



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:50 AM UTC

PDB ID : 1VZ8 / pdb_00001vz8
Title : Ornithine Acetyltransferase (ORF6 Gene Product - Clavulanic Acid Biosynthesis) from Streptomyces clavuligerus (SeMet structure)
Authors : Elkins, J.M.; Kershaw, N.J.; Schofield, C.J.
Deposited on : 2004-05-14
Resolution : 2.75 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

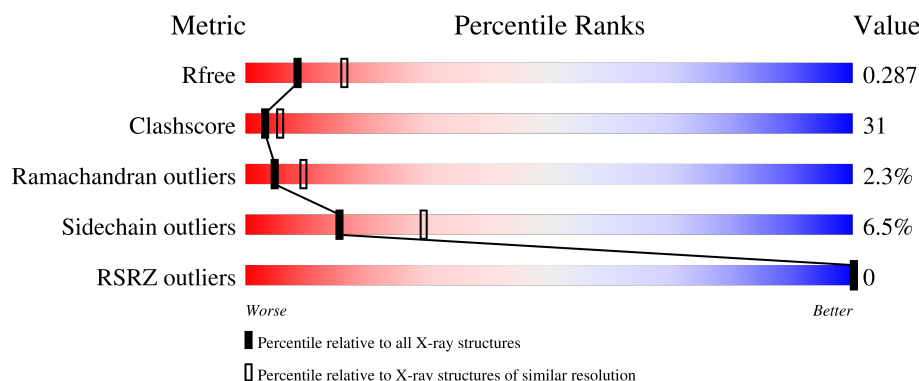
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 $\leq 5\%$. 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	393	
1	B	393	
1	C	393	
1	D	393	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10851 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 ORNITHINE ACETYL-TRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	Se	0	0	0
			2720	1694	482	533	4	7			
1	B	379	Total	C	N	O	S	Se	0	0	0
			2757	1715	485	546	4	7			
1	C	372	Total	C	N	O	S	Se	0	0	0
			2645	1652	464	518	4	7			
1	D	376	Total	C	N	O	S	Se	0	0	0
			2656	1659	469	517	4	7			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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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		

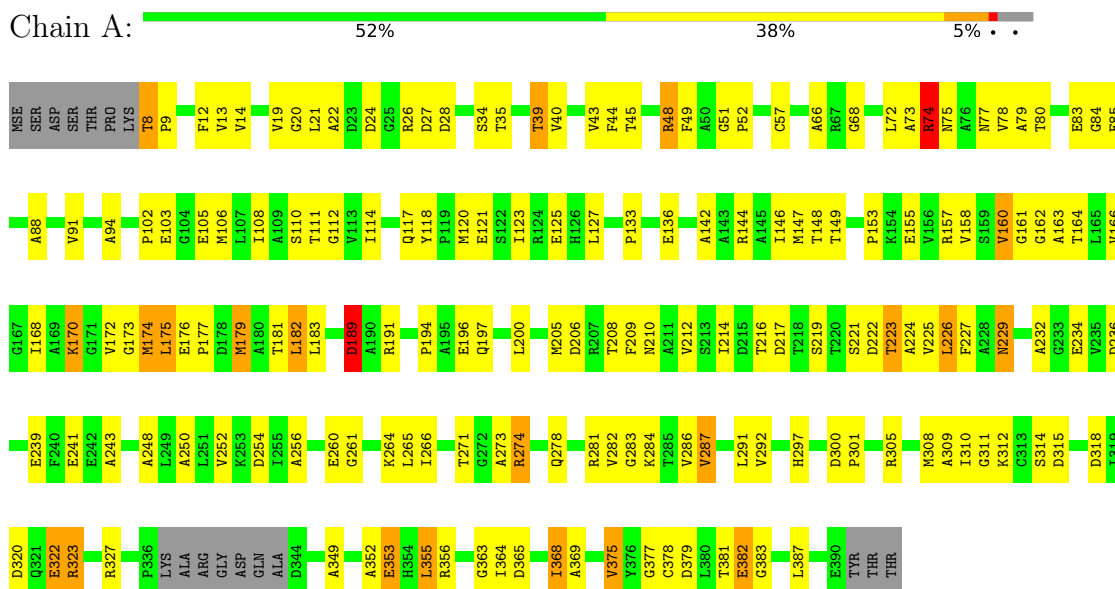
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	17	Total	O	0	0
			17	17		
3	C	7	Total	O	0	0
			7	7		
3	D	8	Total	O	0	0
			8	8		

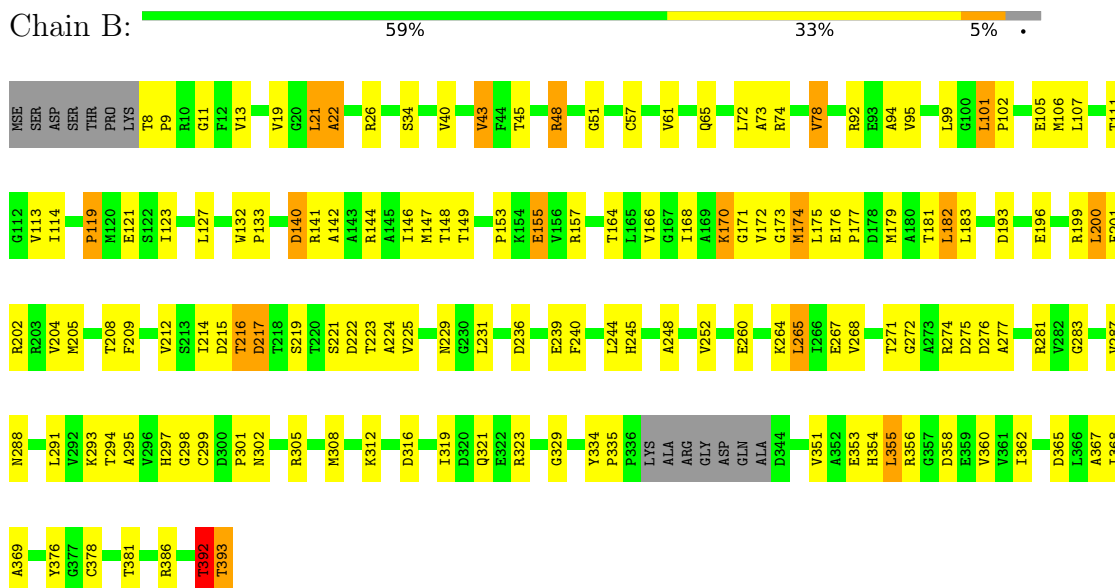
3 Residue-property plots

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: ORNITHINE ACETYL-TRANSFERASE

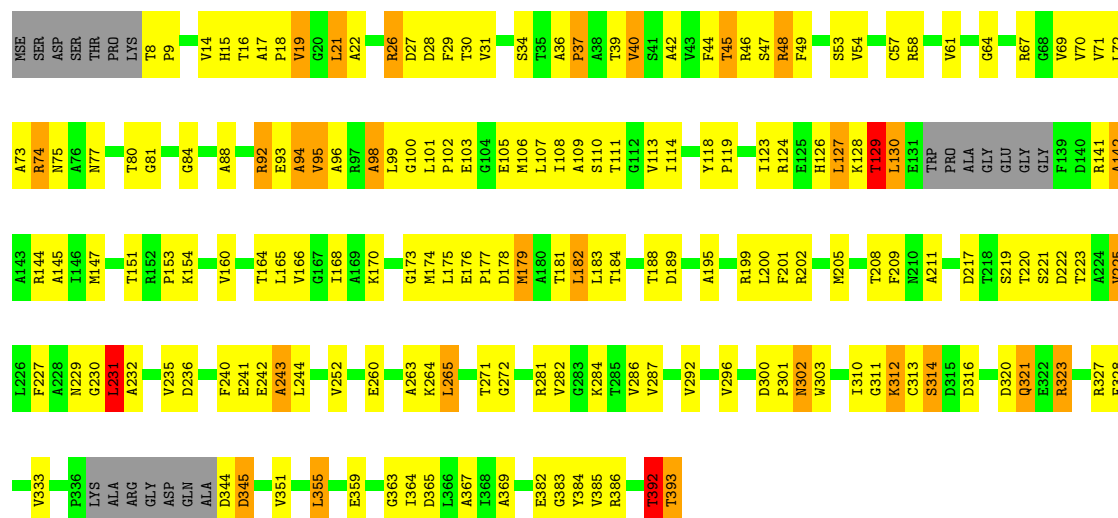


• Molecule 1: ORNITHINE ACETYL-TRANSFERASE

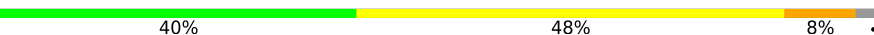


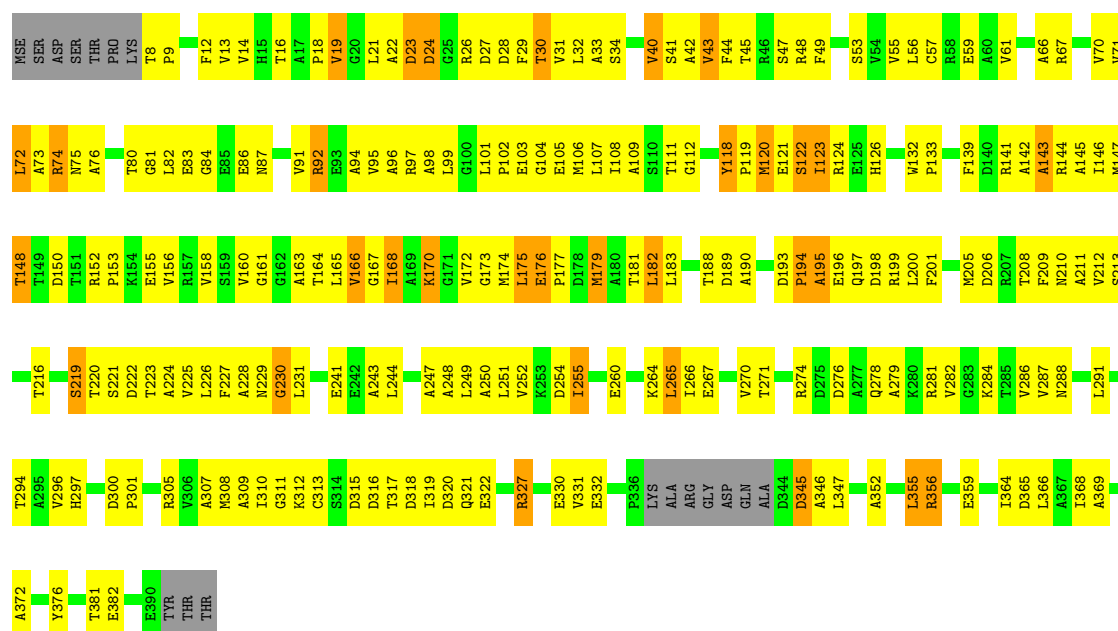
• Molecule 1: ORNITHINE ACETYL-TRANSFERASE

Chain C:  49% 37% 7% • 5%



• Molecule 1: ORNITHINE ACETYL-TRANSFERASE

Chain D:  40% 48% 8% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.79Å 180.19Å 73.33Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	23.67 – 2.75 23.67 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (23.67-2.75) 99.6 (23.67-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.288 0.235 , 0.287	Depositor DCC
R_{free} test set	2047 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 21.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.197 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10851	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 18.15% 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, 0.333 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	0.56	0/2750	1.07	16/3732 (0.4%)
1	B	0.56	0/2788	1.06	19/3783 (0.5%)
1	C	0.49	0/2672	1.04	18/3631 (0.5%)
1	D	0.48	0/2686	1.02	14/3653 (0.4%)
All	All	0.52	0/10896	1.05	67/14799 (0.5%)

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ASN	N-CA-C	-10.79	97.14	110.41
1	C	392	THR	N-CA-C	10.66	127.04	110.20
1	B	392	THR	N-CA-C	10.61	126.96	110.20
1	C	175	LEU	N-CA-C	8.85	123.01	107.61
1	C	142	ALA	N-CA-C	-7.90	102.60	111.14
1	A	21	LEU	N-CA-C	-7.74	103.94	113.15
1	C	292	VAL	N-CA-C	-7.46	103.52	110.53
1	B	175	LEU	N-CA-C	7.19	120.19	108.26
1	A	175	LEU	N-CA-C	7.00	119.91	107.80
1	D	255	ILE	N-CA-C	6.74	116.87	110.53
1	D	175	LEU	N-CA-C	6.70	119.39	108.26
1	B	225	VAL	N-CA-C	6.62	118.24	108.45
1	D	179	MSE	N-CA-C	6.55	120.73	110.32
1	A	174	MSE	N-CA-C	-6.44	102.50	111.52
1	C	179	MSE	N-CA-C	6.42	119.22	110.55
1	D	330	GLU	N-CA-C	-6.37	105.15	114.39
1	C	19	VAL	N-CA-C	-6.36	105.15	111.77
1	B	142	ALA	N-CA-C	-6.35	104.27	111.07
1	C	323	ARG	N-CA-C	-6.31	105.62	113.38
1	C	48	ARG	N-CA-C	-6.24	104.93	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	MSE	N-CA-C	6.08	117.88	110.41
1	B	132	TRP	CA-C-N	-6.06	114.03	120.03
1	B	132	TRP	C-N-CA	-6.06	114.03	120.03
1	A	48	ARG	N-CA-C	-6.00	105.93	113.18
1	D	120	MSE	N-CA-C	5.98	118.31	111.02
1	B	119	PRO	N-CA-C	-5.96	104.44	112.48
1	A	189	ASP	N-CA-C	-5.93	105.96	112.72
1	B	329	GLY	N-CA-C	-5.93	101.27	111.47
1	A	323	ARG	N-CA-C	-5.88	104.61	113.89
1	A	292	VAL	N-CA-C	-5.86	106.00	111.45
1	B	351	VAL	N-CA-C	-5.85	104.80	110.42
1	C	40	VAL	N-CA-C	5.79	116.97	107.24
1	B	40	VAL	N-CA-C	5.73	117.59	108.89
1	C	21	LEU	N-CA-C	-5.71	105.15	111.71
1	D	174	MSE	N-CA-C	-5.67	103.41	111.24
1	C	263	ALA	N-CA-C	-5.66	107.02	114.31
1	B	21	LEU	N-CA-C	-5.64	106.36	113.18
1	C	382	GLU	N-CA-C	-5.53	105.25	111.28
1	C	37	PRO	N-CA-C	-5.51	103.14	111.41
1	A	274	ARG	N-CA-C	-5.50	105.82	112.54
1	C	54	VAL	N-CA-C	5.48	115.68	110.42
1	A	368	ILE	N-CA-C	-5.41	107.34	111.62
1	C	312	LYS	N-CA-C	-5.40	106.69	113.28
1	A	308	MSE	N-CA-C	-5.39	104.64	111.11
1	B	219	SER	N-CA-C	5.34	117.43	110.43
1	B	174	MSE	N-CA-C	-5.33	103.89	111.24
1	D	228	ALA	N-CA-C	5.32	118.80	107.67
1	B	392	THR	CA-C-N	5.31	131.25	121.70
1	B	392	THR	C-N-CA	5.31	131.25	121.70
1	D	219	SER	N-CA-C	5.29	117.52	110.53
1	D	152	ARG	CA-C-N	5.28	125.28	119.89
1	D	152	ARG	C-N-CA	5.28	125.28	119.89
1	D	40	VAL	N-CA-C	5.26	116.80	109.55
1	B	48	ARG	N-CA-C	-5.23	106.16	112.54
1	B	217	ASP	N-CA-C	5.23	117.62	108.52
1	B	22	ALA	N-CA-C	-5.20	100.22	109.06
1	D	356	ARG	N-CA-C	-5.17	106.48	112.89
1	A	225	VAL	N-CA-C	5.15	116.07	108.45
1	D	220	THR	N-CA-C	-5.13	106.61	112.92
1	C	178	ASP	N-CA-C	-5.11	100.15	109.56
1	A	322	GLU	N-CA-C	5.11	119.00	112.26
1	D	313	CYS	N-CA-C	-5.09	101.30	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	392	THR	CA-C-N	5.08	130.85	121.70
1	C	392	THR	C-N-CA	5.08	130.85	121.70
1	B	199	ARG	N-CA-C	-5.07	105.66	111.14
1	A	40	VAL	N-CA-C	5.06	115.77	108.48
1	A	382	GLU	N-CA-C	-5.04	105.89	112.23

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	2720	0	2652	136	0
1	B	2757	0	2683	116	0
1	C	2645	0	2554	182	0
1	D	2656	0	2551	246	0
2	A	15	0	0	2	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
3	A	11	0	0	0	0
3	B	17	0	0	0	0
3	C	7	0	0	1	0
3	D	8	0	0	1	0
All	All	10851	0	10440	654	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 31.

All (654) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ARG:HA	1:B:147:MSE:HE2	1.38	1.04
1:C:174:MSE:HE2	1:D:308:MSE:HG3	1.39	1.00
1:C:16:THR:HG22	1:C:30:THR:HG23	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:ILE:HD11	1:D:364:ILE:HD13	1.48	0.93
1:D:31:VAL:HG22	1:D:70:VAL:HG23	1.51	0.92
1:A:174:MSE:HE2	1:B:308:MSE:HG3	1.54	0.89
1:D:301:PRO:HB3	1:D:355:LEU:HD13	1.56	0.88
1:C:392:THR:HG21	1:D:300:ASP:OD2	1.75	0.87
1:B:301:PRO:HB3	1:B:355:LEU:HD13	1.57	0.86
1:A:200:LEU:HD21	1:A:241:GLU:HA	1.56	0.86
1:C:124:ARG:HA	1:C:127:LEU:HD12	1.58	0.85
1:C:119:PRO:HD2	1:C:123:ILE:HD11	1.57	0.85
1:C:95:VAL:HG12	1:C:106:MSE:HE3	1.59	0.84
1:D:146:ILE:O	1:D:170:LYS:HG3	1.76	0.84
1:B:179:MSE:HE1	1:B:224:ALA:N	1.93	0.83
1:D:160:VAL:HG21	1:D:243:ALA:CB	2.07	0.83
1:C:14:VAL:HG11	1:C:142:ALA:HB2	1.58	0.83
1:B:144:ARG:CA	1:B:147:MSE:HE2	2.10	0.82
1:B:157:ARG:HG2	1:B:166:VAL:HG22	1.61	0.82
1:C:102:PRO:HG2	1:C:105:GLU:CB	2.09	0.81
1:A:8:THR:HB	1:A:164:THR:HG21	1.61	0.81
1:C:327:ARG:NH1	1:C:363:GLY:HA3	1.96	0.81
1:A:177:PRO:HG2	1:A:209:PHE:O	1.81	0.80
1:C:44:PHE:HA	1:C:179:MSE:HE2	1.61	0.80
1:C:113:VAL:HA	1:C:393:THR:HG21	1.64	0.80
1:A:66:ALA:HA	1:A:105:GLU:HG2	1.62	0.79
1:D:92:ARG:HD3	1:D:106:MSE:HB3	1.63	0.79
1:C:230:GLY:O	1:C:232:ALA:N	2.15	0.78
1:C:179:MSE:HE1	1:C:223:THR:CA	2.14	0.78
1:D:179:MSE:HE3	1:D:222:ASP:HB3	1.65	0.78
1:D:160:VAL:HG21	1:D:243:ALA:HB2	1.64	0.78
1:D:177:PRO:HG2	1:D:209:PHE:O	1.83	0.77
1:B:200:LEU:HD11	1:B:240:PHE:HD2	1.48	0.77
1:A:19:VAL:HG11	1:A:123:ILE:HG12	1.67	0.77
1:D:281:ARG:NH1	1:D:316:ASP:OD2	2.17	0.77
1:C:73:ALA:O	1:C:74:ARG:HB2	1.85	0.76
1:B:114:ILE:H	1:B:393:THR:HG21	1.51	0.76
1:B:301:PRO:HB3	1:B:355:LEU:CD1	2.16	0.76
1:B:19:VAL:HG11	1:B:123:ILE:HG12	1.68	0.76
1:B:43:VAL:O	1:B:179:MSE:HE2	1.86	0.75
1:B:193:ASP:OD2	1:B:196:GLU:HG3	1.86	0.75
1:A:300:ASP:OD2	1:B:392:THR:HG21	1.86	0.75
1:D:67:ARG:NE	1:D:101:LEU:HD21	2.01	0.75
1:C:70:VAL:HG13	1:C:108:ILE:HG13	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:THR:HG21	1:A:170:LYS:HE2	1.69	0.74
1:D:27:ASP:O	1:D:145:ALA:HA	1.87	0.74
1:C:179:MSE:HE1	1:C:223:THR:HA	1.69	0.74
1:C:9:PRO:HG3	1:C:166:VAL:HG21	1.70	0.74
1:A:73:ALA:O	1:A:74:ARG:HB2	1.86	0.73
1:C:177:PRO:HG2	1:C:209:PHE:O	1.87	0.73
1:A:39:THR:HG21	1:A:194:PRO:HG3	1.70	0.72
1:B:73:ALA:O	1:B:74:ARG:HB2	1.88	0.72
1:D:74:ARG:NH1	1:D:74:ARG:HG2	2.04	0.72
1:D:96:ALA:HB1	1:D:101:LEU:O	1.89	0.72
1:D:212:VAL:HG23	1:D:376:TYR:HB2	1.72	0.72
1:C:195:ALA:HB1	1:C:199:ARG:NH1	2.04	0.72
1:D:147:MSE:HE2	1:D:153:PRO:HB3	1.71	0.72
1:A:179:MSE:HE1	1:A:223:THR:C	2.14	0.71
1:D:74:ARG:HG2	1:D:74:ARG:HH11	1.55	0.71
1:D:327:ARG:CB	1:D:332:GLU:HA	2.21	0.71
1:A:200:LEU:HG	1:A:241:GLU:HB2	1.73	0.71
1:D:200:LEU:HD21	1:D:241:GLU:HA	1.72	0.70
1:D:87:ASN:OD1	1:D:120:MSE:HG3	1.91	0.70
1:D:56:LEU:HD12	1:D:108:ILE:HG21	1.71	0.70
1:D:318:ASP:OD2	1:D:368:ILE:HD13	1.91	0.70
1:B:8:THR:HB	1:B:164:THR:HG21	1.74	0.70
1:B:179:MSE:HE1	1:B:223:THR:C	2.15	0.70
1:D:16:THR:HG22	1:D:30:THR:HG23	1.72	0.70
1:D:34:SER:OG	1:D:229:ASN:ND2	2.25	0.69
1:A:14:VAL:HG11	1:A:142:ALA:HB2	1.74	0.69
1:D:72:LEU:HD12	1:D:72:LEU:N	2.07	0.69
1:A:301:PRO:HB3	1:A:355:LEU:HD13	1.73	0.69
1:B:148:THR:HG23	1:B:170:LYS:HE2	1.75	0.69
1:D:139:PHE:CD2	1:D:166:VAL:HG11	2.27	0.69
1:D:144:ARG:HA	1:D:147:MSE:HE2	1.75	0.68
1:C:31:VAL:HG11	1:C:99:LEU:HD11	1.74	0.68
1:A:44:PHE:HD2	1:A:223:THR:HG23	1.58	0.68
1:B:291:LEU:HB3	1:B:305:ARG:HD3	1.74	0.68
1:B:214:ILE:HG23	1:B:378:CYS:SG	2.34	0.68
1:D:301:PRO:HB3	1:D:355:LEU:CD1	2.24	0.68
1:C:128:LYS:O	1:C:129:THR:HG22	1.95	0.67
1:C:201:PHE:O	1:C:205:MSE:HG2	1.94	0.67
1:B:99:LEU:HB2	1:B:101:LEU:HD11	1.75	0.67
1:C:58:ARG:HG3	1:C:58:ARG:HH11	1.59	0.67
1:B:113:VAL:HA	1:B:393:THR:HG21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:MSE:HE3	1:D:222:ASP:C	2.19	0.67
1:D:265:LEU:HB3	1:D:359:GLU:HG2	1.77	0.67
1:D:16:THR:HG21	1:D:141:ARG:O	1.95	0.67
1:D:72:LEU:HD22	1:D:118:TYR:CZ	2.29	0.67
1:D:83:GLU:HG2	1:D:87:ASN:HD21	1.58	0.67
1:C:182:LEU:C	1:C:182:LEU:HD13	2.20	0.66
1:D:291:LEU:HB3	1:D:305:ARG:HD3	1.76	0.66
1:A:179:MSE:HE1	1:A:224:ALA:N	2.10	0.66
1:D:248:ALA:O	1:D:252:VAL:HG23	1.95	0.66
1:C:144:ARG:NH1	1:C:153:PRO:HG3	2.11	0.66
1:D:13:VAL:HB	1:D:133:PRO:HG2	1.78	0.66
1:B:177:PRO:HG2	1:B:209:PHE:O	1.95	0.66
1:D:265:LEU:C	1:D:265:LEU:HD23	2.22	0.65
1:C:119:PRO:CD	1:C:123:ILE:HD11	2.23	0.65
1:B:8:THR:N	1:B:9:PRO:HD2	2.11	0.65
1:D:14:VAL:HG11	1:D:142:ALA:HB2	1.79	0.65
1:B:172:VAL:O	1:B:260:GLU:HG3	1.96	0.65
1:C:320:ASP:HB3	1:C:323:ARG:HG3	1.79	0.65
1:D:22:ALA:O	1:D:24:ASP:N	2.28	0.65
1:B:13:VAL:HB	1:B:133:PRO:HG2	1.79	0.65
1:A:173:GLY:HA3	1:A:260:GLU:OE2	1.97	0.65
1:D:300:ASP:C	1:D:355:LEU:HD22	2.22	0.65
1:C:48:ARG:HB2	1:D:311:GLY:HA2	1.80	0.64
1:A:26:ARG:HD2	1:A:27:ASP:O	1.96	0.64
1:C:8:THR:N	1:C:9:PRO:CD	2.60	0.64
1:C:300:ASP:OD2	1:C:302:ASN:HB2	1.98	0.64
1:D:265:LEU:HD23	1:D:266:ILE:N	2.13	0.64
1:D:19:VAL:HG11	1:D:123:ILE:HG12	1.80	0.64
1:D:327:ARG:HB2	1:D:332:GLU:HA	1.79	0.64
1:A:83:GLU:HG2	1:A:117:GLN:OE1	1.97	0.64
1:A:310:ILE:HD11	1:A:364:ILE:HD13	1.80	0.64
1:C:195:ALA:HB1	1:C:199:ARG:HH12	1.60	0.64
1:D:67:ARG:CZ	1:D:101:LEU:HD21	2.28	0.64
1:D:119:PRO:O	1:D:122:SER:HB3	1.98	0.64
1:B:173:GLY:HA3	1:B:260:GLU:OE2	1.99	0.63
1:B:267:GLU:HG3	1:B:376:TYR:CE2	2.34	0.63
1:C:316:ASP:O	1:D:48:ARG:HD2	1.99	0.63
1:C:173:GLY:HA3	1:C:260:GLU:OE2	1.99	0.63
1:C:173:GLY:O	1:C:174:MSE:C	2.41	0.63
1:D:212:VAL:HG23	1:D:376:TYR:CB	2.28	0.62
1:B:99:LEU:HB2	1:B:101:LEU:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLU:O	1:C:96:ALA:HB3	1.99	0.62
1:A:20:GLY:C	1:A:22:ALA:H	2.08	0.62
1:D:226:LEU:HD12	1:D:227:PHE:H	1.63	0.62
1:A:191:ARG:HB3	1:A:234:GLU:HA	1.81	0.62
1:D:111:THR:OG1	1:D:170:LYS:HE3	2.00	0.61
1:C:301:PRO:HB3	1:C:355:LEU:HD13	1.81	0.61
1:B:268:VAL:HG22	1:B:362:ILE:HB	1.81	0.61
1:D:297:HIS:ND1	1:D:381:THR:HG22	2.15	0.61
1:C:284:LYS:HA	1:C:287:VAL:HG12	1.81	0.61
1:D:76:ALA:HB2	1:D:112:GLY:H	1.64	0.61
1:D:155:GLU:HG2	1:D:156:VAL:N	2.15	0.61
1:C:265:LEU:HD22	1:C:359:GLU:HG2	1.83	0.61
1:C:42:ALA:HB2	1:C:225:VAL:HG13	1.83	0.61
1:A:189:ASP:HB2	1:A:232:ALA:H	1.65	0.60
1:B:22:ALA:HB2	1:B:74:ARG:HG2	1.83	0.60
1:C:77:ASN:HD21	1:C:88:ALA:HB2	1.66	0.60
1:C:114:ILE:H	1:C:393:THR:HG21	1.67	0.60
1:D:155:GLU:HG2	1:D:156:VAL:H	1.67	0.60
1:A:181:THR:HG21	1:A:221:SER:HB2	1.83	0.60
1:C:22:ALA:HB2	1:C:74:ARG:HG2	1.83	0.60
1:A:8:THR:N	1:A:9:PRO:HD2	2.16	0.60
1:A:315:ASP:OD2	1:C:386:ARG:NH2	2.34	0.60
1:D:66:ALA:HA	1:D:105:GLU:HG2	1.82	0.60
1:D:83:GLU:O	1:D:87:ASN:ND2	2.34	0.60
1:C:114:ILE:N	1:C:393:THR:HG21	2.17	0.60
1:A:43:VAL:O	1:A:179:MSE:HE2	2.02	0.60
1:A:80:THR:OG1	1:A:84:GLY:HA3	2.02	0.60
1:A:381:THR:HB	2:A:1392:SO4:O2	2.02	0.60
1:C:111:THR:HB	1:C:183:LEU:HD11	1.84	0.60
1:D:156:VAL:O	1:D:166:VAL:HG22	2.02	0.60
1:D:179:MSE:HE3	1:D:222:ASP:CB	2.31	0.60
1:D:264:LYS:HD2	1:D:296:VAL:O	2.00	0.60
1:A:327:ARG:NH1	1:A:363:GLY:HA3	2.17	0.60
1:C:179:MSE:HE1	1:C:223:THR:N	2.16	0.60
1:D:173:GLY:HA3	1:D:260:GLU:OE2	2.01	0.60
1:A:383:GLY:O	1:A:387:LEU:HG	2.00	0.59
1:D:206:ASP:HA	1:D:210:ASN:HB2	1.84	0.59
1:A:274:ARG:NH1	1:A:318:ASP:CG	2.61	0.59
1:A:158:VAL:HG11	1:A:243:ALA:HB1	1.85	0.59
1:C:26:ARG:HH22	1:C:147:MSE:C	2.10	0.59
1:D:99:LEU:CA	1:D:132:TRP:HE1	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:ILE:CD1	1:D:364:ILE:HD13	2.28	0.59
1:B:229:ASN:OD1	1:B:229:ASN:O	2.20	0.58
1:C:205:MSE:HE2	1:C:205:MSE:HA	1.85	0.58
1:D:13:VAL:HG22	1:D:33:ALA:O	2.03	0.58
1:D:71:VAL:HG22	1:D:109:ALA:HB3	1.84	0.58
1:D:120:MSE:O	1:D:121:GLU:C	2.46	0.58
1:A:274:ARG:HH12	1:A:318:ASP:CG	2.10	0.58
1:C:80:THR:OG1	1:C:84:GLY:HA3	2.03	0.58
1:D:75:ASN:N	1:D:112:GLY:HA3	2.18	0.58
1:B:43:VAL:O	1:B:179:MSE:CE	2.52	0.58
1:A:176:GLU:OE1	1:A:216:THR:HA	2.03	0.58
1:C:69:VAL:HA	1:C:107:LEU:O	2.02	0.58
1:D:278:GLN:HG3	1:D:281:ARG:NH1	2.18	0.58
1:A:26:ARG:NH1	1:A:27:ASP:O	2.35	0.58
1:B:272:GLY:HA2	1:B:369:ALA:O	2.04	0.58
1:C:126:HIS:O	1:C:129:THR:HG23	2.03	0.58
1:B:140:ASP:OD2	1:B:140:ASP:N	2.32	0.58
1:D:278:GLN:HG3	1:D:281:ARG:HH12	1.69	0.58
1:B:144:ARG:HG2	1:B:147:MSE:HE2	1.86	0.58
1:B:334:TYR:HA	1:B:335:PRO:C	2.27	0.58
1:D:13:VAL:HB	1:D:133:PRO:CG	2.34	0.58
1:D:96:ALA:C	1:D:98:ALA:H	2.11	0.57
1:A:8:THR:N	1:A:9:PRO:CD	2.66	0.57
1:A:248:ALA:O	1:A:252:VAL:HG23	2.04	0.57
1:D:57:CYS:SG	1:D:107:LEU:HD22	2.45	0.57
1:A:19:VAL:HG12	1:A:19:VAL:O	2.05	0.57
1:A:45:THR:HB	1:A:222:ASP:HB2	1.86	0.57
1:C:129:THR:O	1:C:129:THR:OG1	2.22	0.57
1:C:58:ARG:HG3	1:C:58:ARG:NH1	2.19	0.57
1:D:99:LEU:HA	1:D:132:TRP:HE1	1.70	0.57
1:D:267:GLU:HG3	1:D:376:TYR:CE2	2.39	0.57
1:B:43:VAL:HG23	1:B:224:ALA:HB3	1.85	0.57
1:D:99:LEU:HA	1:D:132:TRP:NE1	2.19	0.57
1:D:165:LEU:HD13	1:D:188:THR:HB	1.86	0.57
1:A:52:PRO:HD2	1:A:77:ASN:O	2.05	0.56
1:A:191:ARG:NH1	2:A:1393:SO4:O3	2.38	0.56
1:B:265:LEU:HD23	1:B:265:LEU:C	2.29	0.56
1:C:231:LEU:HD23	1:C:231:LEU:H	1.70	0.56
1:D:21:LEU:HD13	1:D:73:ALA:O	2.05	0.56
1:C:164:THR:O	1:C:188:THR:HA	2.05	0.56
1:C:182:LEU:HD22	1:C:183:LEU:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:THR:HG21	1:C:221:SER:HB2	1.87	0.56
1:D:99:LEU:HB3	1:D:132:TRP:CE2	2.41	0.56
1:D:148:THR:HG21	2:D:1391:SO4:O4	2.05	0.56
1:D:182:LEU:HD22	1:D:183:LEU:N	2.21	0.56
1:D:200:LEU:HG	1:D:241:GLU:OE1	2.05	0.56
1:C:8:THR:HG22	1:C:8:THR:O	2.06	0.56
1:A:278:GLN:HG3	1:A:281:ARG:HH12	1.69	0.56
1:D:8:THR:HG22	1:D:164:THR:HG21	1.87	0.56
1:D:44:PHE:CE2	1:D:57:CYS:HB3	2.40	0.56
1:C:182:LEU:HD11	1:C:184:THR:HG22	1.88	0.56
1:D:19:VAL:CG1	1:D:123:ILE:HG12	2.35	0.56
1:D:99:LEU:HB3	1:D:132:TRP:CZ2	2.41	0.56
1:A:271:THR:O	1:A:365:ASP:HA	2.06	0.56
1:B:144:ARG:HG2	1:B:147:MSE:CE	2.35	0.56
1:C:113:VAL:HA	1:C:393:THR:CG2	2.33	0.56
1:D:91:VAL:O	1:D:95:VAL:HG23	2.05	0.56
1:B:94:ALA:HB1	1:B:127:LEU:HD22	1.88	0.55
1:A:282:VAL:O	1:A:286:VAL:HG23	2.06	0.55
1:C:229:ASN:CG	1:C:231:LEU:HG	2.31	0.55
1:B:202:ARG:HG3	1:B:202:ARG:HH11	1.71	0.55
1:D:83:GLU:HG2	1:D:87:ASN:ND2	2.21	0.55
1:A:9:PRO:HD3	1:A:166:VAL:CG2	2.37	0.55
1:A:68:GLY:HA3	1:A:106:MSE:HE1	1.89	0.55
1:D:47:SER:C	1:D:49:PHE:H	2.13	0.55
1:A:102:PRO:HG2	1:A:105:GLU:HB2	1.89	0.55
1:C:323:ARG:HG2	1:C:323:ARG:HH11	1.72	0.55
1:D:247:ALA:O	1:D:250:ALA:HB3	2.06	0.55
1:A:144:ARG:NH1	1:A:153:PRO:HG3	2.21	0.54
1:C:9:PRO:HA	1:C:164:THR:HB	1.89	0.54
1:C:170:LYS:HD3	1:C:170:LYS:C	2.32	0.54
1:C:271:THR:O	1:C:365:ASP:HA	2.07	0.54
1:A:160:VAL:O	1:A:163:ALA:N	2.40	0.54
1:C:321:GLN:HG3	1:D:49:PHE:CD2	2.42	0.54
1:D:318:ASP:OD2	1:D:368:ILE:HG21	2.06	0.54
1:A:318:ASP:OD2	1:A:368:ILE:HD13	2.07	0.54
1:B:281:ARG:NH1	1:B:316:ASP:OD2	2.41	0.54
1:B:95:VAL:HG12	1:B:106:MSE:HE3	1.89	0.54
1:B:111:THR:OG1	1:B:170:LYS:HE3	2.08	0.54
1:B:200:LEU:HD11	1:B:240:PHE:CD2	2.38	0.54
1:C:301:PRO:O	1:C:328:PHE:CE2	2.61	0.54
1:B:268:VAL:HG11	1:B:283:GLY:HA2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:THR:HG21	1:D:221:SER:HB2	1.89	0.54
1:D:179:MSE:CE	1:D:222:ASP:C	2.81	0.53
1:A:205:MSE:O	1:A:210:ASN:HB2	2.07	0.53
1:B:179:MSE:HE1	1:B:224:ALA:CB	2.38	0.53
1:C:310:ILE:HD11	1:C:364:ILE:HD13	1.89	0.53
1:D:271:THR:O	1:D:365:ASP:HA	2.09	0.53
1:A:44:PHE:CD2	1:A:223:THR:HG23	2.40	0.53
1:B:208:THR:HB	1:B:252:VAL:HG21	1.90	0.53
1:D:74:ARG:HH11	1:D:74:ARG:CG	2.21	0.53
1:C:303:TRP:HB3	1:C:333:VAL:HG21	1.89	0.53
1:D:209:PHE:C	1:D:211:ALA:H	2.16	0.53
1:D:8:THR:N	1:D:9:PRO:HD2	2.24	0.53
1:D:19:VAL:HB	1:D:29:PHE:HB2	1.90	0.53
1:D:307:ALA:O	1:D:308:MSE:C	2.52	0.53
1:A:297:HIS:HB2	1:A:379:ASP:HB2	1.90	0.52
1:C:311:GLY:HA2	1:D:48:ARG:HB2	1.91	0.52
1:D:53:SER:HB3	1:D:108:ILE:O	2.09	0.52
1:D:319:ILE:HD11	1:D:366:LEU:HD13	1.91	0.52
1:D:179:MSE:HE1	1:D:223:THR:C	2.33	0.52
1:D:225:VAL:HG12	1:D:226:LEU:N	2.23	0.52
1:B:295:ALA:HB2	1:B:305:ARG:NH1	2.24	0.52
1:C:272:GLY:HA2	1:C:369:ALA:O	2.09	0.52
1:B:353:GLU:OE2	1:B:356:ARG:NH1	2.43	0.52
1:C:71:VAL:HA	1:C:109:ALA:O	2.10	0.52
1:C:128:LYS:C	1:C:129:THR:CG2	2.83	0.52
1:C:386:ARG:NH1	1:D:382:GLU:OE1	2.42	0.52
1:A:85:GLU:O	1:A:88:ALA:HB3	2.09	0.52
1:B:113:VAL:HA	1:B:393:THR:CG2	2.39	0.52
1:A:13:VAL:HG12	1:A:136:GLU:HA	1.91	0.52
1:B:114:ILE:N	1:B:393:THR:HG21	2.23	0.52
1:C:265:LEU:C	1:C:265:LEU:HD23	2.35	0.52
1:D:19:VAL:HG21	1:D:29:PHE:CD1	2.45	0.52
1:B:301:PRO:CB	1:B:355:LEU:HD13	2.35	0.52
1:C:235:VAL:HG12	1:C:236:ASP:N	2.24	0.52
1:C:264:LYS:HD2	1:C:296:VAL:O	2.10	0.52
1:C:208:THR:OG1	1:C:209:PHE:N	2.43	0.51
1:D:9:PRO:HB3	1:D:164:THR:HG22	1.91	0.51
1:D:66:ALA:HA	1:D:105:GLU:CB	2.40	0.51
1:D:345:ASP:O	1:D:347:LEU:N	2.43	0.51
1:B:182:LEU:HD22	1:B:183:LEU:N	2.25	0.51
1:C:217:ASP:OD2	1:D:291:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ASP:HA	1:D:145:ALA:O	2.09	0.51
1:A:320:ASP:HB3	1:A:323:ARG:HD3	1.92	0.51
1:D:12:PHE:CE1	1:D:34:SER:HB2	2.45	0.51
1:D:72:LEU:HB2	1:D:118:TYR:OH	2.11	0.51
1:D:172:VAL:O	1:D:260:GLU:HG3	2.10	0.51
1:D:274:ARG:HA	1:D:369:ALA:HB3	1.91	0.51
1:D:181:THR:CG2	1:D:221:SER:HB2	2.40	0.51
1:D:247:ALA:O	1:D:251:LEU:HD12	2.10	0.51
1:D:327:ARG:HH11	1:D:327:ARG:HG2	1.74	0.51
1:B:19:VAL:HG11	1:B:123:ILE:CG1	2.40	0.51
1:C:17:ALA:HA	1:C:27:ASP:OD1	2.10	0.51
1:C:160:VAL:HG21	1:C:243:ALA:CB	2.40	0.51
1:D:96:ALA:O	1:D:98:ALA:N	2.41	0.51
1:D:251:LEU:HD12	1:D:251:LEU:H	1.76	0.51
1:D:315:ASP:O	1:D:317:THR:HG23	2.10	0.51
1:C:19:VAL:CG1	1:C:123:ILE:HA	2.41	0.51
1:C:282:VAL:O	1:C:286:VAL:HG23	2.11	0.51
1:C:179:MSE:CE	1:C:222:ASP:C	2.84	0.51
1:D:70:VAL:HG13	1:D:70:VAL:O	2.11	0.51
1:A:155:GLU:HG3	1:A:168:ILE:HG22	1.92	0.51
1:C:75:ASN:O	1:C:110:SER:OG	2.28	0.51
1:A:206:ASP:HA	1:A:210:ASN:HB2	1.93	0.51
1:C:47:SER:HA	1:D:311:GLY:O	2.11	0.51
1:A:48:ARG:NH1	1:B:319:ILE:O	2.44	0.50
1:A:311:GLY:HA2	1:B:48:ARG:HB2	1.93	0.50
1:A:8:THR:OG1	1:A:157:ARG:HD3	2.12	0.50
1:D:212:VAL:HB	1:D:252:VAL:HG13	1.92	0.50
1:D:139:PHE:CE2	1:D:166:VAL:HG11	2.46	0.50
1:A:229:ASN:C	1:A:229:ASN:OD1	2.55	0.50
1:D:80:THR:OG1	1:D:84:GLY:HA3	2.12	0.50
1:D:216:THR:HG22	1:D:288:ASN:CG	2.36	0.50
1:A:77:ASN:HB2	1:A:118:TYR:CE1	2.47	0.50
1:A:91:VAL:HG23	1:A:120:MSE:HE1	1.94	0.50
1:A:327:ARG:CZ	1:A:363:GLY:HA3	2.42	0.50
1:D:12:PHE:HE2	1:D:188:THR:O	1.95	0.50
1:D:43:VAL:HG23	1:D:224:ALA:HB3	1.93	0.50
1:D:66:ALA:HA	1:D:105:GLU:HA	1.93	0.50
1:C:70:VAL:HG13	1:C:70:VAL:O	2.11	0.50
1:A:9:PRO:HD3	1:A:166:VAL:HG23	1.93	0.49
1:A:179:MSE:HE3	1:A:222:ASP:C	2.36	0.49
1:A:200:LEU:CD2	1:A:241:GLU:HA	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ILE:O	1:B:170:LYS:HG3	2.11	0.49
1:C:281:ARG:NH1	1:C:316:ASP:OD2	2.45	0.49
1:D:276:ASP:O	1:D:279:ALA:HB3	2.12	0.49
1:A:175:LEU:HD22	1:A:214:ILE:HG12	1.94	0.49
1:C:241:GLU:C	1:C:243:ALA:N	2.67	0.49
1:B:295:ALA:HB2	1:B:305:ARG:HH11	1.76	0.49
1:C:19:VAL:HG12	1:C:19:VAL:O	2.12	0.49
1:C:92:ARG:HD2	1:C:92:ARG:C	2.38	0.49
1:D:229:ASN:O	1:D:231:LEU:N	2.37	0.49
1:D:309:ALA:O	1:D:312:LYS:HB2	2.12	0.49
1:B:291:LEU:HD12	1:B:308:MSE:HE2	1.93	0.49
1:C:16:THR:HA	1:C:29:PHE:O	2.13	0.49
1:C:385:VAL:HG11	1:D:381:THR:HA	1.95	0.49
1:B:94:ALA:CB	1:B:127:LEU:HD22	2.42	0.49
1:C:200:LEU:HD12	1:C:241:GLU:OE1	2.11	0.49
1:D:16:THR:CG2	1:D:142:ALA:HA	2.43	0.49
1:D:16:THR:CG2	1:D:30:THR:HG23	2.42	0.49
1:D:249:LEU:O	1:D:249:LEU:HG	2.13	0.49
1:A:217:ASP:HA	1:B:312:LYS:HD3	1.93	0.49
1:B:13:VAL:HB	1:B:133:PRO:CG	2.43	0.49
1:A:78:VAL:O	1:A:79:ALA:HB3	2.12	0.49
1:C:177:PRO:HB2	1:C:179:MSE:HG3	1.93	0.49
1:D:327:ARG:HB2	1:D:331:VAL:O	2.11	0.49
1:A:320:ASP:CB	1:A:323:ARG:HD3	2.41	0.49
1:C:94:ALA:O	1:C:96:ALA:N	2.46	0.49
1:D:229:ASN:O	1:D:229:ASN:OD1	2.30	0.49
1:A:273:ALA:O	1:A:369:ALA:HB3	2.12	0.49
1:C:48:ARG:NH1	1:D:317:THR:HA	2.28	0.49
1:C:323:ARG:HB3	1:C:367:ALA:HB3	1.94	0.49
1:A:291:LEU:O	1:A:305:ARG:HD3	2.12	0.49
1:C:179:MSE:HE3	1:C:222:ASP:C	2.38	0.49
1:D:16:THR:OG1	1:D:141:ARG:NH1	2.46	0.49
1:A:196:GLU:O	1:A:197:GLN:C	2.56	0.48
1:D:47:SER:C	1:D:49:PHE:N	2.71	0.48
1:D:176:GLU:O	1:D:176:GLU:HG3	2.13	0.48
1:A:114:ILE:CD1	1:A:174:MSE:HE1	2.43	0.48
1:A:172:VAL:HG23	1:A:260:GLU:HG2	1.94	0.48
1:D:144:ARG:HA	1:D:147:MSE:CE	2.43	0.48
1:A:57:CYS:SG	1:A:108:ILE:O	2.71	0.48
1:C:36:ALA:HB1	1:C:37:PRO:CD	2.43	0.48
1:D:99:LEU:CA	1:D:132:TRP:NE1	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:PHE:CG	1:D:166:VAL:HG11	2.48	0.48
1:B:57:CYS:O	1:B:61:VAL:HG22	2.13	0.48
1:C:22:ALA:HB3	1:C:74:ARG:NH1	2.29	0.48
1:C:101:LEU:HD22	1:C:102:PRO:HD2	1.95	0.48
1:C:240:PHE:O	1:C:243:ALA:HB3	2.13	0.48
1:D:9:PRO:CG	1:D:139:PHE:HE2	2.26	0.48
1:B:248:ALA:O	1:B:252:VAL:HG23	2.13	0.48
1:C:301:PRO:N	1:C:355:LEU:HD22	2.29	0.48
1:C:181:THR:HG23	1:C:219:SER:OG	2.13	0.48
1:C:72:LEU:HD13	1:C:118:TYR:OH	2.13	0.48
1:A:320:ASP:OD1	1:A:322:GLU:HG2	2.13	0.48
1:B:8:THR:N	1:B:9:PRO:CD	2.76	0.48
1:B:148:THR:OG1	1:B:149:THR:N	2.46	0.48
1:D:22:ALA:O	1:D:23:ASP:C	2.57	0.48
1:A:349:ALA:O	1:A:353:GLU:HB2	2.13	0.47
1:C:107:LEU:HD12	1:C:227:PHE:CZ	2.49	0.47
1:D:73:ALA:O	1:D:74:ARG:HB2	2.13	0.47
1:D:123:ILE:O	1:D:126:HIS:N	2.47	0.47
1:B:21:LEU:HD23	1:B:119:PRO:CD	2.44	0.47
1:C:229:ASN:OD1	1:C:231:LEU:HG	2.14	0.47
1:A:172:VAL:O	1:A:260:GLU:HG3	2.14	0.47
1:A:172:VAL:HG23	1:A:260:GLU:CG	2.44	0.47
1:D:123:ILE:O	1:D:124:ARG:C	2.56	0.47
1:D:193:ASP:O	1:D:194:PRO:C	2.58	0.47
1:C:28:ASP:N	1:C:28:ASP:OD1	2.47	0.47
1:C:113:VAL:CA	1:C:393:THR:HG21	2.42	0.47
1:C:202:ARG:HG3	1:C:202:ARG:HH11	1.80	0.47
1:C:124:ARG:CA	1:C:127:LEU:HD12	2.38	0.47
1:A:13:VAL:HB	1:A:133:PRO:HG2	1.96	0.47
1:A:123:ILE:HG22	1:A:127:LEU:HD12	1.94	0.47
1:A:236:ASP:HB3	1:A:239:GLU:HG3	1.97	0.47
1:B:19:VAL:HG12	1:B:19:VAL:O	2.14	0.47
1:C:168:ILE:HG13	1:C:168:ILE:O	2.14	0.47
1:D:73:ALA:C	1:D:74:ARG:HD3	2.39	0.47
1:D:194:PRO:O	1:D:197:GLN:HB3	2.14	0.47
1:A:181:THR:HG23	1:A:219:SER:OG	2.15	0.47
1:A:278:GLN:HG3	1:A:281:ARG:NH1	2.29	0.47
1:C:9:PRO:HG3	1:C:166:VAL:CG2	2.43	0.47
1:C:15:HIS:HB3	1:C:31:VAL:HB	1.95	0.47
1:C:18:PRO:HA	1:C:28:ASP:OD1	2.15	0.47
1:D:45:THR:HB	1:D:222:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:VAL:HG21	1:D:319:ILE:HD11	1.95	0.47
1:C:300:ASP:C	1:C:355:LEU:HD22	2.40	0.47
1:D:108:ILE:O	1:D:108:ILE:HG23	2.14	0.47
1:D:165:LEU:HD21	1:D:244:LEU:HD13	1.96	0.47
1:D:284:LYS:HA	1:D:287:VAL:HG12	1.97	0.47
1:B:204:VAL:HG21	1:B:244:LEU:HD23	1.97	0.47
1:C:95:VAL:O	1:C:98:ALA:HB3	2.15	0.47
1:C:264:LYS:NZ	1:C:355:LEU:O	2.41	0.47
1:D:190:ALA:C	1:D:230:GLY:HA2	2.39	0.47
1:A:170:LYS:C	1:A:170:LYS:HD3	2.40	0.46
1:A:256:ALA:HB1	1:A:377:GLY:O	2.15	0.46
1:D:198:ASP:C	1:D:200:LEU:N	2.71	0.46
1:A:168:ILE:O	1:A:168:ILE:HG13	2.14	0.46
1:A:309:ALA:O	1:A:312:LYS:HG3	2.15	0.46
1:C:241:GLU:O	1:C:242:GLU:C	2.58	0.46
1:D:208:THR:HG21	1:D:248:ALA:HB3	1.96	0.46
1:A:28:ASP:OD1	1:A:28:ASP:N	2.49	0.46
1:C:19:VAL:HG23	1:C:29:PHE:HB2	1.95	0.46
1:C:111:THR:HG21	1:C:170:LYS:HE2	1.97	0.46
1:D:55:VAL:O	1:D:59:GLU:HG3	2.15	0.46
1:D:163:ALA:CB	1:D:190:ALA:HB2	2.45	0.46
1:C:49:PHE:CD2	1:D:321:GLN:HG3	2.51	0.46
1:B:170:LYS:HG2	1:B:171:GLY:N	2.31	0.46
1:C:208:THR:HB	1:C:252:VAL:HG21	1.97	0.46
1:D:179:MSE:CE	1:D:223:THR:N	2.79	0.46
1:B:182:LEU:HD22	1:B:182:LEU:C	2.41	0.46
1:C:300:ASP:C	1:C:302:ASN:H	2.22	0.46
1:D:265:LEU:C	1:D:265:LEU:CD2	2.88	0.46
1:C:92:ARG:C	1:C:92:ARG:CD	2.89	0.46
1:D:42:ALA:HB3	1:D:61:VAL:HG21	1.98	0.46
1:D:66:ALA:HA	1:D:105:GLU:CG	2.46	0.46
1:D:270:VAL:HG11	1:D:279:ALA:HA	1.96	0.46
1:A:142:ALA:O	1:A:146:ILE:HG23	2.16	0.46
1:A:160:VAL:O	1:A:162:GLY:N	2.48	0.46
1:D:291:LEU:HD12	1:D:308:MSE:HE2	1.96	0.46
1:A:12:PHE:CE1	1:A:34:SER:HB2	2.50	0.46
1:C:57:CYS:O	1:C:61:VAL:HG22	2.16	0.46
1:C:221:SER:HB3	3:C:2003:HOH:O	2.15	0.46
1:D:44:PHE:N	1:D:44:PHE:CD1	2.83	0.46
1:D:282:VAL:O	1:D:286:VAL:HG23	2.16	0.46
1:B:179:MSE:CE	1:B:224:ALA:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:LEU:CD2	1:D:102:PRO:HD2	2.46	0.45
1:D:327:ARG:HB3	1:D:332:GLU:HA	1.97	0.45
1:D:103:GLU:C	1:D:105:GLU:H	2.24	0.45
1:A:312:LYS:O	1:A:314:SER:N	2.48	0.45
1:B:323:ARG:HB3	1:B:367:ALA:HB3	1.97	0.45
1:D:12:PHE:HE1	1:D:34:SER:HB2	1.81	0.45
1:B:297:HIS:ND1	1:B:381:THR:HG22	2.31	0.45
1:C:26:ARG:HB3	1:C:74:ARG:HH22	1.82	0.45
1:C:102:PRO:O	1:C:103:GLU:C	2.60	0.45
1:A:200:LEU:HD21	1:A:241:GLU:CA	2.37	0.45
1:A:284:LYS:O	1:A:287:VAL:HG12	2.16	0.45
1:D:92:ARG:NE	1:D:106:MSE:O	2.49	0.45
1:D:182:LEU:HB3	1:D:222:ASP:OD1	2.16	0.45
1:A:208:THR:HB	1:A:252:VAL:HG21	1.99	0.45
1:A:274:ARG:NH1	1:A:318:ASP:OD2	2.50	0.45
1:C:27:ASP:HB3	1:C:145:ALA:HB2	1.98	0.45
1:D:179:MSE:HE1	1:D:223:THR:CA	2.47	0.45
1:D:101:LEU:HD23	1:D:102:PRO:HD2	1.99	0.45
1:D:271:THR:HA	1:D:372:ALA:HB2	1.99	0.45
1:A:261:GLY:O	1:A:381:THR:HG21	2.17	0.45
1:B:144:ARG:HG3	1:B:144:ARG:HH11	1.81	0.45
1:D:8:THR:N	1:D:9:PRO:CD	2.80	0.45
1:B:11:GLY:O	1:B:34:SER:HA	2.16	0.45
1:C:94:ALA:O	1:C:95:VAL:C	2.59	0.45
1:D:16:THR:HG21	1:D:141:ARG:C	2.42	0.45
1:D:179:MSE:HE1	1:D:223:THR:N	2.32	0.45
1:D:297:HIS:CE1	1:D:381:THR:HG22	2.52	0.45
1:A:250:ALA:O	1:A:254:ASP:OD1	2.34	0.44
1:C:73:ALA:O	1:C:74:ARG:HD3	2.17	0.44
1:D:175:LEU:C	1:D:175:LEU:HD23	2.42	0.44
1:B:73:ALA:O	1:B:74:ARG:CB	2.63	0.44
1:C:45:THR:HB	1:C:222:ASP:HB2	1.98	0.44
1:C:209:PHE:C	1:C:211:ALA:H	2.24	0.44
1:D:146:ILE:O	1:D:170:LYS:CG	2.58	0.44
1:A:20:GLY:C	1:A:22:ALA:N	2.73	0.44
1:B:204:VAL:HG13	1:B:245:HIS:HA	2.00	0.44
1:C:70:VAL:HG21	1:C:95:VAL:HG21	1.99	0.44
1:D:160:VAL:CG2	1:D:243:ALA:HB2	2.42	0.44
1:B:22:ALA:HB3	1:B:74:ARG:NH1	2.33	0.44
1:D:96:ALA:C	1:D:98:ALA:N	2.76	0.44
1:A:208:THR:C	1:A:252:VAL:HG21	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:HB3	1:B:74:ARG:NH2	2.32	0.44
1:B:102:PRO:HG2	1:B:105:GLU:HB2	1.98	0.44
1:C:320:ASP:HB3	1:C:323:ARG:CG	2.47	0.44
1:D:87:ASN:OD1	1:D:120:MSE:HE2	2.18	0.44
1:A:300:ASP:C	1:A:355:LEU:HD22	2.43	0.44
1:B:354:HIS:NE2	1:B:360:VAL:HA	2.32	0.44
1:A:182:LEU:O	1:A:182:LEU:HD13	2.17	0.44
1:A:352:ALA:O	1:A:356:ARG:HG3	2.17	0.44
1:B:78:VAL:HG12	1:B:114:ILE:HG23	1.98	0.44
1:D:40:VAL:HG22	1:D:41:SER:N	2.33	0.44
1:A:181:THR:CG2	1:A:221:SER:HB2	2.47	0.44
1:B:141:ARG:H	1:B:141:ARG:HG2	1.69	0.44
1:C:34:SER:OG	1:C:229:ASN:ND2	2.42	0.44
1:D:76:ALA:HB2	1:D:112:GLY:N	2.30	0.44
1:D:156:VAL:HG12	1:D:167:GLY:O	2.18	0.44
1:A:102:PRO:O	1:A:103:GLU:C	2.60	0.44
1:C:128:LYS:C	1:C:129:THR:HG22	2.42	0.43
1:C:165:LEU:HD21	1:C:244:LEU:HA	1.99	0.43
1:D:18:PRO:HA	1:D:26:ARG:O	2.18	0.43
1:D:42:ALA:HB1	1:D:44:PHE:CZ	2.52	0.43
1:D:143:ALA:HB2	1:D:168:ILE:HG22	1.99	0.43
1:B:144:ARG:CZ	1:B:153:PRO:HG3	2.49	0.43
1:B:173:GLY:O	1:B:174:MSE:C	2.61	0.43
1:C:14:VAL:CG1	1:C:142:ALA:HB2	2.39	0.43
1:B:236:ASP:HB3	1:B:239:GLU:OE1	2.17	0.43
1:D:32:LEU:HD11	1:D:139:PHE:CE1	2.53	0.43
1:D:71:VAL:C	1:D:72:LEU:HD12	2.43	0.43
1:D:198:ASP:O	1:D:199:ARG:C	2.61	0.43
1:B:216:THR:HG22	1:B:288:ASN:CG	2.44	0.43
1:C:118:TYR:HB3	1:C:123:ILE:CD1	2.47	0.43
1:D:82:LEU:O	1:D:86:GLU:HG3	2.18	0.43
1:D:163:ALA:HA	1:D:189:ASP:OD1	2.18	0.43
1:D:319:ILE:CD1	1:D:366:LEU:HD13	2.48	0.43
1:C:14:VAL:O	1:C:141:ARG:NH2	2.52	0.43
1:C:18:PRO:HD3	1:C:27:ASP:OD1	2.19	0.43
1:D:111:THR:CB	1:D:170:LYS:HE3	2.48	0.43
1:D:176:GLU:O	1:D:176:GLU:CG	2.66	0.43
1:D:201:PHE:CE1	1:D:205:MSE:HE3	2.52	0.43
1:A:144:ARG:O	1:A:147:MSE:HE2	2.19	0.43
1:D:267:GLU:OE1	1:D:376:TYR:HE2	2.01	0.43
1:B:212:VAL:HB	1:B:252:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ARG:HD3	1:D:319:ILE:O	2.19	0.43
1:D:158:VAL:HG12	1:D:160:VAL:HG23	2.01	0.43
1:B:45:THR:HB	1:B:222:ASP:HB2	2.00	0.43
1:C:108:ILE:O	1:C:108:ILE:HG23	2.18	0.43
1:C:129:THR:C	1:C:130:LEU:HD23	2.44	0.43
1:D:251:LEU:HA	1:D:254:ASP:HB2	2.01	0.43
1:B:276:ASP:O	1:B:277:ALA:C	2.61	0.43
1:C:344:ASP:O	1:C:345:ASP:C	2.62	0.43
1:D:226:LEU:HD12	1:D:227:PHE:N	2.32	0.43
1:D:14:VAL:HG22	1:D:32:LEU:CD1	2.49	0.43
1:D:320:ASP:OD1	1:D:322:GLU:N	2.51	0.43
1:A:170:LYS:HD3	1:A:170:LYS:O	2.19	0.42
1:B:21:LEU:HD11	1:B:72:LEU:HD23	2.01	0.42
1:B:51:GLY:CA	1:B:78:VAL:HG22	2.49	0.42
1:B:181:THR:HG21	1:B:221:SER:HB2	2.01	0.42
1:D:71:VAL:HA	1:D:109:ALA:O	2.18	0.42
1:D:195:ALA:O	1:D:197:GLN:N	2.52	0.42
1:A:226:LEU:HD12	1:A:227:PHE:N	2.33	0.42
1:C:189:ASP:HA	1:C:229:ASN:OD1	2.19	0.42
1:D:148:THR:OG1	1:D:170:LYS:NZ	2.50	0.42
1:D:276:ASP:O	1:D:279:ALA:N	2.52	0.42
1:D:301:PRO:CB	1:D:355:LEU:HD13	2.39	0.42
1:A:182:LEU:HD22	1:A:183:LEU:N	2.35	0.42
1:A:382:GLU:CD	1:B:386:ARG:NH1	2.77	0.42
1:B:264:LYS:HB3	1:B:358:ASP:HA	1.99	0.42
1:C:98:ALA:C	1:C:100:GLY:H	2.26	0.42
1:C:160:VAL:HG21	1:C:243:ALA:HB2	2.01	0.42
1:B:155:GLU:HB2	1:B:168:ILE:HG22	2.00	0.42
1:C:45:THR:OG1	1:C:46:ARG:N	2.52	0.42
1:C:312:LYS:C	1:C:314:SER:H	2.28	0.42
1:C:313:CYS:HB3	1:C:316:ASP:OD1	2.18	0.42
1:D:61:VAL:HG13	1:D:107:LEU:HD21	2.00	0.42
1:D:165:LEU:CD1	1:D:188:THR:HB	2.48	0.42
1:D:175:LEU:HA	3:D:2004:HOH:O	2.19	0.42
1:A:75:ASN:O	1:A:110:SER:OG	2.37	0.42
1:A:284:LYS:HE3	1:A:375:VAL:HG12	2.01	0.42
1:B:271:THR:O	1:B:365:ASP:HA	2.20	0.42
1:C:123:ILE:O	1:C:127:LEU:HG	2.20	0.42
1:D:99:LEU:C	1:D:132:TRP:HE1	2.26	0.42
1:C:176:GLU:O	1:C:176:GLU:HG2	2.19	0.42
1:C:205:MSE:HE1	1:C:209:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:THR:HG22	1:D:288:ASN:OD1	2.20	0.42
1:B:174:MSE:O	1:B:174:MSE:HG2	2.19	0.42
1:C:42:ALA:HA	1:C:201:PHE:CE2	2.54	0.42
1:C:44:PHE:HA	1:C:179:MSE:CE	2.42	0.42
1:C:179:MSE:HE1	1:C:222:ASP:C	2.45	0.42
1:C:179:MSE:HE3	1:C:222:ASP:HB3	2.01	0.42
1:C:323:ARG:HG2	1:C:323:ARG:NH1	2.33	0.42
1:A:148:THR:OG1	1:A:149:THR:N	2.52	0.42
1:A:226:LEU:HD12	1:A:226:LEU:C	2.45	0.42
1:A:283:GLY:C	1:A:375:VAL:HG21	2.45	0.42
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.77	0.42
1:C:40:VAL:HG12	1:C:64:GLY:O	2.19	0.42
1:C:67:ARG:CB	1:C:101:LEU:HD13	2.50	0.42
1:D:30:THR:OG1	1:D:145:ALA:HB3	2.19	0.42
1:D:118:TYR:HD1	1:D:119:PRO:HD2	1.84	0.42
1:A:49:PHE:CD2	1:B:321:GLN:HG3	2.55	0.42
1:A:266:ILE:HD12	1:A:378:CYS:C	2.45	0.42
1:A:382:GLU:OE1	1:B:386:ARG:NH1	2.53	0.42
1:D:143:ALA:HB2	1:D:168:ILE:CG2	2.50	0.42
1:B:274:ARG:O	1:B:275:ASP:HB3	2.18	0.41
1:B:298:GLY:O	1:B:299:CYS:HB2	2.20	0.41
1:A:24:ASP:OD2	1:A:74:ARG:NH2	2.52	0.41
1:B:200:LEU:HD23	1:B:200:LEU:C	2.45	0.41
1:C:47:SER:OG	1:C:220:THR:HG22	2.20	0.41
1:D:219:SER:HB3	1:D:222:ASP:OD2	2.20	0.41
1:C:21:LEU:HD11	1:C:72:LEU:HB3	2.02	0.41
1:C:217:ASP:HA	1:D:312:LYS:HD3	2.01	0.41
1:D:142:ALA:C	1:D:144:ARG:N	2.78	0.41
1:D:176:GLU:OE2	1:D:284:LYS:CE	2.68	0.41
1:A:114:ILE:HD11	1:A:174:MSE:HE1	2.02	0.41
1:D:94:ALA:O	1:D:95:VAL:C	2.62	0.41
1:D:294:THR:O	1:D:297:HIS:HB3	2.20	0.41
1:C:208:THR:O	1:C:211:ALA:HB3	2.20	0.41
1:D:170:LYS:HD3	1:D:170:LYS:O	2.21	0.41
1:A:75:ASN:N	1:A:112:GLY:HA3	2.35	0.41
1:A:322:GLU:HG2	1:A:322:GLU:H	1.73	0.41
1:B:176:GLU:O	1:B:176:GLU:HG2	2.21	0.41
1:D:19:VAL:HG21	1:D:29:PHE:CG	2.56	0.41
1:D:21:LEU:HD11	1:D:72:LEU:HB3	2.03	0.41
1:B:223:THR:HG22	1:B:224:ALA:N	2.35	0.41
1:C:21:LEU:N	1:C:28:ASP:OD2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LYS:NZ	1:B:217:ASP:HA	2.36	0.41
1:C:111:THR:OG1	2:C:1394:SO4:O4	2.38	0.41
1:C:383:GLY:O	1:C:384:TYR:C	2.64	0.41
1:D:95:VAL:O	1:D:98:ALA:HB3	2.20	0.41
1:A:19:VAL:HG11	1:A:123:ILE:CG1	2.45	0.41
1:A:51:GLY:HA3	1:A:78:VAL:HG22	2.03	0.41
1:A:72:LEU:N	1:A:72:LEU:HD12	2.36	0.41
1:B:201:PHE:O	1:B:205:MSE:HG2	2.21	0.41
1:B:215:ASP:C	1:B:216:THR:HG23	2.45	0.41
1:C:123:ILE:HG22	1:C:127:LEU:HD11	2.03	0.41
1:C:154:LYS:O	1:C:168:ILE:HA	2.21	0.41
1:D:264:LYS:HE2	1:D:264:LYS:HB3	1.89	0.41
1:C:102:PRO:O	1:C:105:GLU:N	2.50	0.41
1:D:274:ARG:NH1	1:D:318:ASP:OD1	2.54	0.41
1:D:315:ASP:O	1:D:317:THR:N	2.49	0.41
1:D:352:ALA:O	1:D:356:ARG:HG3	2.21	0.41
1:A:212:VAL:HB	1:A:252:VAL:HG13	2.02	0.40
1:C:9:PRO:CG	1:C:166:VAL:HG21	2.45	0.40
1:C:80:THR:O	1:C:84:GLY:N	2.51	0.40
1:D:213:SER:N	1:D:376:TYR:O	2.42	0.40
1:B:294:THR:O	1:B:297:HIS:HB3	2.21	0.40
1:C:301:PRO:O	1:C:302:ASN:C	2.64	0.40
1:C:300:ASP:CG	1:C:302:ASN:HB2	2.45	0.40
1:D:123:ILE:H	1:D:123:ILE:HG13	1.69	0.40
1:A:48:ARG:HD3	1:B:319:ILE:HB	2.03	0.40
1:A:94:ALA:HB1	1:A:127:LEU:HD22	2.03	0.40
1:A:174:MSE:CE	1:B:308:MSE:HG3	2.39	0.40
1:B:9:PRO:HD3	1:B:164:THR:CG2	2.52	0.40
1:C:94:ALA:C	1:C:96:ALA:N	2.79	0.40
1:D:12:PHE:HE2	1:D:188:THR:C	2.29	0.40
1:B:144:ARG:CB	1:B:147:MSE:HE2	2.51	0.40
1:B:272:GLY:O	1:B:368:ILE:HB	2.21	0.40
1:C:219:SER:HG	1:C:222:ASP:CG	2.29	0.40
1:C:235:VAL:CG1	1:C:236:ASP:N	2.83	0.40
1:C:300:ASP:C	1:C:355:LEU:CD2	2.95	0.40
1:D:142:ALA:C	1:D:144:ARG:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	370/393 (94%)	341 (92%)	25 (7%)	4 (1%)	11	22
1	B	373/393 (95%)	343 (92%)	28 (8%)	2 (0%)	24	43
1	C	364/393 (93%)	304 (84%)	46 (13%)	14 (4%)	2	4
1	D	370/393 (94%)	307 (83%)	49 (13%)	14 (4%)	2	4
All	All	1477/1572 (94%)	1295 (88%)	148 (10%)	34 (2%)	5	9

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	81	GLY
1	C	231	LEU
1	C	302	ASN
1	D	23	ASP
1	D	122	SER
1	D	346	ALA
1	A	161	GLY
1	C	94	ALA
1	D	196	GLU
1	D	230	GLY
1	B	231	LEU
1	C	95	VAL
1	C	321	GLN
1	D	97	ARG
1	D	123	ILE
1	D	143	ALA
1	D	345	ASP
1	A	74	ARG
1	C	45	THR
1	C	74	ARG
1	C	129	THR
1	C	243	ALA

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Mol	Chain	Res	Type
1	C	345	ASP
1	D	195	ALA
1	A	35	THR
1	B	302	ASN
1	C	98	ALA
1	C	127	LEU
1	D	194	PRO
1	A	125	GLU
1	C	314	SER
1	D	104	GLY
1	D	161	GLY
1	D	81	GLY

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	269/293 (92%)	253 (94%)	16 (6%)	18	33
1	B	275/293 (94%)	256 (93%)	19 (7%)	14	26
1	C	257/293 (88%)	242 (94%)	15 (6%)	18	34
1	D	254/293 (87%)	235 (92%)	19 (8%)	12	24
All	All	1055/1172 (90%)	986 (94%)	69 (6%)	15	29

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	39	THR
1	A	74	ARG
1	A	121	GLU
1	A	160	VAL
1	A	170	LYS
1	A	182	LEU
1	A	189	ASP
1	A	223	THR

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Mol	Chain	Res	Type
1	A	226	LEU
1	A	264	LYS
1	A	265	LEU
1	A	287	VAL
1	A	353	GLU
1	A	355	LEU
1	A	375	VAL
1	B	43	VAL
1	B	65	GLN
1	B	78	VAL
1	B	92	ARG
1	B	101	LEU
1	B	107	LEU
1	B	121	GLU
1	B	140	ASP
1	B	155	GLU
1	B	170	LYS
1	B	182	LEU
1	B	200	LEU
1	B	216	THR
1	B	265	LEU
1	B	287	VAL
1	B	293	LYS
1	B	355	LEU
1	B	392	THR
1	B	393	THR
1	C	26	ARG
1	C	39	THR
1	C	53	SER
1	C	92	ARG
1	C	129	THR
1	C	130	LEU
1	C	151	THR
1	C	182	LEU
1	C	225	VAL
1	C	231	LEU
1	C	265	LEU
1	C	351	VAL
1	C	355	LEU
1	C	392	THR
1	C	393	THR
1	D	19	VAL

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Mol	Chain	Res	Type
1	D	24	ASP
1	D	30	THR
1	D	43	VAL
1	D	72	LEU
1	D	74	ARG
1	D	92	ARG
1	D	118	TYR
1	D	148	THR
1	D	150	ASP
1	D	166	VAL
1	D	168	ILE
1	D	170	LYS
1	D	176	GLU
1	D	182	LEU
1	D	255	ILE
1	D	265	LEU
1	D	327	ARG
1	D	355	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	B	65	GLN
1	B	117	GLN
1	B	302	ASN
1	B	321	GLN
1	C	77	ASN
1	C	87	ASN
1	C	229	ASN
1	C	321	GLN
1	D	229	ASN
1	D	321	GLN
1	D	388	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	1391	-	4,4,4	0.38	0	6,6,6	0.11	0
2	SO4	A	1393	-	4,4,4	0.69	0	6,6,6	0.35	0
2	SO4	A	1392	-	4,4,4	0.67	0	6,6,6	0.18	0
2	SO4	D	1391	-	4,4,4	0.41	0	6,6,6	0.14	0
2	SO4	B	1394	-	4,4,4	0.41	0	6,6,6	0.12	0
2	SO4	C	1394	-	4,4,4	0.38	0	6,6,6	0.12	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.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1393	SO4	1	0
2	A	1392	SO4	1	0
2	D	1391	SO4	1	0
2	C	1394	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	D	1
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	180:ALA	C	181:THR	N	16.59
1	D	180:ALA	C	181:THR	N	16.46
1	A	180:ALA	C	181:THR	N	16.41
1	C	180:ALA	C	181:THR	N	16.28

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	369/393 (93%)	-1.70	0 100 100	5, 25, 38, 47	0
1	B	372/393 (94%)	-1.69	0 100 100	10, 22, 38, 50	0
1	C	365/393 (92%)	-1.50	0 100 100	15, 41, 63, 71	0
1	D	369/393 (93%)	-1.42	0 100 100	11, 48, 65, 74	0
All	All	1475/1572 (93%)	-1.58	0 100 100	5, 31, 62, 74	0

There are no RSRZ outliers to report.

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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
2	SO4	A	1391	5/5	0.99	0.03	34,36,38,38	0
2	SO4	A	1392	5/5	0.99	0.04	52,53,54,57	0
2	SO4	A	1393	5/5	0.99	0.04	55,57,57,57	0
2	SO4	C	1394	5/5	0.99	0.03	29,29,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	1391	5/5	0.99	0.04	50,50,52,52	0
2	SO4	B	1394	5/5	1.00	0.02	35,35,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.