THR:HB	1:C:408:MSE:HE3	1.20	1.11
1:A:248:LEU:CG	1:A:303:ARG:HG3	1.83	1.07
1:D:420:ASP:HB2	1:D:425:ARG:NH1	1.70	1.05
1:D:108:ASP:HA	1:D:135:ARG:HB3	1.40	1.04
1:B:100:PRO:HA	1:B:111:VAL:O	1.59	1.03
1:A:248:LEU:CD1	1:A:303:ARG:CG	2.38	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:LYS:HA	1:B:429:LEU:HD22	1.42	1.01
1:B:389:LYS:HE2	1:B:390:ASN:H	1.25	1.01
1:A:120:ARG:HD2	1:A:123:THR:HG23	1.39	1.00
1:B:376:LYS:HG2	1:B:429:LEU:HD21	1.43	1.00
1:A:248:LEU:CD1	1:A:303:ARG:HG3	1.92	0.99
1:C:408:MSE:HE2	1:C:419:GLU:OE2	1.62	0.99
1:C:83:ILE:HG12	1:C:85:GLU:HB2	1.45	0.99
1:D:416:ASN:HB3	1:D:429:LEU:HD23	1.44	0.98
1:D:379:VAL:HG21	1:D:429:LEU:HD12	1.45	0.98
1:D:308:PHE:HA	1:D:311:LYS:HB2	1.46	0.97
1:B:108:ASP:HB2	1:B:390:ASN:HD21	1.29	0.97
1:D:124:ARG:NE	1:D:421:PHE:HZ	1.63	0.96
1:C:375:ALA:HB3	1:C:427:ASN:HD22	1.28	0.96
1:D:371:VAL:HG23	1:D:427:ASN:ND2	1.82	0.93
1:D:101:THR:HG23	1:D:111:VAL:HG13	1.49	0.93
1:B:89:VAL:HG22	1:B:406:GLN:NE2	1.83	0.93
1:B:394:PHE:HE1	1:B:426:THR:HG23	1.34	0.91
1:C:99:ARG:CZ	1:C:408:MSE:HE1	2.00	0.91
1:D:394:PHE:HE1	1:D:426:THR:HG23	1.35	0.91
1:B:99:ARG:O	1:B:113:VAL:HG22	1.72	0.90
1:C:235:ARG:HB3	1:C:235:ARG:HH11	1.36	0.90
1:D:98:ARG:HD3	1:D:146:MSE:HB2	1.53	0.90
1:C:383:LYS:HA	1:C:387:VAL:HG12	1.55	0.89
1:C:103:GLU:HG2	1:C:104:SER:H	1.36	0.88
1:A:83:ILE:CG1	1:A:85:GLU:HB2	2.03	0.88
1:C:417:GLY:H	1:C:428:GLU:HG2	1.39	0.88
1:A:98:ARG:NH1	1:A:112:VAL:HG21	1.89	0.87
1:C:292:GLU:HG3	1:C:293:LEU:HD23	1.58	0.86
1:C:293:LEU:H	1:C:293:LEU:HD23	1.40	0.86
1:D:85:GLU:OE1	1:D:407:LYS:HA	1.76	0.85
1:D:188:ARG:HH11	1:D:188:ARG:HG3	1.41	0.85
1:C:148:TYR:HB3	1:C:163:GLN:HG3	1.57	0.85
1:C:404:ARG:HH11	1:C:404:ARG:HA	1.41	0.85
1:A:120:ARG:HG2	1:A:122:GLU:H	1.41	0.85
1:A:396:ARG:NH2	1:A:424:ASP:HB3	1.92	0.85
1:A:221:PRO:HB2	1:A:223:MSE:CE	2.06	0.85
1:A:344:THR:HG23	1:A:392:SER:HB2	1.59	0.85
1:C:87:ARG:NH1	1:D:84:GLU:HG2	1.90	0.85
1:C:350:HIS:H	1:C:385:ARG:NH1	1.75	0.84
1:A:83:ILE:HG12	1:A:85:GLU:HB2	1.59	0.84
1:A:248:LEU:HG	1:A:303:ARG:CG	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:MSE:O	1:D:143:GLN:HG2	1.76	0.84
1:B:254:VAL:HG21	1:B:361:ILE:HD13	1.59	0.84
1:C:350:HIS:H	1:C:385:ARG:HH12	1.24	0.83
1:A:156:ASN:C	1:A:156:ASN:HD22	1.81	0.83
1:D:221:PRO:HB2	1:D:223:MSE:CE	2.08	0.83
1:B:78:LEU:HD23	1:B:79:ARG:N	1.93	0.83
1:A:248:LEU:HD11	1:A:303:ARG:CD	2.07	0.83
1:C:99:ARG:HG2	1:C:99:ARG:HH11	1.45	0.82
1:A:248:LEU:HD11	1:A:303:ARG:HD2	1.62	0.82
1:B:172:ARG:HH12	1:B:313:GLY:HA2	1.43	0.82
1:D:137:SER:O	1:D:141:LEU:HD23	1.78	0.82
1:C:399:PRO:HB3	1:C:425:ARG:HE	1.46	0.81
1:D:221:PRO:CB	1:D:223:MSE:HE3	2.10	0.81
1:B:181:SER:HB2	1:B:301:MSE:HE1	1.63	0.81
1:D:115:GLY:HA3	1:D:146:MSE:HE3	1.61	0.81
1:A:78:LEU:HD21	1:A:413:SER:HB2	1.63	0.81
1:C:101:THR:HG22	1:C:111:VAL:HG22	1.63	0.81
1:C:375:ALA:HB3	1:C:427:ASN:ND2	1.94	0.81
1:A:91:ALA:HB1	1:A:97:ASN:HB3	1.62	0.80
1:C:236:ALA:HB1	1:C:239:GLY:O	1.80	0.80
1:B:238:LYS:NZ	1:B:400:GLU:HB3	1.97	0.80
1:C:360:ALA:HA	1:C:363:LEU:HD23	1.61	0.80
1:C:96:ARG:HD3	1:C:118:ARG:CZ	2.11	0.80
1:C:87:ARG:HH11	1:D:84:GLU:CG	1.90	0.80
1:C:375:ALA:CB	1:C:427:ASN:HD22	1.93	0.80
1:C:78:LEU:HG	1:C:81:LEU:HD23	1.63	0.79
1:D:402:ARG:HG2	1:D:403:THR:HG22	1.63	0.79
1:D:139:MSE:HE2	1:D:143:GLN:OE1	1.82	0.79
1:B:83:ILE:H	1:B:83:ILE:HD12	1.46	0.79
1:B:108:ASP:HB2	1:B:390:ASN:ND2	1.96	0.78
1:D:124:ARG:HH21	1:D:421:PHE:HE2	1.30	0.78
1:A:78:LEU:HG	1:A:376:LYS:HZ2	1.48	0.78
1:C:402:ARG:NH1	1:C:422:SER:HB2	1.99	0.78
1:C:88:THR:HB	1:C:408:MSE:CE	2.10	0.78
1:D:371:VAL:CG2	1:D:427:ASN:HD22	1.89	0.78
1:B:119:GLY:O	1:B:121:PRO:HD3	1.83	0.78
1:C:96:ARG:HG2	1:C:118:ARG:HB3	1.64	0.78
1:C:403:THR:HG22	1:C:405:SER:H	1.49	0.78
1:A:392:SER:HA	1:A:430:THR:HG22	1.66	0.77
1:C:292:GLU:HG3	1:C:293:LEU:H	1.49	0.77
1:B:186:PHE:HB2	1:B:244:HIS:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:GLU:O	1:C:104:SER:HB2	1.85	0.77
1:C:85:GLU:O	1:C:88:THR:HG22	1.83	0.77
1:D:368:PRO:HG2	1:D:369:GLU:OE2	1.83	0.77
1:A:222:LEU:HD23	1:A:223:MSE:N	2.00	0.77
1:A:222:LEU:HD23	1:A:223:MSE:H	1.50	0.76
1:A:248:LEU:HD11	1:A:303:ARG:CG	2.15	0.76
1:C:262:ILE:HD11	3:C:480:HOH:O	1.85	0.76
1:D:416:ASN:HB3	1:D:429:LEU:CD2	2.15	0.76
1:A:223:MSE:HG2	1:A:224:PRO:HD2	1.66	0.76
1:A:229:ASN:HD21	1:A:231:ARG:HB2	1.50	0.76
1:B:98:ARG:HG2	1:B:146:MSE:CG	2.13	0.76
1:D:83:ILE:C	1:D:85:GLU:H	1.85	0.76
1:A:163:GLN:HE22	1:A:166:ARG:HE	1.30	0.76
1:B:384:ARG:NH1	1:B:384:ARG:HB3	2.01	0.76
1:A:179:GLY:H	1:A:306:GLY:HA3	1.49	0.76
1:A:264:LEU:O	1:A:330:THR:HG21	1.85	0.76
1:A:84:GLU:HG2	1:A:87:ARG:HD2	1.67	0.76
1:C:126:HIS:CE1	1:C:426:THR:HG21	2.21	0.75
1:D:429:LEU:HD13	1:D:430:THR:N	2.01	0.75
1:B:344:THR:HG23	1:B:392:SER:HB2	1.68	0.75
1:B:394:PHE:CE1	1:B:426:THR:HG23	2.21	0.75
1:A:89:VAL:HG22	1:A:406:GLN:NE2	2.02	0.75
1:B:254:VAL:CG2	1:B:341:VAL:HB	2.17	0.75
1:B:402:ARG:HA	1:B:423:ILE:HG13	1.68	0.74
1:D:98:ARG:HG3	1:D:146:MSE:HE2	1.67	0.74
1:B:101:THR:HG22	1:B:111:VAL:HB	1.70	0.74
1:A:89:VAL:HG13	1:A:406:GLN:HE22	1.52	0.74
1:A:248:LEU:HD12	1:A:303:ARG:CG	2.18	0.74
1:C:292:GLU:HG3	1:C:293:LEU:N	2.03	0.74
1:D:423:ILE:O	1:D:423:ILE:HG23	1.87	0.74
1:B:153:ARG:HG2	1:C:192:LYS:NZ	2.02	0.74
1:A:289:VAL:HB	1:A:294:LEU:HD22	1.71	0.73
1:A:408:MSE:HG3	1:A:419:GLU:HG2	1.69	0.73
1:D:84:GLU:O	1:D:87:ARG:HB3	1.87	0.73
1:D:112:VAL:O	1:D:112:VAL:HG22	1.88	0.73
1:C:417:GLY:H	1:C:428:GLU:CG	2.01	0.73
1:B:78:LEU:HA	1:B:413:SER:OG	1.89	0.73
1:D:394:PHE:CE1	1:D:426:THR:HG23	2.22	0.73
1:A:78:LEU:CD2	1:A:412:THR:O	2.37	0.73
1:A:186:PHE:HB2	1:A:244:HIS:HB2	1.69	0.73
1:A:85:GLU:O	1:A:88:THR:HG22	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:GLU:O	1:B:89:VAL:HG23	1.88	0.72
1:C:235:ARG:CB	1:C:235:ARG:HH11	2.01	0.72
1:B:372:LEU:HA	1:B:427:ASN:CG	2.10	0.72
1:C:83:ILE:CG1	1:C:85:GLU:HB2	2.17	0.72
1:C:198:VAL:HG13	1:C:202:GLN:O	1.88	0.72
1:A:248:LEU:CD1	1:A:303:ARG:HD2	2.19	0.72
1:B:135:ARG:HB3	1:B:135:ARG:HH11	1.54	0.72
1:B:89:VAL:HG22	1:B:406:GLN:HE21	1.53	0.72
1:A:243:ILE:HD13	1:A:340:ILE:HD11	1.72	0.71
1:D:113:VAL:HG23	1:D:426:THR:HG21	1.71	0.71
1:A:124:ARG:NE	1:A:421:PHE:HZ	1.89	0.71
1:D:199:VAL:HG11	1:D:211:PHE:CE1	2.25	0.71
1:D:79:ARG:HB3	1:D:79:ARG:CZ	2.20	0.71
1:B:223:MSE:HA	1:B:223:MSE:HE3	1.73	0.71
1:C:78:LEU:N	1:C:413:SER:HB3	2.04	0.71
1:D:403:THR:OG1	1:D:404:ARG:N	2.19	0.71
1:B:428:GLU:O	1:B:429:LEU:HD12	1.89	0.71
1:D:159:GLU:O	1:D:162:ARG:HB3	1.91	0.71
1:A:126:HIS:CE1	1:A:396:ARG:HH11	2.09	0.71
1:B:317:LYS:NZ	1:B:317:LYS:HB3	2.04	0.71
1:C:252:ARG:HB2	1:C:348:PHE:CE1	2.25	0.71
1:C:396:ARG:HB2	1:C:426:THR:HG22	1.71	0.71
1:A:126:HIS:HE1	1:A:396:ARG:HH11	1.38	0.71
1:A:115:GLY:HA3	1:A:146:MSE:HE2	1.73	0.71
1:A:352:ARG:H	1:A:352:ARG:NH1	1.89	0.71
1:B:336:PRO:HB3	1:B:400:GLU:HA	1.71	0.71
1:C:202:GLN:HE22	1:C:213:SER:HB3	1.54	0.70
1:C:78:LEU:HD21	1:C:81:LEU:HB3	1.73	0.70
1:D:289:VAL:HB	1:D:294:LEU:HD12	1.73	0.70
1:A:248:LEU:HD11	1:A:303:ARG:HG3	1.72	0.70
1:D:203:ILE:HD12	1:D:331:THR:HG22	1.74	0.70
1:B:181:SER:HB2	1:B:301:MSE:CE	2.21	0.70
1:C:83:ILE:O	1:C:83:ILE:HG23	1.91	0.70
1:A:351:PHE:HA	1:A:352:ARG:NH1	2.07	0.70
1:A:78:LEU:CD2	1:A:413:SER:HB2	2.21	0.70
1:D:317:LYS:O	1:D:317:LYS:HG2	1.90	0.70
1:A:97:ASN:HB2	1:A:99:ARG:NH1	2.07	0.69
1:A:370:THR:HB	3:A:476:HOH:O	1.90	0.69
1:C:194:THR:HA	1:C:231:ARG:HH11	1.55	0.69
1:D:400:GLU:CD	1:D:400:GLU:H	1.95	0.69
1:B:289:VAL:HB	1:B:294:LEU:HD13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LYS:HD3	1:B:391:ILE:HD12	1.74	0.69
1:D:415:GLU:O	1:D:429:LEU:HD22	1.93	0.69
1:B:99:ARG:HD3	1:B:408:MSE:SE	2.42	0.69
1:D:118:ARG:HG2	1:D:150:ASN:OD1	1.92	0.69
1:D:115:GLY:HA3	1:D:146:MSE:CE	2.23	0.69
1:D:84:GLU:HB3	1:D:408:MSE:HE2	1.73	0.69
1:A:248:LEU:CD1	1:A:303:ARG:CD	2.68	0.69
1:A:139:MSE:O	1:A:139:MSE:HE3	1.93	0.69
1:C:417:GLY:HA3	1:C:428:GLU:CD	2.14	0.69
1:B:403:THR:HG22	1:B:422:SER:CA	2.23	0.69
1:C:372:LEU:HA	1:C:427:ASN:CG	2.13	0.69
1:A:98:ARG:HD2	1:A:146:MSE:HG2	1.73	0.68
1:D:420:ASP:HB2	1:D:425:ARG:CZ	2.24	0.68
1:D:222:LEU:O	1:D:223:MSE:CE	2.35	0.68
1:B:139:MSE:O	1:B:143:GLN:HG3	1.93	0.68
1:A:84:GLU:CD	1:A:87:ARG:HH11	1.97	0.68
1:C:117:LEU:HD21	1:C:149:LEU:HB3	1.74	0.68
1:D:403:THR:OG1	1:D:404:ARG:O	2.12	0.68
1:C:124:ARG:NE	1:C:421:PHE:HZ	1.91	0.68
1:C:98:ARG:HB3	1:C:146:MSE:HG3	1.76	0.68
1:B:389:LYS:HE2	1:B:390:ASN:N	2.03	0.68
1:C:390:ASN:H	1:C:390:ASN:ND2	1.90	0.68
1:A:221:PRO:HB2	1:A:223:MSE:HE3	1.76	0.68
1:B:216:GLU:HG3	1:B:222:LEU:HB3	1.76	0.68
1:C:202:GLN:HE22	1:C:213:SER:CB	2.06	0.68
1:D:163:GLN:HE22	1:D:166:ARG:NH2	1.92	0.68
1:B:162:ARG:NH2	1:B:166:ARG:NH2	2.42	0.67
1:A:256:LYS:NZ	1:A:364:TYR:O	2.27	0.67
1:B:172:ARG:HH12	1:B:313:GLY:CA	2.06	0.67
1:C:124:ARG:HE	1:C:421:PHE:HZ	1.39	0.67
1:D:372:LEU:HD13	1:D:427:ASN:OD1	1.94	0.67
1:C:344:THR:HG23	1:C:392:SER:HB2	1.76	0.67
1:D:139:MSE:HE3	1:D:139:MSE:O	1.95	0.67
1:D:140:TRP:HE3	1:D:141:LEU:HD22	1.58	0.67
1:D:418:GLU:OE1	1:D:425:ARG:NH1	2.27	0.67
1:D:89:VAL:HG22	1:D:406:GLN:HG2	1.77	0.67
1:A:163:GLN:NE2	1:A:166:ARG:HE	1.93	0.67
1:C:87:ARG:NH1	1:D:84:GLU:HA	2.08	0.67
1:A:91:ALA:CB	1:A:99:ARG:HH12	2.08	0.67
1:D:407:LYS:HB3	1:D:420:ASP:HB3	1.77	0.67
1:A:396:ARG:CZ	1:A:424:ASP:HB3	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:CYS:O	1:B:94:THR:HG23	1.95	0.67
1:A:78:LEU:HD22	1:A:412:THR:O	1.95	0.66
1:D:426:THR:HG22	1:D:427:ASN:N	2.10	0.66
1:B:376:LYS:HG2	1:B:429:LEU:CD2	2.23	0.66
1:D:193:PRO:HG3	1:D:240:ILE:HG12	1.77	0.66
1:B:269:THR:HG22	1:B:270:ALA:N	2.10	0.66
1:C:259:ARG:HG2	1:C:259:ARG:HH11	1.60	0.66
1:B:222:LEU:O	1:B:222:LEU:HD12	1.96	0.66
1:B:146:MSE:HE3	3:B:476:HOH:O	1.95	0.66
1:A:259:ARG:N	1:A:259:ARG:HD2	2.11	0.66
1:B:161:THR:HG22	1:B:327:PRO:HG2	1.77	0.65
1:A:218:LEU:HD21	1:A:266:THR:HG22	1.78	0.65
1:C:293:LEU:H	1:C:293:LEU:CD2	2.07	0.65
1:A:172:ARG:NH1	1:D:153:ARG:HH12	1.95	0.65
1:D:372:LEU:HB2	1:D:427:ASN:HD21	1.62	0.65
1:A:164:PHE:HA	1:A:167:MSE:HE3	1.78	0.65
1:B:419:GLU:HB2	1:B:426:THR:HB	1.78	0.65
1:D:78:LEU:HD21	1:D:81:LEU:HD23	1.79	0.65
1:A:404:ARG:HA	1:A:404:ARG:NE	2.12	0.64
1:B:94:THR:O	1:B:95:SER:HB3	1.97	0.64
1:C:412:THR:HA	1:C:414:GLY:O	1.96	0.64
1:C:268:HIS:CD2	1:C:303:ARG:HD2	2.32	0.64
1:C:365:PRO:O	1:C:367:SER:N	2.30	0.64
1:A:108:ASP:HA	1:A:135:ARG:HG3	1.79	0.64
1:A:126:HIS:HE1	1:A:396:ARG:NH1	1.95	0.64
1:B:203:ILE:HD12	1:B:331:THR:HG22	1.79	0.64
1:C:417:GLY:N	1:C:428:GLU:CG	2.61	0.64
1:D:229:ASN:OD1	1:D:231:ARG:HG2	1.97	0.64
1:A:101:THR:HG23	1:A:111:VAL:HB	1.79	0.64
1:A:99:ARG:HG2	1:A:408:MSE:SE	2.48	0.64
1:D:96:ARG:CZ	1:D:118:ARG:HH21	2.11	0.64
1:C:383:LYS:HA	1:C:387:VAL:CG1	2.27	0.64
1:A:368:PRO:HG3	1:A:397:HIS:CD2	2.33	0.64
1:C:408:MSE:CE	1:C:419:GLU:OE2	2.42	0.64
1:B:145:VAL:O	1:B:149:LEU:HD13	1.96	0.64
1:B:206:GLU:HB3	1:C:206:GLU:OE2	1.98	0.64
1:A:134:GLY:O	1:A:135:ARG:HB3	1.97	0.63
1:B:97:ASN:O	1:B:146:MSE:HE2	1.98	0.63
1:C:91:ALA:CB	1:C:99:ARG:HH21	2.10	0.63
1:D:163:GLN:HE22	1:D:166:ARG:HH21	1.47	0.63
1:A:108:ASP:HB2	1:A:390:ASN:ND2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ARG:NE	1:C:408:MSE:HE1	2.13	0.63
1:C:87:ARG:HH12	1:D:84:GLU:HA	1.63	0.63
1:A:371:VAL:HG13	1:A:395:VAL:HG12	1.79	0.63
1:A:112:VAL:HG11	1:A:127:ALA:HB3	1.79	0.63
1:A:250:ASN:ND2	1:A:345:ALA:HB2	2.14	0.63
1:A:123:THR:HG22	1:A:188:ARG:HB2	1.81	0.63
1:B:110:VAL:HG21	1:B:142:ALA:HB2	1.81	0.63
1:C:186:PHE:HB2	1:C:244:HIS:HB2	1.81	0.63
1:A:248:LEU:HD12	1:A:303:ARG:HG2	1.81	0.63
1:D:91:ALA:HB1	1:D:97:ASN:HB3	1.80	0.63
1:D:95:SER:HA	1:D:116:MSE:SE	2.49	0.63
1:A:351:PHE:HA	1:A:352:ARG:HH11	1.64	0.62
1:A:87:ARG:NH1	1:B:87:ARG:HD2	2.13	0.62
1:A:375:ALA:HB2	1:A:427:ASN:HD22	1.64	0.62
1:B:403:THR:HG22	1:B:422:SER:O	1.98	0.62
1:C:132:PHE:CE2	1:C:179:GLY:HA2	2.35	0.62
1:A:112:VAL:CG1	1:A:127:ALA:HB3	2.29	0.62
1:A:124:ARG:NE	1:A:421:PHE:CZ	2.66	0.62
1:D:301:MSE:HE3	1:D:301:MSE:HA	1.81	0.62
1:A:78:LEU:HD12	1:A:376:LYS:HZ3	1.65	0.62
3:B:469:HOH:O	1:C:423:ILE:HD11	1.99	0.62
1:B:407:LYS:HB3	1:B:420:ASP:HB3	1.82	0.62
1:A:172:ARG:NH1	1:D:153:ARG:NH1	2.48	0.62
1:A:344:THR:CG2	1:A:392:SER:HB2	2.28	0.62
1:B:91:ALA:HB1	1:B:97:ASN:HB3	1.82	0.62
1:B:84:GLU:O	1:B:87:ARG:HG2	2.00	0.61
1:A:352:ARG:HH11	1:A:352:ARG:H	1.48	0.61
1:D:250:ASN:ND2	1:D:345:ALA:HB2	2.15	0.61
1:A:303:ARG:HD3	1:A:324:SER:HB3	1.82	0.61
1:C:344:THR:CG2	1:C:392:SER:HB2	2.31	0.61
1:C:81:LEU:HB2	1:C:411:GLY:HA3	1.82	0.61
1:C:97:ASN:C	1:C:98:ARG:HD3	2.20	0.61
1:A:349:ALA:O	1:A:350:HIS:HB2	2.00	0.61
1:B:83:ILE:CG2	1:B:85:GLU:OE2	2.49	0.61
1:C:417:GLY:N	1:C:428:GLU:HG2	2.11	0.61
1:C:99:ARG:HG2	1:C:99:ARG:NH1	2.14	0.61
1:D:188:ARG:HG3	1:D:188:ARG:NH1	2.13	0.61
1:D:83:ILE:C	1:D:85:GLU:N	2.54	0.61
1:A:163:GLN:HE22	1:A:166:ARG:NE	1.99	0.61
1:A:373:ASP:N	1:A:373:ASP:OD2	2.34	0.61
1:A:259:ARG:H	1:A:259:ARG:HD2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ALA:C	1:B:219:GLY:H	2.02	0.61
1:C:392:SER:OG	1:C:430:THR:HG23	2.01	0.61
1:A:100:PRO:HA	1:A:112:VAL:HA	1.82	0.61
1:A:352:ARG:HD2	1:A:352:ARG:N	2.15	0.61
1:A:84:GLU:CG	1:A:87:ARG:HH11	2.14	0.60
1:A:94:THR:O	1:A:95:SER:HB3	2.00	0.60
1:B:254:VAL:HG23	1:B:341:VAL:HB	1.83	0.60
1:B:124:ARG:NH1	1:B:421:PHE:CZ	2.69	0.60
1:B:114:GLU:HA	1:B:125:VAL:O	2.01	0.60
1:B:229:ASN:OD1	1:B:231:ARG:HB2	2.00	0.60
1:D:192:LYS:HE2	1:D:193:PRO:O	2.01	0.60
1:A:120:ARG:HH11	1:A:120:ARG:HG3	1.65	0.60
1:A:365:PRO:O	1:A:366:VAL:HG12	2.01	0.60
1:A:379:VAL:O	1:A:383:LYS:HG3	2.01	0.60
1:B:222:LEU:O	1:B:223:MSE:HE3	2.02	0.60
1:A:78:LEU:HD12	1:A:376:LYS:NZ	2.16	0.60
1:A:120:ARG:HD3	1:A:122:GLU:HB2	1.84	0.60
1:B:195:GLU:HG2	1:B:229:ASN:HA	1.84	0.60
1:D:165:GLU:OE1	1:D:165:GLU:HA	2.01	0.60
1:D:163:GLN:NE2	1:D:166:ARG:HH21	2.00	0.60
1:D:157:GLU:HG3	1:D:329:VAL:CG1	2.32	0.60
1:B:99:ARG:CD	1:B:408:MSE:SE	3.00	0.60
1:C:268:HIS:CE1	1:C:303:ARG:HD2	2.37	0.60
1:C:84:GLU:HG2	1:C:87:ARG:NE	2.16	0.60
1:D:157:GLU:HG3	1:D:329:VAL:HG11	1.83	0.60
1:A:195:GLU:HB3	1:A:229:ASN:HA	1.84	0.59
1:A:194:THR:HB	1:A:231:ARG:NH2	2.17	0.59
1:D:250:ASN:HA	1:D:267:PRO:HB3	1.83	0.59
1:A:349:ALA:O	1:A:385:ARG:NH1	2.35	0.59
1:D:175:ASN:O	1:D:176:LEU:HD23	2.01	0.59
1:A:181:SER:HB3	1:A:301:MSE:SE	2.53	0.59
1:A:85:GLU:HG2	1:A:407:LYS:HA	1.83	0.59
1:B:431:GLN:OE1	1:B:432:ALA:N	2.36	0.59
1:D:266:THR:HG23	1:D:268:HIS:HE1	1.66	0.59
1:B:100:PRO:CA	1:B:111:VAL:O	2.44	0.59
1:B:386:LYS:HZ2	1:B:386:LYS:HB3	1.68	0.59
1:A:201:ARG:HD2	1:A:333:PHE:CZ	2.37	0.59
1:A:421:PHE:CE2	1:A:422:SER:OG	2.55	0.59
1:A:91:ALA:HB2	1:A:99:ARG:HH12	1.68	0.59
1:A:156:ASN:ND2	1:A:159:GLU:H	2.01	0.59
1:C:252:ARG:HD3	1:C:348:PHE:HD1	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:SER:OG	1:D:430:THR:HG22	2.03	0.59
1:B:158:GLU:HG3	1:C:194:THR:HG22	1.83	0.58
1:D:419:GLU:HB2	1:D:426:THR:HB	1.84	0.58
1:B:384:ARG:HH11	1:B:384:ARG:HB3	1.68	0.58
1:C:107:SER:HA	3:C:479:HOH:O	2.03	0.58
1:C:117:LEU:CD2	1:C:149:LEU:HB3	2.33	0.58
1:C:84:GLU:OE2	1:C:87:ARG:NH2	2.35	0.58
1:D:402:ARG:C	1:D:403:THR:HG22	2.23	0.58
1:B:372:LEU:HB2	1:B:427:ASN:ND2	2.18	0.58
1:D:84:GLU:HB3	1:D:408:MSE:CE	2.33	0.58
1:A:84:GLU:HG2	1:A:87:ARG:NH1	2.19	0.58
1:C:77:SER:C	1:C:413:SER:HB3	2.24	0.58
1:D:241:TYR:OH	1:D:423:ILE:HG12	2.03	0.58
1:A:115:GLY:CA	1:A:146:MSE:HE2	2.32	0.58
1:A:162:ARG:O	1:A:165:GLU:HG2	2.04	0.58
1:C:379:VAL:HG21	1:C:429:LEU:HD22	1.84	0.58
1:D:113:VAL:HG23	1:D:426:THR:CG2	2.34	0.58
1:A:124:ARG:CZ	1:A:421:PHE:HZ	2.17	0.58
1:C:367:SER:O	1:C:397:HIS:CD2	2.56	0.58
1:A:98:ARG:HH12	1:A:112:VAL:HG21	1.68	0.58
1:A:112:VAL:HG13	1:A:127:ALA:H	1.69	0.58
1:A:371:VAL:HG12	1:A:427:ASN:HD21	1.68	0.58
1:A:84:GLU:CG	1:A:87:ARG:NH1	2.67	0.57
1:B:241:TYR:HE1	1:B:423:ILE:HG21	1.69	0.57
1:C:350:HIS:HB2	1:C:385:ARG:HH11	1.69	0.57
1:D:248:LEU:HD12	1:D:303:ARG:HB3	1.86	0.57
1:C:197:ARG:HD2	3:C:495:HOH:O	2.04	0.57
1:D:257:SER:HB2	3:D:460:HOH:O	2.03	0.57
1:D:375:ALA:HB2	1:D:395:VAL:HG12	1.86	0.57
1:A:248:LEU:HD21	1:A:325:ALA:HA	1.85	0.57
1:A:372:LEU:HA	1:A:427:ASN:ND2	2.19	0.57
1:B:418:GLU:HB2	1:B:427:ASN:ND2	2.19	0.57
1:C:348:PHE:N	1:C:348:PHE:CD2	2.72	0.57
1:C:399:PRO:HB3	1:C:425:ARG:NE	2.18	0.57
1:D:336:PRO:HB3	1:D:400:GLU:HA	1.86	0.57
1:B:311:LYS:C	1:B:313:GLY:H	2.06	0.57
1:C:312:LYS:HD3	1:C:321:ASP:OD2	2.04	0.57
1:C:360:ALA:CA	1:C:363:LEU:HD23	2.33	0.57
1:D:367:SER:C	1:D:369:GLU:H	2.07	0.57
1:D:386:LYS:HZ2	1:D:386:LYS:HB2	1.69	0.57
1:A:134:GLY:O	1:A:135:ARG:CB	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:LEU:HB2	1:B:427:ASN:HD21	1.69	0.57
1:B:238:LYS:HZ3	1:B:400:GLU:HB3	1.69	0.57
1:C:156:ASN:O	1:C:160:ILE:HG13	2.04	0.57
1:D:418:GLU:HG2	1:D:427:ASN:ND2	2.19	0.57
1:C:131:GLY:HA2	1:C:180:SER:HA	1.86	0.56
1:C:312:LYS:HA	1:C:318:LEU:O	2.05	0.56
1:C:376:LYS:HG3	1:C:429:LEU:HD11	1.85	0.56
1:D:402:ARG:HG3	1:D:402:ARG:HH11	1.69	0.56
1:C:145:VAL:HG22	1:C:149:LEU:HD22	1.87	0.56
1:D:199:VAL:HG11	1:D:211:PHE:HE1	1.70	0.56
1:D:266:THR:HG23	1:D:268:HIS:CE1	2.40	0.56
1:A:366:VAL:O	1:A:366:VAL:HG22	2.06	0.56
1:B:191:LYS:O	1:B:192:LYS:HB2	2.03	0.56
1:B:367:SER:OG	1:B:370:THR:HB	2.06	0.56
1:C:124:ARG:NE	1:C:421:PHE:CZ	2.70	0.56
1:C:372:LEU:HA	1:C:427:ASN:ND2	2.20	0.56
1:C:82:TYR:OH	1:D:410:GLU:HB3	2.05	0.56
1:A:146:MSE:O	1:A:150:ASN:HB2	2.05	0.56
1:A:392:SER:CA	1:A:430:THR:HG22	2.34	0.56
1:A:179:GLY:N	1:A:306:GLY:HA3	2.18	0.56
1:B:191:LYS:O	1:B:191:LYS:HG3	2.04	0.56
1:C:416:ASN:HB3	1:C:429:LEU:HG	1.88	0.56
1:A:132:PHE:CZ	1:A:179:GLY:HA2	2.40	0.56
1:A:330:THR:HG23	1:A:332:PHE:CE1	2.41	0.56
1:B:89:VAL:HG22	1:B:406:GLN:HE22	1.66	0.56
1:C:235:ARG:CG	1:C:235:ARG:HH11	2.17	0.56
1:D:248:LEU:CD1	1:D:303:ARG:HB3	2.35	0.56
1:D:78:LEU:HD21	1:D:81:LEU:CD2	2.35	0.56
1:A:259:ARG:CD	1:A:259:ARG:N	2.67	0.56
1:B:164:PHE:CE2	1:B:327:PRO:HB3	2.41	0.56
1:B:387:VAL:CG1	1:B:391:ILE:HD11	2.36	0.56
1:C:404:ARG:NH1	1:C:404:ARG:HA	2.15	0.56
1:B:408:MSE:HA	1:B:418:GLU:O	2.05	0.56
1:A:175:ASN:ND2	1:D:153:ARG:HH21	2.04	0.56
1:D:400:GLU:CD	1:D:400:GLU:N	2.59	0.56
1:D:426:THR:CG2	1:D:427:ASN:N	2.68	0.56
1:A:156:ASN:O	1:A:160:ILE:HG12	2.06	0.55
1:A:318:LEU:N	1:A:318:LEU:HD12	2.21	0.55
1:C:431:GLN:O	1:C:432:ALA:HB2	2.06	0.55
1:C:89:VAL:HG22	1:C:406:GLN:OE1	2.06	0.55
1:A:101:THR:HG23	1:A:101:THR:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:HIS:NE2	1:C:303:ARG:HD2	2.22	0.55
1:C:88:THR:CB	1:C:408:MSE:HE3	2.13	0.55
1:A:172:ARG:HH12	1:D:153:ARG:NH1	2.03	0.55
1:A:163:GLN:HE22	1:A:166:ARG:HH21	1.55	0.55
1:A:371:VAL:HG12	1:A:427:ASN:ND2	2.21	0.55
1:C:341:VAL:HG22	1:C:395:VAL:HG22	1.89	0.55
1:C:390:ASN:N	1:C:390:ASN:ND2	2.54	0.55
1:C:91:ALA:HB1	1:C:97:ASN:HB3	1.88	0.55
1:B:269:THR:CG2	1:B:270:ALA:N	2.69	0.55
1:B:371:VAL:HG13	1:B:395:VAL:HG22	1.89	0.55
1:D:272:SER:O	1:D:276:ARG:HB2	2.07	0.55
1:D:96:ARG:CZ	1:D:118:ARG:NH2	2.69	0.55
1:C:423:ILE:O	1:C:423:ILE:CG2	2.55	0.55
1:D:145:VAL:HA	1:D:167:MSE:HE3	1.89	0.55
1:D:85:GLU:O	1:D:88:THR:HG22	2.07	0.55
1:C:229:ASN:HB3	1:C:232:ARG:HG2	1.88	0.55
1:C:293:LEU:N	1:C:293:LEU:HD23	2.12	0.55
1:D:379:VAL:CG2	1:D:429:LEU:HD12	2.27	0.55
1:A:78:LEU:CG	1:A:376:LYS:HZ2	2.17	0.54
1:A:78:LEU:HD11	1:A:416:ASN:OD1	2.07	0.54
1:A:109:ASP:OD1	1:A:390:ASN:CB	2.55	0.54
1:A:389:LYS:HG3	3:A:473:HOH:O	2.07	0.54
1:B:83:ILE:HB	1:B:85:GLU:OE2	2.07	0.54
1:B:326:VAL:HG12	1:B:326:VAL:O	2.08	0.54
1:B:83:ILE:HG22	1:B:85:GLU:OE2	2.08	0.54
1:C:81:LEU:HA	1:C:411:GLY:HA2	1.88	0.54
1:D:103:GLU:HG3	1:D:432:ALA:HA	1.88	0.54
1:A:168:ASP:OD1	1:A:305:PHE:O	2.25	0.54
1:A:98:ARG:HH11	1:A:146:MSE:HG2	1.72	0.54
1:C:376:LYS:HA	1:C:429:LEU:HD13	1.90	0.54
1:C:78:LEU:HD22	1:C:79:ARG:N	2.23	0.54
1:C:276:ARG:HD2	2:C:453:SO4:O4	2.07	0.54
1:C:124:ARG:NH2	1:C:421:PHE:HZ	2.05	0.54
1:C:100:PRO:HA	1:C:111:VAL:O	2.08	0.54
1:D:149:LEU:O	1:D:152:LEU:HG	2.07	0.54
1:D:317:LYS:O	1:D:317:LYS:CG	2.54	0.54
1:D:89:VAL:HG22	1:D:406:GLN:CG	2.38	0.54
1:C:368:PRO:HD2	1:C:370:THR:HG22	1.89	0.54
1:C:251:SER:HB2	3:C:461:HOH:O	2.07	0.54
1:C:369:GLU:HG2	1:C:369:GLU:O	2.08	0.54
1:C:402:ARG:HG2	1:C:403:THR:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ASN:OD1	1:D:231:ARG:CG	2.55	0.54
1:D:218:LEU:HD23	1:D:263:HIS:CD2	2.43	0.54
1:A:145:VAL:HG13	1:A:146:MSE:N	2.22	0.53
1:D:380:VAL:O	1:D:383:LYS:HB2	2.08	0.53
1:D:111:VAL:HG11	1:D:428:GLU:CD	2.28	0.53
1:B:187:VAL:HG11	1:B:396:ARG:NH1	2.23	0.53
1:D:353:SER:C	1:D:355:ALA:N	2.60	0.53
1:B:354:HIS:N	1:B:354:HIS:ND1	2.56	0.53
1:B:418:GLU:HB2	1:B:427:ASN:HD22	1.72	0.53
1:B:403:THR:HG22	1:B:422:SER:N	2.24	0.53
1:D:344:THR:HG23	1:D:392:SER:HB2	1.90	0.53
1:A:299:VAL:HG12	1:A:301:MSE:H	1.73	0.53
1:B:135:ARG:HE	1:B:139:MSE:HE3	1.72	0.53
1:D:353:SER:O	1:D:354:HIS:C	2.47	0.53
1:B:254:VAL:HG22	1:B:341:VAL:HB	1.91	0.53
1:D:116:MSE:HE2	1:D:124:ARG:CZ	2.38	0.53
1:B:198:VAL:O	1:B:226:VAL:HG12	2.08	0.53
1:B:326:VAL:CG1	1:B:326:VAL:O	2.56	0.53
1:C:124:ARG:CZ	1:C:421:PHE:HZ	2.21	0.53
1:A:95:SER:O	1:A:116:MSE:HE2	2.09	0.53
1:A:108:ASP:HB2	1:A:390:ASN:HD21	1.72	0.53
1:C:326:VAL:HG23	3:C:469:HOH:O	2.08	0.53
1:A:115:GLY:C	1:A:146:MSE:HE2	2.28	0.53
1:B:135:ARG:HE	1:B:139:MSE:CE	2.21	0.53
1:C:371:VAL:O	1:C:374:ALA:HB3	2.09	0.53
1:D:377:ALA:HA	1:D:380:VAL:HG22	1.90	0.53
1:A:396:ARG:HG3	1:A:426:THR:HG22	1.91	0.53
1:A:98:ARG:HH11	1:A:98:ARG:HG3	1.74	0.53
1:B:115:GLY:HA3	1:B:146:MSE:HE2	1.91	0.53
1:B:82:TYR:OH	1:B:87:ARG:NH2	2.42	0.53
1:C:103:GLU:HG2	1:C:104:SER:N	2.15	0.53
1:B:159:GLU:OE1	1:C:192:LYS:HE2	2.09	0.53
1:C:414:GLY:HA3	1:C:431:GLN:OE1	2.08	0.53
1:D:424:ASP:OD2	1:D:425:ARG:N	2.41	0.53
1:B:257:SER:HA	1:B:338:ASP:OD1	2.08	0.53
1:C:371:VAL:HG12	1:C:427:ASN:HB2	1.90	0.53
1:D:202:GLN:HE22	1:D:214:VAL:HG23	1.74	0.53
1:D:103:GLU:CD	1:D:432:ALA:HA	2.29	0.53
1:B:295:LEU:C	1:B:295:LEU:HD23	2.29	0.52
1:C:241:TYR:CD1	1:C:398:LEU:HD22	2.44	0.52
1:C:81:LEU:CB	1:C:411:GLY:HA3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ALA:O	1:D:176:LEU:HG	2.08	0.52
1:D:269:THR:HG22	1:D:301:MSE:HE1	1.89	0.52
1:D:85:GLU:O	1:D:89:VAL:HG23	2.08	0.52
1:B:114:GLU:OE1	1:B:124:ARG:HD2	2.09	0.52
1:C:254:VAL:HG21	1:C:361:ILE:HG21	1.91	0.52
1:D:77:SER:O	1:D:78:LEU:CB	2.56	0.52
1:C:423:ILE:HG23	1:C:423:ILE:O	2.09	0.52
1:B:154:ASP:O	1:B:159:GLU:HG2	2.09	0.52
1:B:303:ARG:O	1:B:304:ALA:HB2	2.10	0.52
1:C:390:ASN:H	1:C:390:ASN:HD22	1.57	0.52
1:A:172:ARG:NE	1:D:162:ARG:HD2	2.25	0.52
1:A:341:VAL:HG11	1:A:361:ILE:HG21	1.91	0.52
1:C:82:TYR:OH	1:D:410:GLU:CD	2.47	0.52
1:A:248:LEU:HD23	1:A:304:ALA:HA	1.90	0.52
1:A:98:ARG:NH1	1:A:98:ARG:HG3	2.25	0.52
1:C:183:LEU:HD11	1:C:253:CYS:HB2	1.92	0.52
1:A:238:LYS:HD2	1:A:400:GLU:OE1	2.09	0.52
1:B:110:VAL:CG2	1:B:142:ALA:HB2	2.40	0.52
1:C:241:TYR:CE2	1:C:398:LEU:HB3	2.45	0.52
1:C:126:HIS:HE1	1:C:426:THR:HG21	1.71	0.52
1:A:223:MSE:CG	1:A:224:PRO:HD2	2.36	0.52
1:C:82:TYR:C	1:C:82:TYR:CD2	2.83	0.52
1:D:99:ARG:HH11	1:D:99:ARG:HA	1.75	0.52
1:A:248:LEU:CG	1:A:303:ARG:CG	2.64	0.52
1:C:181:SER:HB3	1:C:301:MSE:SE	2.60	0.52
1:A:109:ASP:OD1	1:A:390:ASN:HB3	2.09	0.51
1:B:110:VAL:HG21	1:B:142:ALA:CB	2.40	0.51
1:B:372:LEU:HA	1:B:427:ASN:OD1	2.08	0.51
1:D:141:LEU:HD12	1:D:167:MSE:HE2	1.92	0.51
1:A:318:LEU:HD23	1:A:322:LEU:HG	1.91	0.51
1:C:181:SER:HB2	1:C:249:GLY:HA3	1.93	0.51
1:D:101:THR:HG22	1:D:113:VAL:HG12	1.90	0.51
1:B:426:THR:HG22	1:B:427:ASN:N	2.25	0.51
1:C:390:ASN:N	1:C:390:ASN:HD22	2.07	0.51
1:A:396:ARG:CG	1:A:426:THR:HG22	2.40	0.51
1:A:96:ARG:HG3	1:A:96:ARG:O	2.10	0.51
1:C:200:GLY:O	1:C:201:ARG:HB2	2.10	0.51
1:D:272:SER:HB3	1:D:275:GLU:HB3	1.91	0.51
1:B:409:LEU:O	1:B:417:GLY:HA2	2.10	0.51
1:C:417:GLY:CA	1:C:428:GLU:CD	2.78	0.51
1:D:228:MSE:HE2	1:D:230:PHE:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:LEU:HD23	1:B:296:GLY:N	2.25	0.51
1:B:317:LYS:HZ3	1:B:317:LYS:HB3	1.73	0.51
1:C:367:SER:OG	1:C:371:VAL:N	2.44	0.51
1:A:365:PRO:O	1:A:366:VAL:CG1	2.57	0.51
1:B:238:LYS:HZ1	1:B:400:GLU:HB3	1.72	0.51
1:D:130:ASP:HB3	1:D:181:SER:HB2	1.93	0.51
1:D:98:ARG:HG3	1:D:146:MSE:CE	2.39	0.51
1:A:199:VAL:HG12	1:A:199:VAL:O	2.11	0.51
1:B:78:LEU:HA	1:B:413:SER:HG	1.74	0.51
1:C:148:TYR:O	1:C:151:ASP:HB2	2.10	0.51
1:C:168:ASP:OD2	1:C:305:PHE:O	2.29	0.51
1:C:99:ARG:CG	1:C:99:ARG:NH1	2.74	0.51
1:A:111:VAL:HG22	1:A:128:MSE:HG3	1.93	0.50
1:B:135:ARG:O	1:B:135:ARG:HG2	2.11	0.50
1:C:145:VAL:HG13	1:C:146:MSE:HE2	1.93	0.50
1:D:117:LEU:HD21	1:D:149:LEU:HB3	1.92	0.50
1:B:110:VAL:HG22	1:B:129:PHE:HB2	1.92	0.50
1:C:99:ARG:NH1	1:C:408:MSE:HE1	2.24	0.50
1:A:378:MSE:O	1:A:382:ALA:HB2	2.11	0.50
1:D:386:LYS:NZ	1:D:386:LYS:CB	2.74	0.50
1:B:254:VAL:HG21	1:B:361:ILE:CD1	2.37	0.50
1:A:87:ARG:HH12	1:B:87:ARG:HG3	1.76	0.50
1:C:172:ARG:HB2	1:C:308:PHE:CE2	2.46	0.50
1:C:197:ARG:HH22	1:C:206:GLU:CG	2.25	0.50
1:A:280:GLN:HA	1:A:284:GLY:O	2.11	0.50
1:A:352:ARG:N	1:A:352:ARG:HH11	2.10	0.50
1:A:78:LEU:CD1	1:A:376:LYS:NZ	2.74	0.50
1:B:375:ALA:HB2	1:B:395:VAL:HG12	1.93	0.50
1:C:82:TYR:OH	1:D:410:GLU:CG	2.60	0.50
1:D:386:LYS:NZ	1:D:386:LYS:HB2	2.27	0.50
1:A:392:SER:HA	1:A:430:THR:CG2	2.39	0.50
1:C:197:ARG:CD	3:C:495:HOH:O	2.58	0.50
1:C:109:ASP:OD1	1:C:344:THR:HG21	2.11	0.50
1:C:381:ASN:HD21	1:C:384:ARG:NH2	2.10	0.50
1:C:424:ASP:O	1:C:425:ARG:HG3	2.11	0.50
1:A:421:PHE:CG	1:A:422:SER:N	2.79	0.50
1:C:114:GLU:HG3	1:C:115:GLY:N	2.26	0.50
1:C:229:ASN:OD1	1:C:231:ARG:HG3	2.11	0.50
1:D:313:GLY:HA3	3:D:454:HOH:O	2.10	0.50
1:D:94:THR:O	1:D:95:SER:HB3	2.10	0.50
1:A:101:THR:CG2	1:A:111:VAL:HB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:HH22	1:D:175:ASN:HB3	1.77	0.50
1:D:112:VAL:HG13	1:D:127:ALA:HB3	1.94	0.49
1:D:124:ARG:NE	1:D:421:PHE:CZ	2.52	0.49
1:D:418:GLU:CD	1:D:425:ARG:NH1	2.65	0.49
1:A:188:ARG:HH11	1:A:188:ARG:HG2	1.77	0.49
1:B:81:LEU:HA	1:B:411:GLY:HA2	1.93	0.49
1:C:90:CYS:O	1:C:93:ALA:HB3	2.12	0.49
1:D:379:VAL:O	1:D:382:ALA:HB3	2.11	0.49
1:A:396:ARG:CB	1:A:426:THR:HG22	2.42	0.49
1:D:99:ARG:HD2	1:D:408:MSE:HE1	1.94	0.49
1:A:254:VAL:HB	1:A:341:VAL:HG13	1.95	0.49
1:A:424:ASP:C	1:A:425:ARG:HD3	2.32	0.49
1:C:96:ARG:CD	1:C:118:ARG:NH2	2.75	0.49
1:D:116:MSE:HE2	1:D:124:ARG:NH2	2.27	0.49
1:D:201:ARG:HG3	1:D:333:PHE:O	2.12	0.49
1:D:172:ARG:HG3	1:D:308:PHE:CE2	2.48	0.49
1:B:145:VAL:HG13	1:B:146:MSE:N	2.27	0.49
1:D:382:ALA:C	1:D:384:ARG:H	2.15	0.49
1:A:108:ASP:HA	1:A:135:ARG:CG	2.43	0.49
1:A:366:VAL:HG13	1:A:366:VAL:O	2.13	0.49
1:B:98:ARG:O	1:B:99:ARG:HG3	2.13	0.49
1:D:255:LEU:HD12	1:D:339:ASP:O	2.12	0.49
1:D:376:LYS:HA	1:D:429:LEU:HG	1.94	0.49
1:A:157:GLU:HA	1:A:329:VAL:HG21	1.93	0.48
1:B:81:LEU:O	1:B:81:LEU:HG	2.13	0.48
1:C:124:ARG:HH21	1:C:421:PHE:HZ	1.61	0.48
1:C:91:ALA:CB	1:C:99:ARG:NH2	2.76	0.48
1:D:145:VAL:HG23	1:D:167:MSE:HE1	1.95	0.48
1:D:286:PHE:HB3	1:D:293:LEU:HD11	1.96	0.48
1:A:120:ARG:CD	1:A:122:GLU:HB2	2.42	0.48
1:A:88:THR:HB	1:A:408:MSE:HE3	1.95	0.48
1:B:85:GLU:O	1:B:88:THR:HG22	2.13	0.48
1:C:381:ASN:ND2	1:C:384:ARG:NH2	2.62	0.48
1:D:145:VAL:O	1:D:149:LEU:HD13	2.13	0.48
1:C:214:VAL:HG11	1:C:263:HIS:O	2.14	0.48
1:D:96:ARG:O	1:D:96:ARG:HG3	2.13	0.48
1:A:120:ARG:HG2	1:A:122:GLU:N	2.21	0.48
1:A:109:ASP:CG	1:A:390:ASN:HB3	2.33	0.48
1:B:153:ARG:HG2	1:C:192:LYS:HZ3	1.78	0.48
1:C:409:LEU:O	1:C:417:GLY:HA2	2.13	0.48
1:D:303:ARG:HA	1:D:324:SER:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ASP:OD1	1:D:311:LYS:HE2	2.13	0.48
1:A:423:ILE:O	1:A:423:ILE:HG23	2.12	0.48
1:B:153:ARG:HG2	1:C:192:LYS:HZ1	1.73	0.48
1:D:88:THR:O	1:D:92:SER:HB2	2.13	0.48
1:A:120:ARG:NE	1:A:188:ARG:HE	2.11	0.48
1:A:368:PRO:O	1:A:371:VAL:HG23	2.13	0.48
1:B:241:TYR:HE1	1:B:423:ILE:CG2	2.25	0.48
1:D:112:VAL:HG21	1:D:146:MSE:HE1	1.94	0.48
1:B:107:SER:O	1:B:135:ARG:HB2	2.14	0.48
1:B:423:ILE:CG2	1:B:423:ILE:O	2.61	0.48
1:C:359:ALA:O	1:C:362:ALA:HB3	2.13	0.48
1:D:372:LEU:HB2	1:D:427:ASN:ND2	2.28	0.48
1:A:156:ASN:HD21	1:A:159:GLU:H	1.60	0.48
1:B:97:ASN:O	1:B:115:GLY:HA2	2.14	0.48
1:C:299:VAL:HA	1:C:300:PRO:HD3	1.73	0.48
1:D:378:MSE:HE2	1:D:393:THR:HG22	1.96	0.48
1:C:165:GLU:OE2	1:C:166:ARG:N	2.47	0.48
1:C:376:LYS:HE2	1:C:413:SER:OG	2.14	0.48
1:D:188:ARG:HH11	1:D:188:ARG:CG	2.19	0.48
1:A:132:PHE:CE2	1:A:179:GLY:HA2	2.49	0.48
1:B:133:GLN:HG3	1:B:133:GLN:O	2.13	0.48
1:B:255:LEU:HB2	1:B:264:LEU:HD21	1.96	0.48
1:B:386:LYS:HA	1:B:386:LYS:HZ3	1.79	0.48
1:D:85:GLU:HA	1:D:85:GLU:OE2	2.13	0.48
1:A:156:ASN:ND2	1:A:156:ASN:C	2.55	0.47
1:B:83:ILE:CB	1:B:85:GLU:OE2	2.62	0.47
1:C:91:ALA:HB3	1:C:99:ARG:HH21	1.76	0.47
1:D:368:PRO:HG2	1:D:369:GLU:CD	2.34	0.47
1:A:393:THR:O	1:A:428:GLU:HA	2.13	0.47
1:B:101:THR:HG21	1:B:428:GLU:HG3	1.96	0.47
1:C:359:ALA:O	1:C:363:LEU:CD2	2.63	0.47
1:C:350:HIS:N	1:C:385:ARG:NH1	2.54	0.47
1:C:259:ARG:CG	1:C:259:ARG:HH11	2.26	0.47
1:D:126:HIS:NE2	1:D:396:ARG:NH1	2.58	0.47
1:B:146:MSE:HB3	3:B:476:HOH:O	2.14	0.47
1:B:393:THR:O	1:B:428:GLU:CD	2.53	0.47
1:D:199:VAL:HG13	1:D:199:VAL:O	2.15	0.47
1:A:98:ARG:HB2	1:A:146:MSE:HG3	1.96	0.47
1:B:422:SER:OG	1:B:423:ILE:N	2.47	0.47
1:B:394:PHE:HB2	1:B:428:GLU:OE2	2.13	0.47
1:B:158:GLU:HG3	1:C:194:THR:CG2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ARG:HG3	1:C:96:ARG:HH11	1.80	0.47
1:D:156:ASN:O	1:D:160:ILE:HG13	2.14	0.47
1:A:219:GLY:O	1:A:220:GLY:O	2.33	0.47
1:A:392:SER:OG	1:A:430:THR:HG22	2.15	0.47
1:B:316:GLY:O	1:B:317:LYS:HG2	2.13	0.47
1:D:353:SER:O	1:D:355:ALA:N	2.47	0.47
1:D:406:GLN:N	1:D:406:GLN:OE1	2.47	0.47
1:D:424:ASP:OD2	1:D:424:ASP:C	2.52	0.47
1:D:372:LEU:CA	1:D:427:ASN:ND2	2.78	0.47
1:A:124:ARG:NH2	1:A:421:PHE:HZ	2.13	0.47
1:D:112:VAL:CG1	1:D:127:ALA:HB3	2.44	0.47
1:D:139:MSE:HE2	1:D:143:GLN:CD	2.35	0.47
1:D:334:ALA:HB1	1:D:338:ASP:OD1	2.15	0.47
1:A:396:ARG:HB2	1:A:426:THR:HG22	1.96	0.47
1:B:123:THR:O	1:B:124:ARG:NE	2.46	0.47
1:A:384:ARG:HD3	1:A:384:ARG:C	2.35	0.47
1:A:398:LEU:HA	1:A:399:PRO:HD3	1.71	0.47
1:B:99:ARG:HG3	1:B:99:ARG:NH1	2.29	0.47
1:C:95:SER:OG	1:C:118:ARG:HA	2.15	0.47
1:B:364:TYR:HA	1:B:365:PRO:HD3	1.68	0.46
1:A:396:ARG:HH21	1:A:424:ASP:HB3	1.78	0.46
1:A:417:GLY:O	1:A:427:ASN:HA	2.15	0.46
1:C:155:VAL:HG11	3:C:483:HOH:O	2.14	0.46
1:B:403:THR:HG22	1:B:422:SER:HA	1.96	0.46
1:C:396:ARG:CB	1:C:426:THR:HG22	2.42	0.46
1:D:429:LEU:HD13	1:D:430:THR:H	1.78	0.46
1:B:384:ARG:C	1:B:386:LYS:H	2.17	0.46
1:C:201:ARG:HA	1:C:333:PHE:CE1	2.51	0.46
1:C:226:VAL:CG2	1:C:227:ALA:N	2.79	0.46
1:D:103:GLU:CG	1:D:432:ALA:HA	2.45	0.46
1:A:189:TYR:HB2	1:A:241:TYR:CE1	2.50	0.46
1:A:218:LEU:HD23	1:A:218:LEU:N	2.30	0.46
1:A:229:ASN:ND2	1:A:231:ARG:HB2	2.25	0.46
1:A:415:GLU:O	1:A:429:LEU:HA	2.16	0.46
1:B:372:LEU:HA	1:B:427:ASN:ND2	2.30	0.46
1:C:179:GLY:O	1:C:180:SER:HB2	2.15	0.46
1:D:201:ARG:CG	1:D:201:ARG:HH11	2.29	0.46
1:A:192:LYS:HA	1:A:192:LYS:HD2	1.87	0.46
1:A:391:ILE:O	1:A:430:THR:HG22	2.14	0.46
1:B:201:ARG:HH11	1:B:201:ARG:HG2	1.81	0.46
1:C:97:ASN:O	1:C:98:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ARG:CG	1:D:188:ARG:NH1	2.77	0.46
1:D:201:ARG:HG2	1:D:201:ARG:NH1	2.29	0.46
1:A:194:THR:O	1:A:195:GLU:O	2.33	0.46
1:A:89:VAL:HG22	1:A:406:GLN:HE21	1.78	0.46
1:B:82:TYR:CD1	1:B:83:ILE:HD12	2.51	0.46
1:C:120:ARG:HH11	1:C:120:ARG:HG3	1.80	0.46
1:D:96:ARG:NH1	1:D:118:ARG:NH2	2.63	0.46
1:D:418:GLU:OE2	1:D:425:ARG:NH1	2.49	0.46
1:B:78:LEU:HB2	1:B:376:LYS:NZ	2.31	0.46
1:D:163:GLN:CD	1:D:166:ARG:HH21	2.19	0.46
1:D:257:SER:HA	1:D:338:ASP:HB3	1.98	0.46
1:D:353:SER:HB2	1:D:356:ALA:H	1.80	0.46
1:D:409:LEU:N	1:D:409:LEU:HD22	2.31	0.46
1:A:84:GLU:CG	1:A:87:ARG:HD2	2.42	0.46
1:A:91:ALA:HB1	1:A:97:ASN:CB	2.41	0.46
1:C:256:LYS:NZ	1:C:362:ALA:HA	2.31	0.46
1:C:397:HIS:O	1:C:399:PRO:HD3	2.16	0.46
1:B:253:CYS:SG	1:B:264:LEU:HD12	2.55	0.46
1:C:256:LYS:HZ3	1:C:362:ALA:HA	1.81	0.46
1:D:353:SER:O	1:D:356:ALA:N	2.49	0.46
1:C:132:PHE:CZ	1:C:179:GLY:HA2	2.51	0.45
1:C:231:ARG:HH11	1:C:231:ARG:HG2	1.81	0.45
1:A:163:GLN:HE22	1:A:166:ARG:NH2	2.14	0.45
1:A:408:MSE:HE2	1:A:419:GLU:OE1	2.17	0.45
1:B:287:THR:C	1:B:293:LEU:HD12	2.37	0.45
1:C:380:VAL:O	1:C:384:ARG:N	2.50	0.45
1:A:189:TYR:OH	1:A:191:LYS:HA	2.17	0.45
1:B:200:GLY:O	1:B:201:ARG:HB2	2.16	0.45
1:B:372:LEU:HD13	1:B:427:ASN:HD21	1.80	0.45
1:B:84:GLU:HB3	1:B:408:MSE:CE	2.47	0.45
1:C:123:THR:OG1	1:C:188:ARG:CZ	2.64	0.45
1:A:168:ASP:HB2	1:A:305:PHE:HE2	1.80	0.45
1:B:367:SER:O	1:B:371:VAL:HG23	2.16	0.45
1:D:210:GLU:N	1:D:210:GLU:OE1	2.49	0.45
1:D:256:LYS:NZ	1:D:258:GLY:O	2.46	0.45
1:D:301:MSE:CA	1:D:301:MSE:HE3	2.46	0.45
1:D:99:ARG:NH1	1:D:99:ARG:HA	2.32	0.45
1:B:350:HIS:HB3	1:B:356:ALA:HB3	1.98	0.45
1:C:372:LEU:HD12	1:C:427:ASN:HD21	1.81	0.45
1:D:423:ILE:O	1:D:423:ILE:CG2	2.60	0.45
1:A:163:GLN:NE2	1:A:166:ARG:HH21	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:THR:HG23	1:A:332:PHE:HE1	1.78	0.45
1:A:371:VAL:C	1:A:427:ASN:HD21	2.20	0.45
1:A:81:LEU:C	1:A:81:LEU:HD12	2.37	0.45
1:B:317:LYS:CG	1:B:317:LYS:O	2.65	0.45
1:B:240:ILE:HD12	1:B:333:PHE:HB2	1.99	0.45
1:C:133:GLN:OE1	1:C:133:GLN:HA	2.15	0.45
1:C:252:ARG:HB2	1:C:348:PHE:CD1	2.51	0.45
1:C:241:TYR:CD2	1:C:398:LEU:HB3	2.52	0.45
1:D:403:THR:HA	1:D:422:SER:O	2.16	0.45
1:A:192:LYS:HE3	1:A:192:LYS:CA	2.46	0.45
1:A:78:LEU:CD1	1:A:376:LYS:HZ2	2.30	0.45
1:B:78:LEU:HB2	1:B:376:LYS:HZ3	1.82	0.45
1:B:85:GLU:HG2	1:B:407:LYS:HA	1.99	0.45
1:B:412:THR:C	1:B:413:SER:HG	2.20	0.45
1:A:108:ASP:HA	1:A:135:ARG:HB2	1.97	0.45
1:A:303:ARG:HD3	1:A:324:SER:O	2.16	0.45
1:B:263:HIS:O	1:B:264:LEU:HD23	2.16	0.45
1:C:103:GLU:CG	1:C:104:SER:H	2.09	0.45
1:C:96:ARG:HD3	1:C:118:ARG:NH2	2.31	0.45
1:D:276:ARG:HG2	1:D:280:GLN:OE1	2.16	0.45
1:D:378:MSE:CB	1:D:393:THR:HG21	2.47	0.45
1:A:352:ARG:HG2	1:A:353:SER:N	2.32	0.45
1:B:96:ARG:HA	1:B:116:MSE:HB3	1.98	0.45
1:C:197:ARG:HH22	1:C:206:GLU:HG2	1.82	0.45
1:C:412:THR:HG23	1:C:412:THR:O	2.17	0.45
1:A:109:ASP:OD1	1:A:390:ASN:HB2	2.17	0.45
1:C:96:ARG:CD	1:C:118:ARG:CZ	2.90	0.45
1:C:143:GLN:HE21	1:C:143:GLN:HB3	1.59	0.45
1:C:162:ARG:O	1:C:165:GLU:HB3	2.16	0.45
1:D:112:VAL:O	1:D:112:VAL:CG2	2.59	0.45
1:D:117:LEU:CD2	1:D:149:LEU:HB3	2.46	0.45
1:D:172:ARG:HD2	3:D:454:HOH:O	2.15	0.45
1:D:308:PHE:HB3	3:D:454:HOH:O	2.17	0.45
1:A:83:ILE:O	1:A:83:ILE:HG23	2.16	0.44
1:B:85:GLU:O	1:B:88:THR:CG2	2.65	0.44
1:D:326:VAL:HG12	1:D:326:VAL:O	2.17	0.44
1:A:124:ARG:NH2	1:A:421:PHE:CZ	2.86	0.44
1:A:83:ILE:HG13	1:A:85:GLU:HB2	1.95	0.44
1:B:428:GLU:C	1:B:429:LEU:HD12	2.37	0.44
1:D:282:ALA:HB1	1:D:320:GLN:NE2	2.33	0.44
1:A:421:PHE:CD2	1:A:422:SER:OG	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:CZ	1:B:87:ARG:HB3	2.47	0.44
1:B:379:VAL:O	1:B:383:LYS:HG2	2.17	0.44
1:A:164:PHE:CD2	1:A:327:PRO:HG3	2.51	0.44
1:A:303:ARG:CD	1:A:324:SER:HB3	2.46	0.44
1:B:382:ALA:O	1:B:387:VAL:HG12	2.17	0.44
1:B:82:TYR:CE1	1:B:83:ILE:HD12	2.53	0.44
1:C:348:PHE:HB3	1:C:357:ILE:HD13	1.99	0.44
1:B:317:LYS:HZ2	1:B:317:LYS:HB3	1.79	0.44
1:B:376:LYS:HA	1:B:429:LEU:CD2	2.31	0.44
1:A:87:ARG:NH1	1:B:87:ARG:CG	2.80	0.44
1:C:98:ARG:HD2	1:C:146:MSE:HG3	1.99	0.44
1:C:402:ARG:HG2	1:C:403:THR:N	2.33	0.44
1:C:90:CYS:O	1:C:94:THR:HG22	2.17	0.44
1:A:109:ASP:OD2	1:A:390:ASN:HB3	2.18	0.44
1:B:384:ARG:HB3	1:B:384:ARG:CZ	2.48	0.44
1:B:426:THR:CG2	1:B:427:ASN:N	2.81	0.44
1:A:87:ARG:HH12	1:B:87:ARG:CG	2.31	0.44
1:D:377:ALA:HA	1:D:380:VAL:CG2	2.46	0.44
1:D:85:GLU:CA	1:D:85:GLU:OE2	2.66	0.44
1:A:123:THR:O	1:A:124:ARG:NH1	2.50	0.44
1:B:376:LYS:O	1:B:380:VAL:HG23	2.17	0.44
1:B:428:GLU:OE1	1:B:429:LEU:O	2.35	0.44
1:C:268:HIS:CG	1:C:303:ARG:HD2	2.53	0.44
1:D:367:SER:C	1:D:369:GLU:N	2.71	0.44
1:D:78:LEU:C	1:D:79:ARG:HE	2.21	0.44
1:A:245:VAL:HB	1:A:330:THR:HG22	1.99	0.44
1:B:85:GLU:HA	1:B:88:THR:HG22	2.00	0.44
1:A:214:VAL:HG13	1:A:266:THR:HG23	1.99	0.43
1:B:375:ALA:HB2	1:B:395:VAL:CG1	2.48	0.43
1:B:187:VAL:CG1	1:B:396:ARG:NH1	2.80	0.43
1:D:193:PRO:HG2	1:D:240:ILE:HG23	2.00	0.43
1:A:108:ASP:OD1	1:A:135:ARG:HB2	2.17	0.43
1:A:145:VAL:CG1	1:A:146:MSE:N	2.81	0.43
1:A:218:LEU:O	1:A:219:GLY:C	2.55	0.43
1:A:371:VAL:HG13	1:A:395:VAL:CG1	2.46	0.43
1:B:120:ARG:HB3	1:B:123:THR:HB	1.99	0.43
1:C:403:THR:O	1:C:422:SER:HA	2.18	0.43
1:A:126:HIS:CE1	1:A:396:ARG:NH1	2.76	0.43
1:A:78:LEU:CD2	1:A:413:SER:CB	2.93	0.43
1:B:270:ALA:O	1:B:276:ARG:HD3	2.18	0.43
1:C:125:VAL:HG12	1:C:126:HIS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:TYR:CE2	1:D:398:LEU:HB3	2.53	0.43
1:D:78:LEU:C	1:D:78:LEU:HD13	2.38	0.43
1:A:112:VAL:O	1:A:112:VAL:HG22	2.17	0.43
1:A:341:VAL:O	1:A:341:VAL:HG13	2.19	0.43
1:B:121:PRO:HD2	3:B:454:HOH:O	2.17	0.43
1:B:418:GLU:O	1:B:418:GLU:HG3	2.17	0.43
1:B:82:TYR:HE2	1:B:87:ARG:HH21	1.64	0.43
1:B:98:ARG:NH1	3:B:491:HOH:O	2.50	0.43
1:C:367:SER:HA	1:C:370:THR:HG22	1.99	0.43
1:C:96:ARG:HG3	1:C:96:ARG:NH1	2.33	0.43
1:D:96:ARG:NE	1:D:118:ARG:HH21	2.16	0.43
1:A:223:MSE:CB	1:A:224:PRO:HD2	2.49	0.43
1:B:217:ALA:C	1:B:219:GLY:N	2.69	0.43
1:B:403:THR:HG22	1:B:422:SER:C	2.39	0.43
1:C:82:TYR:C	1:C:82:TYR:HD2	2.19	0.43
1:D:248:LEU:HD21	1:D:325:ALA:HA	2.00	0.43
1:B:89:VAL:HG13	1:B:406:GLN:HE22	1.83	0.43
1:C:235:ARG:CG	1:C:235:ARG:NH1	2.78	0.43
1:A:172:ARG:NH2	1:D:162:ARG:HG2	2.33	0.43
1:A:96:ARG:HB3	1:A:118:ARG:CD	2.48	0.43
1:B:269:THR:CG2	1:B:270:ALA:H	2.30	0.43
1:B:346:GLY:HA3	1:B:390:ASN:O	2.19	0.43
1:C:96:ARG:HD3	1:C:118:ARG:NE	2.32	0.43
1:A:101:THR:N	1:A:111:VAL:O	2.48	0.43
1:A:408:MSE:HE2	1:A:419:GLU:HG2	2.00	0.43
1:A:84:GLU:HG2	1:A:87:ARG:HH11	1.77	0.43
1:A:98:ARG:CZ	1:A:145:VAL:HG12	2.48	0.43
1:B:188:ARG:O	1:B:241:TYR:HA	2.18	0.43
1:C:396:ARG:HD2	1:C:426:THR:CG2	2.49	0.43
1:D:202:GLN:NE2	1:D:214:VAL:HG23	2.34	0.43
1:C:99:ARG:HD3	1:C:408:MSE:CE	2.48	0.43
1:C:414:GLY:CA	1:C:431:GLN:OE1	2.67	0.43
1:B:152:LEU:HD22	1:B:159:GLU:HG3	2.01	0.43
1:C:311:LYS:HD2	1:C:323:VAL:O	2.19	0.43
1:C:376:LYS:CG	1:C:429:LEU:HD11	2.49	0.43
1:B:223:MSE:HG3	1:B:224:PRO:HD3	2.01	0.42
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.83	0.42
1:B:124:ARG:NH1	1:B:421:PHE:CE1	2.87	0.42
1:B:97:ASN:O	1:B:115:GLY:CA	2.67	0.42
1:D:189:TYR:HE2	1:D:402:ARG:HH22	1.65	0.42
1:B:207:GLY:N	1:C:206:GLU:OE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ARG:HD3	1:B:362:ALA:O	2.19	0.42
1:B:350:HIS:HB3	1:B:356:ALA:CB	2.49	0.42
1:C:200:GLY:O	1:C:201:ARG:CB	2.66	0.42
1:C:402:ARG:NH1	1:C:422:SER:CB	2.77	0.42
1:D:252:ARG:HB2	1:D:348:PHE:CE1	2.54	0.42
1:A:194:THR:HB	1:A:231:ARG:CZ	2.48	0.42
1:A:371:VAL:HG12	1:A:427:ASN:OD1	2.20	0.42
1:A:392:SER:OG	1:A:430:THR:CG2	2.67	0.42
1:B:268:HIS:CG	1:B:303:ARG:HD2	2.54	0.42
1:C:339:ASP:OD1	1:C:397:HIS:CD2	2.72	0.42
1:A:408:MSE:HE2	1:A:419:GLU:CD	2.40	0.42
1:B:371:VAL:HG12	1:B:427:ASN:HB2	2.01	0.42
1:C:231:ARG:NH1	1:C:231:ARG:HG2	2.35	0.42
1:C:359:ALA:O	1:C:363:LEU:HD22	2.20	0.42
1:C:339:ASP:OD1	1:C:397:HIS:HD2	2.02	0.42
1:C:85:GLU:HG2	1:C:407:LYS:HA	2.02	0.42
1:A:365:PRO:C	1:A:366:VAL:HG12	2.40	0.42
1:A:368:PRO:HG3	1:A:397:HIS:NE2	2.34	0.42
1:A:87:ARG:NH1	1:B:87:ARG:CD	2.81	0.42
1:B:308:PHE:HA	1:B:311:LYS:HB2	2.02	0.42
1:C:408:MSE:O	1:C:409:LEU:HD23	2.20	0.42
1:C:408:MSE:HG3	1:C:419:GLU:OE2	2.20	0.42
1:A:293:LEU:O	1:A:294:LEU:HD12	2.20	0.42
1:A:379:VAL:HG13	1:A:391:ILE:HG21	2.01	0.42
1:A:403:THR:O	1:A:403:THR:HG23	2.20	0.42
1:C:236:ALA:HB2	1:C:335:TYR:HD1	1.84	0.42
1:C:357:ILE:HG22	1:C:361:ILE:HD12	2.01	0.42
1:D:202:GLN:HB2	1:D:332:PHE:CE1	2.55	0.42
1:C:194:THR:HA	1:C:231:ARG:NH1	2.28	0.42
1:A:351:PHE:CA	1:A:352:ARG:HH11	2.32	0.42
1:B:235:ARG:HB2	1:B:335:TYR:CE1	2.55	0.42
1:B:321:ASP:HB3	1:B:323:VAL:O	2.20	0.42
1:B:383:LYS:CD	1:B:391:ILE:HD12	2.47	0.42
1:C:288:THR:HA	1:C:293:LEU:HA	2.02	0.42
1:C:347:ALA:O	1:C:385:ARG:NH2	2.53	0.42
1:A:248:LEU:HD23	1:A:304:ALA:CA	2.49	0.42
1:C:149:LEU:HD12	1:C:149:LEU:HA	1.76	0.42
1:C:171:LEU:HD13	1:C:171:LEU:C	2.40	0.42
1:C:382:ALA:HB3	1:C:391:ILE:HD13	2.02	0.42
1:D:222:LEU:C	1:D:223:MSE:HG2	2.39	0.42
1:D:266:THR:O	1:D:266:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:PHE:HE1	1:B:426:THR:CG2	2.19	0.42
1:B:78:LEU:HD23	1:B:79:ARG:H	1.79	0.42
1:C:184:ILE:HB	1:C:246:ALA:HB3	2.01	0.42
1:D:349:ALA:O	1:D:352:ARG:HG2	2.19	0.42
1:A:408:MSE:HG3	1:A:419:GLU:CG	2.43	0.41
1:C:398:LEU:HA	1:C:399:PRO:HD2	1.91	0.41
1:D:156:ASN:N	1:D:156:ASN:OD1	2.53	0.41
1:A:410:GLU:HA	1:A:416:ASN:O	2.20	0.41
1:A:83:ILE:C	1:A:85:GLU:H	2.23	0.41
1:B:235:ARG:HB2	1:B:335:TYR:CZ	2.55	0.41
1:D:371:VAL:O	1:D:374:ALA:HB3	2.19	0.41
1:A:96:ARG:HE	1:A:96:ARG:HB2	1.69	0.41
1:B:198:VAL:HG13	1:B:202:GLN:O	2.20	0.41
1:B:259:ARG:HD3	1:B:259:ARG:HA	1.77	0.41
1:B:382:ALA:HB1	1:B:387:VAL:HG11	2.01	0.41
1:C:248:LEU:HD12	1:C:303:ARG:HB3	2.02	0.41
1:C:83:ILE:CG2	1:C:83:ILE:O	2.62	0.41
1:D:367:SER:OG	1:D:370:THR:HG23	2.21	0.41
1:B:301:MSE:SE	1:B:304:ALA:HB2	2.71	0.41
1:C:121:PRO:O	1:C:122:GLU:C	2.59	0.41
1:C:243:ILE:CD1	1:C:340:ILE:HD11	2.50	0.41
1:D:114:GLU:OE2	1:D:124:ARG:HD2	2.20	0.41
1:D:141:LEU:N	1:D:141:LEU:HD22	2.35	0.41
1:A:98:ARG:NH2	1:A:112:VAL:HB	2.35	0.41
1:A:268:HIS:CB	1:A:303:ARG:HB3	2.50	0.41
1:A:408:MSE:C	1:A:409:LEU:HD12	2.41	0.41
1:C:351:PHE:HB3	1:C:356:ALA:HB3	2.03	0.41
1:C:361:ILE:HA	1:C:364:TYR:CD1	2.55	0.41
1:D:179:GLY:HA3	1:D:305:PHE:O	2.20	0.41
1:A:127:ALA:HA	1:A:183:LEU:O	2.21	0.41
1:B:387:VAL:HG13	1:B:391:ILE:HD11	2.02	0.41
1:B:372:LEU:CB	1:B:427:ASN:HD21	2.33	0.41
1:C:272:SER:HB3	1:C:275:GLU:HB2	2.02	0.41
1:A:221:PRO:HB2	1:A:223:MSE:HE1	1.97	0.41
1:B:392:SER:HA	1:B:429:LEU:O	2.20	0.41
1:A:352:ARG:HD2	1:A:352:ARG:H	1.82	0.41
1:A:78:LEU:HA	1:A:78:LEU:HD23	1.72	0.41
1:C:101:THR:HG21	1:C:428:GLU:HB2	2.02	0.41
1:D:123:THR:O	1:D:124:ARG:NH1	2.46	0.41
1:A:139:MSE:O	1:A:139:MSE:CE	2.66	0.41
1:B:222:LEU:HG	1:B:222:LEU:H	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:THR:HG23	1:C:111:VAL:HG13	2.03	0.41
1:C:248:LEU:CD1	1:C:303:ARG:HB3	2.51	0.41
1:D:231:ARG:CG	1:D:231:ARG:HH11	2.33	0.41
1:A:78:LEU:HD23	1:A:413:SER:OG	2.20	0.41
1:A:99:ARG:HD2	1:A:99:ARG:N	2.36	0.41
1:C:372:LEU:HD12	1:C:372:LEU:O	2.21	0.41
1:D:382:ALA:C	1:D:384:ARG:N	2.74	0.41
1:B:201:ARG:HG2	1:B:201:ARG:NH1	2.36	0.41
1:B:372:LEU:CB	1:B:427:ASN:ND2	2.83	0.41
1:B:428:GLU:CG	1:B:429:LEU:N	2.84	0.41
1:C:133:GLN:OE1	1:C:133:GLN:CA	2.69	0.41
1:C:218:LEU:O	1:C:354:HIS:HE1	2.04	0.41
1:C:403:THR:HG22	1:C:404:ARG:N	2.36	0.41
1:D:264:LEU:CD1	1:D:264:LEU:N	2.84	0.41
1:A:97:ASN:HB2	1:A:99:ARG:HH11	1.83	0.40
1:B:99:ARG:CG	1:B:99:ARG:HH11	2.34	0.40
1:C:190:GLU:O	1:C:190:GLU:HG2	2.21	0.40
1:D:114:GLU:CD	1:D:421:PHE:HE1	2.25	0.40
1:A:371:VAL:O	1:A:374:ALA:HB3	2.21	0.40
1:A:404:ARG:HA	1:A:404:ARG:HE	1.83	0.40
1:B:115:GLY:HA3	1:B:146:MSE:CE	2.50	0.40
1:B:289:VAL:HB	1:B:294:LEU:CD1	2.49	0.40
1:B:311:LYS:C	1:B:313:GLY:N	2.74	0.40
1:B:206:GLU:CB	1:C:206:GLU:OE2	2.69	0.40
1:D:122:GLU:HA	1:D:122:GLU:OE1	2.21	0.40
1:A:295:LEU:HD13	1:A:323:VAL:HG23	2.02	0.40
1:A:351:PHE:O	1:A:352:ARG:C	2.59	0.40
1:B:423:ILE:HG23	1:B:423:ILE:O	2.21	0.40
1:B:98:ARG:NH1	3:B:492:HOH:O	2.53	0.40
1:C:199:VAL:O	1:C:200:GLY:C	2.59	0.40
1:C:376:LYS:N	1:C:429:LEU:HD13	2.37	0.40
1:D:123:THR:HG22	1:D:124:ARG:N	2.36	0.40
1:D:428:GLU:CD	1:D:429:LEU:N	2.75	0.40
1:B:129:PHE:CE1	1:B:141:LEU:HB3	2.55	0.40
1:B:162:ARG:NH2	1:B:166:ARG:HH22	2.19	0.40
1:B:253:CYS:O	1:B:264:LEU:N	2.54	0.40
1:C:363:LEU:N	1:C:363:LEU:HD22	2.36	0.40
1:C:365:PRO:C	1:C:367:SER:N	2.71	0.40
1:C:394:PHE:HA	1:C:427:ASN:O	2.21	0.40
1:A:195:GLU:HA	1:A:228:MSE:O	2.21	0.40
1:C:293:LEU:N	1:C:293:LEU:CD2	2.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:LYS:HG2	1:C:387:VAL:HG11	2.04	0.40
1:C:430:THR:HG22	1:C:431:GLN:H	1.86	0.40
1:D:114:GLU:OE2	1:D:424:ASP:OD1	2.38	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	340/377 (90%)	302 (89%)	30 (9%)	8 (2%)	6 13
1	B	342/377 (91%)	299 (87%)	36 (10%)	7 (2%)	7 17
1	C	343/377 (91%)	298 (87%)	38 (11%)	7 (2%)	7 17
1	D	336/377 (89%)	296 (88%)	35 (10%)	5 (2%)	10 24
All	All	1361/1508 (90%)	1195 (88%)	139 (10%)	27 (2%)	7 17

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	A	220	GLY
1	A	413	SER
1	C	214	VAL
1	D	78	LEU
1	D	413	SER
1	A	119	GLY
1	B	200	GLY
1	B	313	GLY
1	B	349	ALA
1	B	413	SER
1	C	103	GLU

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Mol	Chain	Res	Type
1	C	178	GLY
1	A	365	PRO
1	B	178	GLY
1	B	314	GLY
1	B	175	ASN
1	C	201	ARG
1	D	108	ASP
1	D	374	ALA
1	A	205	PRO
1	A	307	SER
1	C	200	GLY
1	D	100	PRO
1	C	179	GLY
1	C	366	VAL
1	A	200	GLY

5.3.2 Protein sidechains (i)

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	280/295 (95%)	243 (87%)	37 (13%)	4 8
1	B	283/295 (96%)	246 (87%)	37 (13%)	4 9
1	C	285/295 (97%)	246 (86%)	39 (14%)	3 8
1	D	280/295 (95%)	245 (88%)	35 (12%)	4 10
All	All	1128/1180 (96%)	980 (87%)	148 (13%)	4 9

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	MSE
1	A	79	ARG
1	A	85	GLU
1	A	99	ARG
1	A	103	GLU
1	A	109	ASP

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Mol	Chain	Res	Type
1	A	112	VAL
1	A	135	ARG
1	A	156	ASN
1	A	171	LEU
1	A	175	ASN
1	A	192	LYS
1	A	199	VAL
1	A	218	LEU
1	A	223	MSE
1	A	224	PRO
1	A	259	ARG
1	A	285	VAL
1	A	290	ASN
1	A	305	PHE
1	A	307	SER
1	A	309	ASP
1	A	321	ASP
1	A	330	THR
1	A	350	HIS
1	A	352	ARG
1	A	363	LEU
1	A	373	ASP
1	A	381	ASN
1	A	384	ARG
1	A	387	VAL
1	A	388	THR
1	A	389	LYS
1	A	404	ARG
1	A	418	GLU
1	A	422	SER
1	A	427	ASN
1	B	76	MSE
1	B	81	LEU
1	B	83	ILE
1	B	87	ARG
1	B	102	SER
1	B	103	GLU
1	B	107	SER
1	B	108	ASP
1	B	116	MSE
1	B	117	LEU
1	B	124	ARG

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Mol	Chain	Res	Type
1	B	135	ARG
1	B	158	GLU
1	B	183	LEU
1	B	187	VAL
1	B	201	ARG
1	B	206	GLU
1	B	210	GLU
1	B	222	LEU
1	B	223	MSE
1	B	225	VAL
1	B	228	MSE
1	B	272	SER
1	B	317	LYS
1	B	318	LEU
1	B	326	VAL
1	B	354	HIS
1	B	384	ARG
1	B	389	LYS
1	B	402	ARG
1	B	413	SER
1	B	418	GLU
1	B	419	GLU
1	B	421	PHE
1	B	423	ILE
1	B	430	THR
1	B	431	GLN
1	C	79	ARG
1	C	82	TYR
1	C	85	GLU
1	C	94	THR
1	C	96	ARG
1	C	98	ARG
1	C	99	ARG
1	C	104	SER
1	C	111	VAL
1	C	114	GLU
1	C	122	GLU
1	C	132	PHE
1	C	133	GLN
1	C	149	LEU
1	C	158	GLU
1	C	183	LEU

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Mol	Chain	Res	Type
1	C	188	ARG
1	C	201	ARG
1	C	235	ARG
1	C	255	LEU
1	C	259	ARG
1	C	262	ILE
1	C	264	LEU
1	C	266	THR
1	C	269	THR
1	C	288	THR
1	C	298	VAL
1	C	311	LYS
1	C	320	GLN
1	C	339	ASP
1	C	354	HIS
1	C	369	GLU
1	C	390	ASN
1	C	404	ARG
1	C	413	SER
1	C	421	PHE
1	C	422	SER
1	C	423	ILE
1	C	429	LEU
1	D	79	ARG
1	D	92	SER
1	D	99	ARG
1	D	101	THR
1	D	111	VAL
1	D	112	VAL
1	D	113	VAL
1	D	149	LEU
1	D	152	LEU
1	D	171	LEU
1	D	188	ARG
1	D	198	VAL
1	D	201	ARG
1	D	206	GLU
1	D	210	GLU
1	D	218	LEU
1	D	222	LEU
1	D	231	ARG
1	D	232	ARG

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Mol	Chain	Res	Type
1	D	285	VAL
1	D	309	ASP
1	D	318	LEU
1	D	319	GLN
1	D	320	GLN
1	D	321	ASP
1	D	338	ASP
1	D	339	ASP
1	D	400	GLU
1	D	403	THR
1	D	406	GLN
1	D	416	ASN
1	D	419	GLU
1	D	425	ARG
1	D	427	ASN
1	D	431	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	133	GLN
1	A	136	HIS
1	A	156	ASN
1	A	163	GLN
1	A	175	ASN
1	A	229	ASN
1	A	273	HIS
1	A	280	GLN
1	A	290	ASN
1	A	406	GLN
1	B	144	ASN
1	B	156	ASN
1	B	175	ASN
1	B	280	GLN
1	B	381	ASN
1	B	390	ASN
1	B	406	GLN
1	C	143	GLN
1	C	147	ASN
1	C	163	GLN
1	C	202	GLN

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Mol	Chain	Res	Type
1	C	280	GLN
1	C	354	HIS
1	C	381	ASN
1	C	390	ASN
1	C	397	HIS
1	C	427	ASN
1	D	147	ASN
1	D	163	GLN
1	D	263	HIS
1	D	290	ASN
1	D	320	GLN
1	D	416	ASN
1	D	427	ASN
1	D	431	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	C	454	-	4,4,4	0.16	0	6,6,6	0.14	0
2	SO4	A	453	-	4,4,4	0.09	0	6,6,6	0.12	0
2	SO4	C	453	-	4,4,4	0.26	0	6,6,6	0.14	0
2	SO4	B	453	-	4,4,4	0.20	0	6,6,6	0.10	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	453	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^{th} 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	337/377 (89%)	0.24	13 (3%)	39	39	13, 32, 56, 75	0
1	B	339/377 (89%)	0.22	13 (3%)	40	40	9, 33, 51, 82	0
1	C	341/377 (90%)	0.24	18 (5%)	26	25	10, 29, 55, 65	0
1	D	336/377 (89%)	0.28	16 (4%)	30	29	14, 33, 58, 74	0
All	All	1353/1508 (89%)	0.24	60 (4%)	34	33	9, 32, 56, 82	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	432	ALA	5.1
1	C	78	LEU	4.9
1	D	95	SER	4.2
1	C	414	GLY	4.1
1	A	77	SER	4.0
1	D	317	LYS	4.0
1	B	427	ASN	3.9
1	D	352	ARG	3.8
1	C	82	TYR	3.6
1	C	429	LEU	3.6
1	C	427	ASN	3.6
1	B	82	TYR	3.6
1	A	384	ARG	3.5
1	D	232	ARG	3.4
1	B	77	SER	3.3
1	D	230	PHE	3.3
1	D	429	LEU	3.2
1	A	79	ARG	3.2
1	D	427	ASN	3.1
1	A	98	ARG	3.1
1	A	78	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	384	ARG	2.8
1	B	425	ARG	2.8
1	C	366	VAL	2.8
1	C	367	SER	2.7
1	B	314	GLY	2.7
1	A	387	VAL	2.7
1	A	81	LEU	2.7
1	B	413	SER	2.7
1	A	317	LYS	2.6
1	A	82	TYR	2.6
1	D	107	SER	2.6
1	C	213	SER	2.6
1	D	222	LEU	2.6
1	B	315	GLN	2.6
1	D	94	THR	2.5
1	C	77	SER	2.5
1	A	232	ARG	2.4
1	B	384	ARG	2.4
1	A	413	SER	2.4
1	D	413	SER	2.4
1	A	192	LYS	2.4
1	C	210	GLU	2.4
1	C	428	GLU	2.3
1	B	80	HIS	2.3
1	C	80	HIS	2.3
1	C	208	ALA	2.3
1	D	135	ARG	2.3
1	D	192	LYS	2.3
1	B	78	LEU	2.2
1	D	383	LYS	2.2
1	C	387	VAL	2.2
1	C	236	ALA	2.2
1	B	317	LYS	2.2
1	B	429	LEU	2.1
1	C	319	GLN	2.1
1	D	78	LEU	2.1
1	C	404	ARG	2.1
1	B	95	SER	2.1
1	A	352	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	SO4	C	453	5/5	0.89	0.18	82,82,82,83	0
2	SO4	C	454	5/5	0.94	0.17	61,62,62,63	0
2	SO4	B	453	5/5	0.94	0.18	60,61,62,63	0
2	SO4	A	453	5/5	0.97	0.16	38,39,41,42	0

6.5 Other polymers (i)

There are no such residues in this entry.