



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:23 PM UTC

PDB ID : 5SVC / pdb_00005svc
Title : Mechanism of ATP-Dependent Acetone Carboxylation, Acetone Carboxylase nucleotide-free structure
Authors : Eilers, B.J.; Mus, F.; Alleman, A.B.; Kabasakal, B.V.; Murray, J.W.; Nocek, B.P.; Dubois, J.L.; Peters, J.W.
Deposited on : 2016-08-05
Resolution : 2.70 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

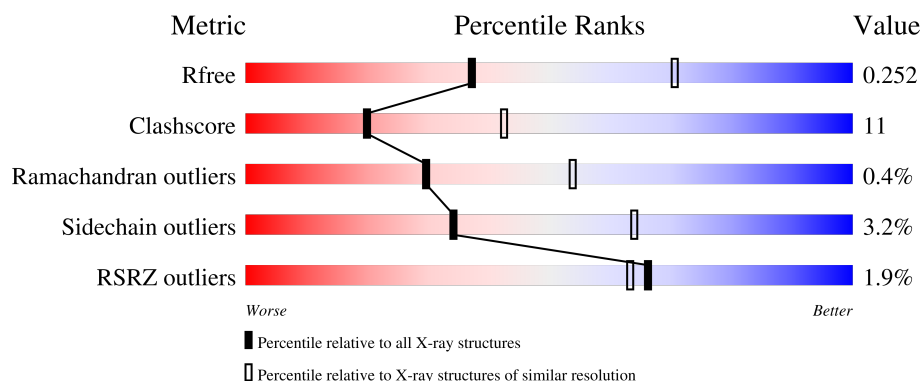
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. 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	776	% 73% 25% ..
1	D	776	70% 27% ..
2	B	727	2% 72% 25% ..
2	E	727	5% 70% 26% ..
3	C	168	% 72% 26% ..

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Mol	Chain	Length	Quality of chain
3	F	168	% 75% 24% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25811 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 Acetone carboxylase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	763	Total	C	N	O	S	0	0	0
			5992	3783	1050	1125	34			
1	D	763	Total	C	N	O	S	0	0	0
			5992	3783	1050	1125	34			

- Molecule 2 is a protein called Acetone carboxylase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	710	Total	C	N	O	S	0	0	0
			5474	3446	954	1050	24			
2	E	710	Total	C	N	O	S	0	0	0
			5470	3443	953	1050	24			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	initiating methionine	UNP Q8RM04
B	-8	HIS	-	expression tag	UNP Q8RM04
B	-7	HIS	-	expression tag	UNP Q8RM04
B	-6	HIS	-	expression tag	UNP Q8RM04
B	-5	HIS	-	expression tag	UNP Q8RM04
B	-4	HIS	-	expression tag	UNP Q8RM04
B	-3	HIS	-	expression tag	UNP Q8RM04
B	-2	SER	-	expression tag	UNP Q8RM04
B	-1	SER	-	expression tag	UNP Q8RM04
B	0	GLY	-	expression tag	UNP Q8RM04
E	-9	MET	-	initiating methionine	UNP Q8RM04
E	-8	HIS	-	expression tag	UNP Q8RM04
E	-7	HIS	-	expression tag	UNP Q8RM04
E	-6	HIS	-	expression tag	UNP Q8RM04
E	-5	HIS	-	expression tag	UNP Q8RM04
E	-4	HIS	-	expression tag	UNP Q8RM04

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	HIS	-	expression tag	UNP Q8RM04
E	-2	SER	-	expression tag	UNP Q8RM04
E	-1	SER	-	expression tag	UNP Q8RM04
E	0	GLY	-	expression tag	UNP Q8RM04

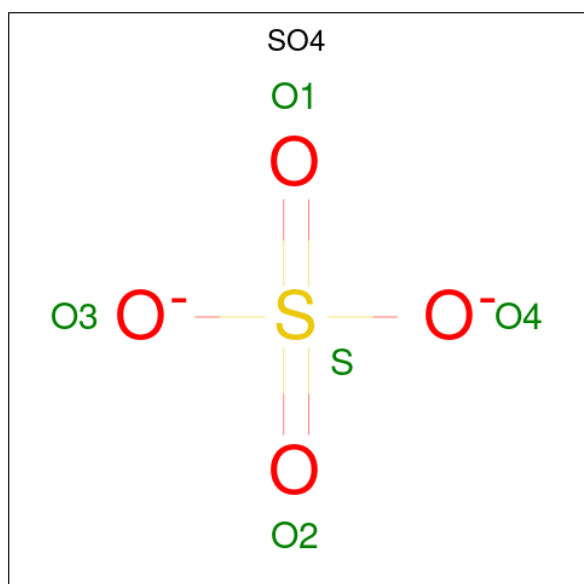
- Molecule 3 is a protein called Acetone carboxylase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	166	Total	C	N	O	S	0	0	0
			1379	892	229	249	9			
3	F	166	Total	C	N	O	S	0	0	0
			1379	892	229	249	9			

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	D	1	Total	Mn	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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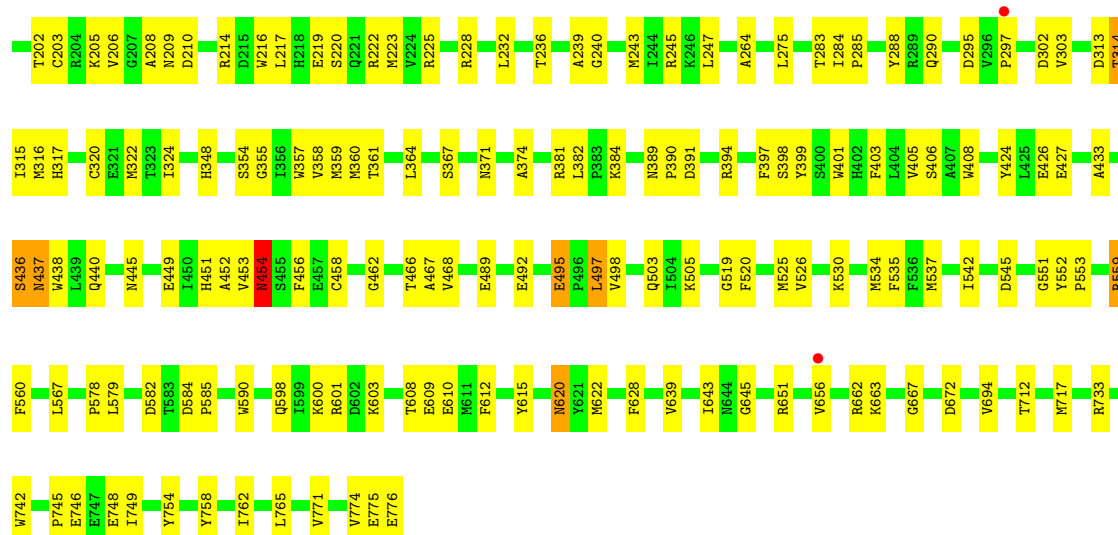
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

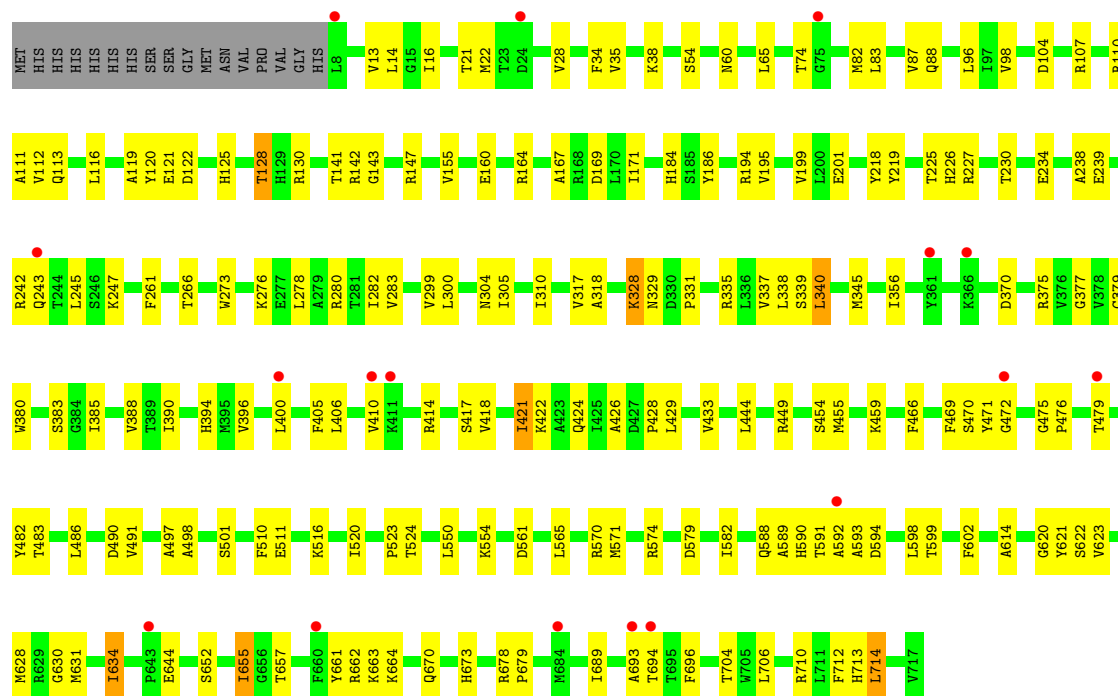
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Zn	0	0
			1	1		
6	F	1	Total	Zn	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	42	Total	O	0	0
			42	42		
7	B	10	Total	O	0	0
			10	10		
7	C	4	Total	O	0	0
			4	4		
7	D	40	Total	O	0	0
			40	40		
7	E	11	Total	O	0	0
			11	11		
7	F	4	Total	O	0	0
			4	4		

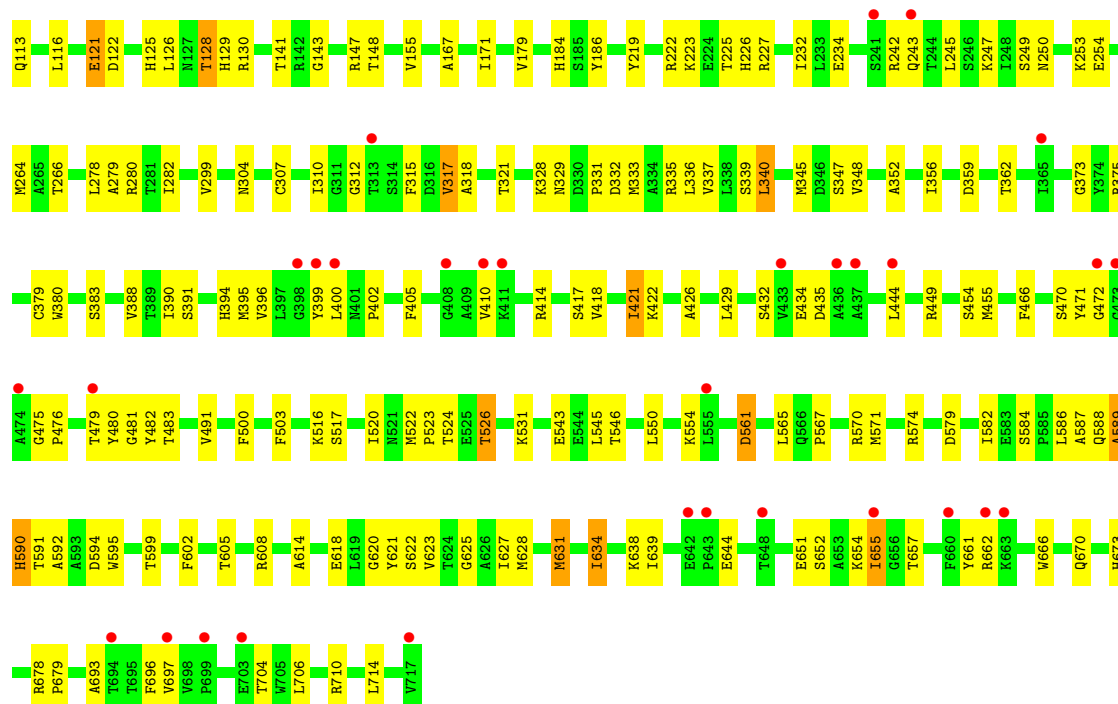


• Molecule 2: Acetone carboxylase beta subunit

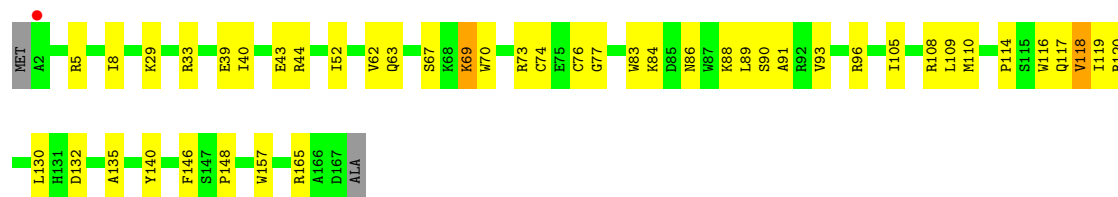


• Molecule 2: Acetone carboxylase beta subunit

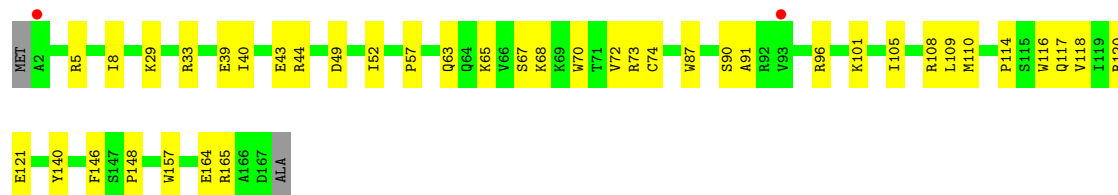
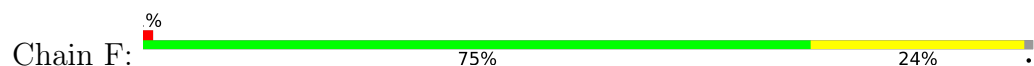




- Molecule 3: Acetone carboxylase gamma subunit



- Molecule 3: Acetone carboxylase gamma subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.76Å 265.16Å 122.17Å 90.00° 92.33° 90.00°	Depositor
Resolution (Å)	38.90 – 2.70 38.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.7 (38.90-2.70) 93.6 (38.90-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.202 , 0.255 0.198 , 0.252	Depositor DCC
R_{free} test set	6962 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.089 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25811	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: MN, ZN, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/6145	0.74	1/8326 (0.0%)
1	D	0.49	0/6145	0.74	1/8326 (0.0%)
2	B	0.38	0/5589	0.62	0/7575
2	E	0.38	0/5585	0.62	1/7571 (0.0%)
3	C	0.49	0/1426	0.68	0/1947
3	F	0.43	0/1426	0.63	0/1947
All	All	0.45	0/26316	0.68	3/35692 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
2	E	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	SER	N-CA-C	8.78	119.82	108.24
1	D	436	SER	N-CA-C	7.22	117.77	108.24
2	E	589	ALA	CB-CA-C	-6.81	108.73	116.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	436	SER	Peptide
1	D	436	SER	Peptide
2	E	587	ALA	Peptide

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	5992	0	5749	144	0
1	D	5992	0	5749	153	0
2	B	5474	0	5391	129	0
2	E	5470	0	5380	129	0
3	C	1379	0	1337	34	0
3	F	1379	0	1337	29	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	B	5	0	0	0	0
5	E	5	0	0	0	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
7	A	42	0	0	2	0
7	B	10	0	0	1	0
7	C	4	0	0	0	0
7	D	40	0	0	5	0
7	E	11	0	0	1	0
7	F	4	0	0	1	0
All	All	25811	0	24943	578	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 11.

All (578) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:MET:HE1	1:A:406:SER:HB2	1.50	0.92
1:A:38:THR:HG21	1:A:43:GLY:HA2	1.53	0.90
1:D:316:MET:HE1	1:D:406:SER:HB2	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:THR:HG21	1:D:43:GLY:HA2	1.56	0.88
1:D:733:ARG:NH2	1:D:742:TRP:O	2.07	0.87
3:F:120:ARG:NH2	3:F:140:TYR:O	2.08	0.87
2:B:394:HIS:HB3	2:B:400:LEU:HG	1.55	0.87
1:A:359:MET:HE1	1:A:411:LEU:HB2	1.58	0.86
1:A:585:PRO:HG3	3:C:110:MET:HE3	1.57	0.86
1:A:733:ARG:NH2	1:A:742:TRP:O	2.09	0.85
1:A:214:ARG:NH1	1:D:126:ASN:O	2.09	0.85
1:D:316:MET:HE2	1:D:403:PHE:HA	1.58	0.84
1:A:194:ARG:HH21	1:D:223:MET:HE1	1.42	0.84
2:B:22:MET:HE2	2:B:38:LYS:HD3	1.58	0.82
1:A:223:MET:HE1	1:D:194:ARG:HH21	1.44	0.82
1:D:48:GLU:OE1	1:D:52:ARG:NH1	2.15	0.80
2:B:483:THR:HG21	2:B:491:VAL:HG21	1.67	0.77
1:A:283:THR:HG22	1:A:284:ILE:H	1.49	0.76
2:B:122:ASP:HB3	2:B:128:THR:HG21	1.65	0.76
1:D:489:GLU:OE2	2:E:227:ARG:NH2	2.19	0.75
2:E:22:MET:HE2	2:E:38:LYS:HD3	1.69	0.74
2:B:35:VAL:HG21	2:B:60:ASN:HB2	1.69	0.74
1:D:78:ILE:HB	1:D:236:THR:HG22	1.70	0.73
1:D:283:THR:HG22	1:D:284:ILE:H	1.54	0.73
1:D:186:SER:N	1:D:454:ASN:OD1	2.16	0.73
2:B:390:ILE:HD13	2:B:444:LEU:HD22	1.71	0.72
1:A:191:GLN:NE2	1:A:197:ASP:OD1	2.22	0.72
2:E:449:ARG:HB2	2:E:482:TYR:HA	1.70	0.72
1:A:297:PRO:HD2	1:A:606:ILE:HD12	1.72	0.71
2:E:130:ARG:O	2:E:335:ARG:NH2	2.23	0.71
2:B:571:MET:HE1	2:B:599:THR:HG22	1.72	0.70
1:A:316:MET:HE2	1:A:403:PHE:HA	1.72	0.70
1:A:126:ASN:O	1:D:214:ARG:NH1	2.24	0.70
1:D:585:PRO:HG3	3:F:110:MET:HE3	1.74	0.70
3:C:73:ARG:HG2	3:C:74:CYS:O	1.91	0.70
1:A:603:LYS:NZ	3:C:109:LEU:O	2.25	0.70
2:E:655:ILE:HD11	2:E:673:HIS:HB2	1.74	0.69
2:B:422:LYS:HA	2:B:426:ALA:HB3	1.73	0.69
1:D:22:GLU:OE2	1:D:30:ARG:NH1	2.26	0.69
2:E:470:SER:HG	2:E:482:TYR:HH	1.34	0.69
1:A:115:MET:SD	1:A:173:VAL:HG23	2.33	0.69
1:D:191:GLN:NE2	1:D:197:ASP:OD1	2.23	0.69
2:E:304:ASN:HB3	2:E:466:PHE:CD1	2.28	0.69
1:A:656:VAL:HG22	3:C:105:ILE:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:MET:SD	1:D:173:VAL:HG23	2.33	0.69
2:E:571:MET:HE1	2:E:599:THR:HG22	1.74	0.68
2:B:104:ASP:OD1	2:B:107:ARG:NH1	2.26	0.68
2:B:510:PHE:HB2	2:B:634:ILE:HD12	1.74	0.68
2:E:317:VAL:HG12	2:E:455:MET:HE3	1.77	0.67
1:D:283:THR:HG22	1:D:284:ILE:N	2.09	0.67
2:E:125:HIS:O	2:E:128:THR:HB	1.95	0.67
2:B:418:VAL:HG13	2:B:433:VAL:HG11	1.76	0.66
2:E:523:PRO:HA	2:E:574:ARG:HH12	1.60	0.66
3:F:52:ILE:HD11	3:F:63:GLN:HB2	1.76	0.66
2:B:470:SER:HG	2:B:482:TYR:HH	1.42	0.66
1:D:584:ASP:OD2	1:D:651:ARG:NH2	2.29	0.66
2:E:526:THR:O	7:E:901:HOH:O	2.14	0.65
2:B:82:MET:HE1	2:B:278:LEU:HB3	1.78	0.65
1:A:78:ILE:HB	1:A:236:THR:HG22	1.77	0.65
1:D:137:ASP:OD2	1:D:205:LYS:NZ	2.26	0.65
1:D:214:ARG:HA	1:D:217:LEU:HD12	1.78	0.65
2:B:375:ARG:HB3	2:B:383:SER:HB2	1.78	0.65
2:E:483:THR:HG21	2:E:491:VAL:HG21	1.79	0.65
2:B:582:ILE:HD13	2:B:602:PHE:HA	1.78	0.64
3:C:8:ILE:HD13	3:C:33:ARG:HD3	1.78	0.64
2:E:375:ARG:HB3	2:E:383:SER:HB2	1.78	0.64
1:D:160:ILE:HD11	1:D:170:VAL:HG23	1.79	0.64
2:B:243:GLN:HB3	2:B:247:LYS:HE3	1.79	0.64
1:D:582:ASP:OD1	1:D:601:ARG:NH2	2.31	0.63
2:E:390:ILE:HD13	2:E:444:LEU:HD22	1.80	0.63
1:A:186:SER:N	1:A:454:ASN:OD1	2.20	0.63
3:C:146:PHE:CZ	3:C:148:PRO:HB3	2.34	0.63
1:D:355:GLY:HA3	1:D:408:TRP:CZ2	2.34	0.63
2:E:122:ASP:HB3	2:E:128:THR:HG21	1.80	0.63
1:D:38:THR:HG23	1:D:40:ARG:H	1.64	0.62
2:E:396:VAL:HG21	2:E:421:ILE:HD12	1.81	0.62
3:C:5:ARG:NH2	3:C:43:GLU:OE1	2.33	0.62
1:A:160:ILE:HD11	1:A:170:VAL:HG23	1.81	0.62
1:A:355:GLY:HA3	1:A:408:TRP:CZ2	2.35	0.62
1:A:283:THR:HG22	1:A:284:ILE:N	2.14	0.62
1:D:38:THR:CG2	1:D:40:ARG:H	2.12	0.62
3:F:73:ARG:HG2	3:F:74:CYS:O	2.00	0.61
2:E:167:ALA:O	2:E:171:ILE:HG13	2.00	0.61
1:A:183:GLY:HA3	1:A:188:ALA:HB1	1.82	0.61
1:A:620:ASN:CG	1:A:622:MET:HE1	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:HIS:O	2:B:128:THR:HB	2.00	0.61
2:E:605:THR:HG22	2:E:608:ARG:HH21	1.64	0.61
2:B:218:TYR:CZ	2:B:276:LYS:HD2	2.36	0.61
3:C:120:ARG:NH2	3:C:140:TYR:O	2.21	0.61
3:F:146:PHE:CZ	3:F:148:PRO:HB3	2.36	0.61
2:B:396:VAL:HG21	2:B:421:ILE:HD12	1.82	0.61
2:B:449:ARG:HB2	2:B:482:TYR:HA	1.82	0.61
1:D:620:ASN:CG	1:D:622:MET:HE1	2.26	0.60
1:D:712:THR:HG22	1:D:749:ILE:HG22	1.83	0.60
2:B:130:ARG:O	2:B:335:ARG:NH2	2.34	0.60
1:D:225:ARG:HD2	1:D:452:ALA:HB2	1.82	0.60
2:E:304:ASN:HD22	2:E:466:PHE:HE1	1.49	0.60
1:A:382:LEU:O	1:A:776:GLU:HA	2.02	0.60
1:D:358:VAL:O	1:D:361:THR:OG1	2.19	0.60
1:A:155:HIS:HD2	1:A:173:VAL:HG22	1.64	0.60
1:A:239:ALA:HB2	2:B:614:ALA:HB2	1.84	0.60
2:E:266:THR:HG21	2:E:340:LEU:HD13	1.84	0.60
1:D:228:ARG:NH2	7:D:902:HOH:O	2.34	0.59
1:D:603:LYS:NZ	3:F:109:LEU:O	2.35	0.59
2:E:104:ASP:OD1	2:E:107:ARG:NH1	2.34	0.59
2:E:696:PHE:HE2	2:E:704:THR:HG21	1.65	0.59
2:B:655:ILE:HD11	2:B:673:HIS:HB2	1.84	0.59
3:C:67:SER:OG	3:C:69:LYS:NZ	2.34	0.59
1:A:79:ALA:HB2	1:A:236:THR:HG21	1.84	0.59
2:B:14:LEU:HD21	2:B:16:ILE:HD11	1.83	0.59
2:E:422:LYS:HA	2:E:426:ALA:HB3	1.84	0.59
1:A:489:GLU:OE2	2:B:227:ARG:NH2	2.36	0.59
3:F:5:ARG:NH2	3:F:43:GLU:OE1	2.36	0.59
2:B:565:LEU:HB3	2:B:628:MET:HE2	1.83	0.58
2:E:299:VAL:HG11	2:E:639:ILE:HG13	1.85	0.58
2:E:570:ARG:NH1	2:E:579:ASP:OD2	2.35	0.58
2:E:304:ASN:HB3	2:E:466:PHE:HD1	1.69	0.58
1:D:578:PRO:O	1:D:579:LEU:HD23	2.03	0.58
2:B:520:ILE:HB	2:B:623:VAL:HB	1.85	0.58
2:B:696:PHE:HE2	2:B:704:THR:HG21	1.67	0.58
2:E:470:SER:OG	2:E:479:THR:HG22	2.04	0.58
1:D:49:LEU:HD23	1:D:57:TYR:HD1	1.69	0.57
1:D:194:ARG:N	1:D:394:ARG:O	2.33	0.57
2:E:226:HIS:CE1	2:E:337:VAL:HB	2.39	0.57
2:B:38:LYS:HD2	2:B:693:ALA:HB1	1.86	0.57
2:B:82:MET:HE2	2:B:238:ALA:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:656:VAL:HG22	3:F:105:ILE:HG22	1.87	0.57
1:D:119:ILE:O	1:D:123:ILE:HG13	2.04	0.57
3:C:52:ILE:HD11	3:C:63:GLN:HB2	1.85	0.57
2:E:312:GLY:HA2	2:E:352:ALA:N	2.20	0.57
2:B:644:GLU:HA	2:B:679:PRO:HB2	1.86	0.57
2:E:35:VAL:HG21	2:E:60:ASN:HB2	1.85	0.57
1:A:119:ILE:O	1:A:123:ILE:HG13	2.04	0.56
1:A:282:MET:HG2	3:C:29:LYS:HZ3	1.69	0.56
2:B:574:ARG:NH1	2:B:620:GLY:HA3	2.19	0.56
1:A:358:VAL:O	1:A:361:THR:OG1	2.21	0.56
1:A:219:GLU:HB2	1:D:202:THR:HB	1.87	0.56
2:B:570:ARG:NH1	2:B:579:ASP:OD2	2.39	0.56
2:E:266:THR:HG23	2:E:280:ARG:O	2.06	0.56
2:B:74:THR:HG21	2:B:634:ILE:HD11	1.87	0.56
2:B:582:ILE:CD1	2:B:602:PHE:HA	2.36	0.56
1:D:155:HIS:HD2	1:D:173:VAL:HG22	1.71	0.56
1:D:645:GLY:O	2:E:107:ARG:NH2	2.38	0.56
2:E:574:ARG:NH1	2:E:620:GLY:HA3	2.21	0.56
1:D:639:VAL:O	1:D:643:ILE:HG12	2.05	0.56
1:D:228:ARG:NH2	1:D:449:GLU:OE1	2.38	0.55
1:D:525:MET:HE2	1:D:615:TYR:HA	1.88	0.55
1:D:534:MET:HE3	1:D:612:PHE:CD2	2.41	0.55
1:A:620:ASN:ND2	1:A:622:MET:HE1	2.22	0.55
2:B:226:HIS:CE1	2:B:337:VAL:HB	2.41	0.55
2:E:582:ILE:CD1	2:E:602:PHE:HA	2.37	0.55
2:E:405:PHE:HD2	2:E:410:VAL:HB	1.70	0.55
1:A:519:GLY:HA3	1:A:622:MET:O	2.07	0.55
2:E:38:LYS:HD2	2:E:693:ALA:HB1	1.88	0.55
1:A:38:THR:CG2	1:A:40:ARG:H	2.19	0.55
2:B:239:GLU:OE1	2:B:242:ARG:NE	2.31	0.55
1:D:316:MET:HB2	1:D:403:PHE:CE1	2.42	0.55
2:E:524:THR:HG21	2:E:618:GLU:HA	1.89	0.55
2:B:164:ARG:NH2	2:B:201:GLU:OE1	2.33	0.54
2:B:476:PRO:HA	2:B:479:THR:HG23	1.87	0.54
1:A:313:ASP:HB3	3:C:116:TRP:CH2	2.42	0.54
1:D:290:GLN:NE2	1:D:320:CYS:O	2.39	0.54
2:E:356:ILE:HB	2:E:388:VAL:HG23	1.88	0.54
1:A:283:THR:HG21	1:A:324:ILE:HD13	1.90	0.54
1:D:160:ILE:HD11	1:D:170:VAL:CG2	2.37	0.54
1:A:283:THR:CG2	1:A:284:ILE:H	2.18	0.54
1:A:542:ILE:HG12	3:C:117:GLN:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:VAL:HG12	2:B:455:MET:HE3	1.90	0.54
2:E:522:MET:HE3	2:E:526:THR:HG21	1.88	0.54
3:F:57:PRO:HD2	7:F:304:HOH:O	2.08	0.54
2:B:318:ALA:HB2	2:B:345:MET:HG2	1.89	0.54
2:E:113:GLN:HG2	2:E:116:LEU:HD12	1.90	0.54
2:E:399:TYR:HD2	2:E:697:VAL:HG21	1.72	0.54
3:F:96:ARG:HG2	3:F:101:LYS:HB3	1.90	0.54
1:A:102:LEU:HD21	1:A:264:ALA:HA	1.90	0.53
1:A:584:ASP:OD2	1:A:651:ARG:NH2	2.42	0.53
2:B:54:SER:HB3	2:B:65:LEU:HD13	1.90	0.53
3:F:5:ARG:NH1	3:F:39:GLU:OE1	2.40	0.53
1:A:645:GLY:O	2:B:107:ARG:NH2	2.40	0.53
1:D:283:THR:HG21	1:D:324:ILE:HD13	1.91	0.53
1:D:552:TYR:OH	3:F:121:GLU:OE1	2.20	0.53
1:A:745:PRO:HG2	1:A:748:GLU:CD	2.33	0.53
3:C:62:VAL:HG11	3:C:73:ARG:HB3	1.90	0.53
2:E:318:ALA:HB2	2:E:345:MET:HG2	1.91	0.53
2:E:678:ARG:NH1	2:E:710:ARG:HH22	2.06	0.53
1:A:466:THR:HG22	1:A:468:VAL:H	1.73	0.53
1:D:54:PRO:O	1:D:58:ASN:ND2	2.38	0.53
1:D:102:LEU:HD21	1:D:264:ALA:HA	1.90	0.53
1:A:384:LYS:HD2	1:A:391:ASP:HB3	1.91	0.53
2:E:500:PHE:O	2:E:503:PHE:HB3	2.09	0.53
1:A:591:ASP:OD1	1:A:601:ARG:NH1	2.42	0.53
1:D:283:THR:CG2	1:D:284:ILE:H	2.20	0.53
1:D:399:TYR:CE1	1:D:401:TRP:HB2	2.43	0.53
2:E:219:TYR:OH	2:E:234:GLU:OE2	2.23	0.53
1:A:526:VAL:HG22	1:A:534:MET:CE	2.39	0.53
1:A:109:ILE:HG13	1:A:358:VAL:HG22	1.91	0.52
1:D:662:ARG:HG3	1:D:672:ASP:HB2	1.90	0.52
1:D:288:TYR:HB2	1:D:322:MET:HB3	1.91	0.52
1:A:177:ILE:HG13	7:A:904:HOH:O	2.10	0.52
1:A:505:LYS:NZ	3:C:110:MET:HE1	2.24	0.52
1:A:585:PRO:CG	3:C:110:MET:HE3	2.34	0.52
3:C:5:ARG:NH1	3:C:39:GLU:OE1	2.42	0.52
1:D:232:LEU:O	1:D:236:THR:HG23	2.08	0.52
2:E:74:THR:HG21	2:E:634:ILE:HD11	1.91	0.52
1:A:177:ILE:O	1:A:186:SER:HB3	2.09	0.52
2:E:565:LEU:HB3	2:E:628:MET:HE2	1.90	0.52
1:A:22:GLU:OE2	1:A:30:ARG:NH1	2.42	0.52
1:A:445:ASN:HD22	1:A:451:HIS:CG	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:TRP:O	1:D:220:SER:OG	2.16	0.52
2:E:32:GLY:HA3	2:E:638:LYS:HB2	1.91	0.52
2:E:543:GLU:HA	2:E:546:THR:HG22	1.90	0.52
2:E:184:HIS:HA	2:E:186:TYR:CE1	2.45	0.52
1:D:438:TRP:HB2	1:D:440:GLN:HE21	1.74	0.52
2:E:520:ILE:HB	2:E:623:VAL:HB	1.91	0.52
1:D:445:ASN:HD22	1:D:451:HIS:CG	2.28	0.51
1:D:367:SER:OG	2:E:121:GLU:OE1	2.21	0.51
1:D:424:TYR:CE1	3:F:29:LYS:HB3	2.45	0.51
1:A:191:GLN:HE21	1:A:197:ASP:HA	1.74	0.51
1:A:639:VAL:O	1:A:643:ILE:HG12	2.11	0.51
2:B:329:ASN:O	2:B:331:PRO:HD3	2.10	0.51
1:D:545:ASP:O	1:D:553:PRO:HB3	2.10	0.51
2:E:82:MET:HE1	2:E:278:LEU:HB3	1.91	0.51
1:D:74:THR:HB	1:D:243:MET:HE1	1.93	0.51
1:D:357:TRP:HA	1:D:360:MET:HG2	1.92	0.51
1:D:526:VAL:HG22	1:D:534:MET:CE	2.40	0.51
2:E:356:ILE:HD11	2:E:390:ILE:HA	1.92	0.51
2:B:591:THR:O	2:B:591:THR:OG1	2.22	0.51
1:D:384:LYS:HG2	1:D:776:GLU:HG3	1.93	0.51
1:A:232:LEU:O	1:A:236:THR:HG23	2.11	0.51
2:B:594:ASP:OD1	2:B:594:ASP:N	2.44	0.51
1:D:745:PRO:HG2	1:D:748:GLU:CD	2.36	0.51
2:E:329:ASN:O	2:E:331:PRO:HD3	2.11	0.51
3:C:83:TRP:CZ2	3:C:84:LYS:HE3	2.46	0.51
1:A:399:TYR:CD2	1:A:537:MET:HE2	2.46	0.50
1:A:578:PRO:O	1:A:579:LEU:HD23	2.10	0.50
1:D:222:ARG:HG3	1:D:223:MET:HE2	1.94	0.50
1:A:534:MET:HE3	1:A:612:PHE:CD2	2.45	0.50
2:B:242:ARG:HA	2:B:278:LEU:HD11	1.92	0.50
2:E:116:LEU:HD11	2:E:337:VAL:HG13	1.93	0.50
1:A:160:ILE:HD11	1:A:170:VAL:CG2	2.41	0.50
2:B:38:LYS:HE2	2:B:498:ALA:HB1	1.94	0.50
2:E:399:TYR:CE2	2:E:697:VAL:HG11	2.46	0.50
1:D:146:ILE:HG22	1:D:146:ILE:O	2.11	0.50
1:D:317:HIS:HB2	1:D:717:MET:SD	2.52	0.50
1:D:542:ILE:HG12	3:F:117:GLN:HB2	1.93	0.50
2:E:307:CYS:HB3	2:E:471:TYR:OH	2.11	0.50
2:E:13:VAL:HB	2:E:28:VAL:HB	1.94	0.50
2:B:167:ALA:O	2:B:171:ILE:HG13	2.12	0.50
1:D:92:PHE:CZ	1:D:240:GLY:HA3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:186:TYR:CZ	2:E:222:ARG:HG3	2.47	0.50
1:A:155:HIS:CD2	1:A:173:VAL:HG22	2.46	0.50
1:A:313:ASP:O	1:A:314:THR:HG23	2.12	0.50
1:A:694:VAL:HG23	3:C:91:ALA:O	2.12	0.50
1:D:382:LEU:O	1:D:776:GLU:HA	2.12	0.50
1:A:545:ASP:HB2	1:A:626:PRO:HG3	1.93	0.50
1:A:598:GLN:HE21	1:A:600:LYS:HE2	1.77	0.50
2:B:470:SER:OG	2:B:479:THR:HG22	2.12	0.50
1:D:239:ALA:HB2	2:E:614:ALA:HB2	1.93	0.50
3:F:8:ILE:HD13	3:F:33:ARG:HD3	1.94	0.50
1:A:516:GLY:HA3	1:A:625:GLY:O	2.11	0.49
1:D:197:ASP:OD1	1:D:398:SER:HB3	2.12	0.49
3:C:86:ASN:HB3	3:C:89:LEU:HG	1.93	0.49
1:D:585:PRO:CG	3:F:110:MET:HE3	2.43	0.49
2:B:304:ASN:HB3	2:B:466:PHE:CD1	2.46	0.49
2:E:312:GLY:HA2	2:E:352:ALA:H	1.77	0.49
1:A:466:THR:HG22	1:A:467:ALA:N	2.27	0.49
1:A:181:ALA:O	1:A:225:ARG:NH1	2.45	0.49
1:A:214:ARG:HA	1:A:217:LEU:HD12	1.94	0.49
1:A:282:MET:HE2	1:A:419:TYR:CE1	2.48	0.49
1:A:505:LYS:HG3	1:A:508:SER:HB3	1.94	0.49
1:A:758:TYR:CZ	1:D:530:LYS:HG2	2.48	0.49
2:E:476:PRO:HA	2:E:479:THR:HG23	1.92	0.49
1:D:101:SER:O	1:D:371:ASN:HB2	2.12	0.49
1:D:610:GLU:O	1:D:612:PHE:HD1	1.96	0.49
1:A:202:THR:HB	1:D:219:GLU:HB2	1.94	0.49
2:B:396:VAL:HG22	2:B:418:VAL:HG22	1.95	0.49
1:D:313:ASP:HB3	3:F:116:TRP:CH2	2.48	0.49
1:A:149:VAL:HG11	1:A:401:TRP:CZ2	2.47	0.49
1:A:540:GLY:O	1:A:556:SER:HB2	2.13	0.49
1:D:384:LYS:HG2	1:D:776:GLU:CG	2.43	0.49
2:E:590:HIS:HB3	2:E:591:THR:HG23	1.95	0.49
1:A:147:GLY:HA2	1:A:348:HIS:CG	2.47	0.48
3:C:108:ARG:O	3:C:109:LEU:HB2	2.13	0.48
1:D:141:ASN:HB2	1:D:203:CYS:HA	1.94	0.48
2:B:662:ARG:NH1	2:B:663:LYS:HE3	2.29	0.48
1:D:399:TYR:HD2	1:D:537:MET:HE2	1.77	0.48
2:E:243:GLN:HB3	2:E:247:LYS:HE3	1.95	0.48
1:A:399:TYR:HD2	1:A:537:MET:HE2	1.79	0.48
2:B:305:ILE:HD13	2:B:469:PHE:CE2	2.48	0.48
2:B:328:LYS:HB2	2:B:331:PRO:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:455:MET:O	2:B:459:LYS:HG3	2.13	0.48
2:B:594:ASP:O	2:B:598:LEU:HG	2.14	0.48
1:D:526:VAL:HG22	1:D:534:MET:HE1	1.94	0.48
2:E:644:GLU:HA	2:E:679:PRO:HB2	1.95	0.48
1:A:475:ALA:O	1:A:483:GLY:HA3	2.13	0.48
2:E:380:TRP:CE3	2:E:383:SER:HB3	2.48	0.48
1:D:492:GLU:OE2	1:D:498:VAL:HA	2.12	0.48
1:A:225:ARG:NH2	7:A:903:HOH:O	2.45	0.48
1:D:83:ILE:HG12	1:D:456:PHE:CD1	2.49	0.48
1:A:225:ARG:HD2	1:A:452:ALA:HB2	1.96	0.48
1:A:578:PRO:HB3	1:A:590:TRP:CD1	2.48	0.48
2:B:523:PRO:HA	2:B:574:ARG:HH12	1.77	0.48
1:D:534:MET:HB2	1:D:612:PHE:CE1	2.49	0.48
1:A:92:PHE:CZ	1:A:240:GLY:HA3	2.48	0.48
1:A:325:ARG:NH2	1:A:379:GLU:OE1	2.46	0.48
1:A:357:TRP:HA	1:A:360:MET:HG2	1.95	0.48
2:E:282:ILE:HD13	2:E:333:MET:HE1	1.94	0.48
2:E:414:ARG:O	2:E:418:VAL:HG23	2.14	0.48
2:E:582:ILE:HD11	2:E:602:PHE:HA	1.94	0.48
2:E:589:ALA:O	2:E:590:HIS:HB2	2.13	0.48
2:E:432:SER:OG	2:E:435:ASP:OD2	2.31	0.47
1:A:530:LYS:HG2	1:D:758:TYR:CZ	2.50	0.47
2:B:110:ARG:HB2	2:B:225:THR:HG21	1.96	0.47
1:A:64:LEU:HD21	1:A:251:VAL:HG11	1.96	0.47
1:A:525:MET:HG3	1:A:615:TYR:HA	1.95	0.47
2:B:160:GLU:CD	2:B:194:ARG:HE	2.20	0.47
1:D:453:VAL:HG13	1:D:495:GLU:HG2	1.97	0.47
2:B:380:TRP:CE3	2:B:383:SER:HB3	2.50	0.47
1:D:313:ASP:O	1:D:314:THR:HG23	2.15	0.47
1:D:437:ASN:OD1	1:D:620:ASN:ND2	2.46	0.47
2:E:245:LEU:HD23	2:E:245:LEU:HA	1.83	0.47
2:E:565:LEU:HD22	2:E:628:MET:HE2	1.96	0.47
1:A:38:THR:HG22	1:A:40:ARG:H	1.78	0.47
1:A:83:ILE:HG12	1:A:456:PHE:CD1	2.50	0.47
1:A:285:PRO:HD3	3:C:157:TRP:CZ3	2.50	0.47
1:D:109:ILE:HG13	1:D:358:VAL:HG22	1.95	0.47
1:D:124:GLU:HG3	1:D:771:VAL:HG22	1.96	0.47
1:A:115:MET:HG2	1:A:155:HIS:CG	2.50	0.47
1:D:466:THR:HG22	1:D:468:VAL:H	1.77	0.47
1:A:492:GLU:HG2	1:A:497:LEU:O	2.15	0.47
1:D:79:ALA:HB2	1:D:236:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ASP:CB	2:B:128:THR:HG21	2.42	0.47
2:B:219:TYR:CE2	2:B:230:THR:HG22	2.50	0.47
1:D:17:ILE:HG23	1:D:128:GLU:OE2	2.15	0.47
2:E:594:ASP:OD1	2:E:594:ASP:N	2.47	0.47
1:A:762:ILE:CD1	1:A:765:LEU:HD12	2.45	0.46
1:D:177:ILE:HG13	7:D:908:HOH:O	2.15	0.46
2:E:242:ARG:HA	2:E:278:LEU:HD11	1.97	0.46
2:B:574:ARG:HG3	2:B:620:GLY:C	2.40	0.46
1:D:65:ARG:O	1:D:69:VAL:HG23	2.15	0.46
2:E:335:ARG:HG2	2:E:335:ARG:HH11	1.81	0.46
2:B:501:SER:HB2	7:B:910:HOH:O	2.15	0.46
1:D:295:ASP:OD2	1:D:297:PRO:HD3	2.15	0.46
2:B:375:ARG:HD2	2:B:385:ILE:HD11	1.97	0.46
1:A:316:MET:HB2	1:A:403:PHE:CE1	2.50	0.46
2:B:22:MET:CE	2:B:406:LEU:HD21	2.46	0.46
2:B:22:MET:HB3	2:B:22:MET:HE3	1.72	0.46
2:E:86:VAL:HG21	2:E:282:ILE:HD11	1.98	0.46
2:E:219:TYR:OH	2:E:279:ALA:HB3	2.16	0.46
2:E:678:ARG:HA	2:E:678:ARG:HD3	1.65	0.46
2:E:332:ASP:HA	2:E:336:LEU:O	2.16	0.46
2:B:406:LEU:HD23	2:B:406:LEU:HA	1.71	0.46
2:B:689:ILE:HB	2:B:696:PHE:HB3	1.98	0.46
2:B:706:LEU:HD11	2:B:710:ARG:HA	1.98	0.46
2:E:359:ASP:HB3	2:E:362:THR:HB	1.97	0.46
1:A:124:GLU:HG3	1:A:771:VAL:HG22	1.98	0.45
2:B:96:LEU:O	2:B:141:THR:HA	2.16	0.45
2:B:405:PHE:HD2	2:B:410:VAL:HB	1.82	0.45
2:E:83:LEU:HB2	2:E:282:ILE:O	2.16	0.45
2:E:379:CYS:HB3	2:E:417:SER:OG	2.15	0.45
2:B:83:LEU:O	2:B:87:VAL:HG23	2.17	0.45
3:C:70:TRP:HB2	3:C:83:TRP:CD1	2.52	0.45
1:D:492:GLU:HG2	1:D:497:LEU:O	2.17	0.45
1:D:663:LYS:HE3	1:D:667:GLY:O	2.14	0.45
2:E:706:LEU:HD11	2:E:710:ARG:HA	1.98	0.45
2:B:184:HIS:CE1	2:B:186:TYR:HH	2.33	0.45
3:C:114:PRO:HA	3:C:117:GLN:O	2.15	0.45
1:D:381:ARG:HA	1:D:775:GLU:HB2	1.98	0.45
2:B:266:THR:HG21	2:B:340:LEU:HD13	1.99	0.45
1:D:364:LEU:HD23	1:D:364:LEU:HA	1.68	0.45
2:B:98:VAL:O	2:B:143:GLY:HA2	2.17	0.45
1:D:302:ASP:OD2	1:D:559:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:PRO:HB3	1:A:590:TRP:CG	2.51	0.45
3:C:40:ILE:O	3:C:44:ARG:HD2	2.17	0.45
1:D:505:LYS:HD3	1:D:505:LYS:HA	1.75	0.45
2:E:21:THR:HG23	2:E:373:GLY:O	2.16	0.45
1:A:381:ARG:HA	1:A:775:GLU:HB2	1.99	0.45
1:A:384:LYS:NZ	1:A:390:PRO:O	2.48	0.45
2:B:113:GLN:HG2	2:B:116:LEU:HD12	1.98	0.45
2:B:714:LEU:HA	2:B:714:LEU:HD23	1.72	0.45
1:D:426:GLU:HG2	1:D:427:GLU:HG2	1.98	0.45
2:E:394:HIS:HB3	2:E:400:LEU:HG	1.99	0.45
2:E:434:GLU:HB3	2:E:661:TYR:CE2	2.52	0.45
2:E:714:LEU:HD23	2:E:714:LEU:HA	1.73	0.45
2:B:657:THR:HG22	2:B:670:GLN:HA	1.98	0.45
1:D:162:TRP:NE1	1:D:163:GLU:HG3	2.32	0.45
7:D:921:HOH:O	2:E:129:HIS:HD2	1.99	0.45
3:F:40:ILE:O	3:F:44:ARG:HD2	2.17	0.45
2:B:379:CYS:HB3	2:B:417:SER:OG	2.17	0.45
1:D:598:GLN:NE2	1:D:600:LYS:HE2	2.31	0.45
1:D:694:VAL:HG23	3:F:91:ALA:O	2.17	0.44
1:A:316:MET:HE1	1:A:406:SER:CB	2.34	0.44
1:A:322:MET:HE3	1:A:324:ILE:HD11	1.98	0.44
2:B:483:THR:HG21	2:B:491:VAL:CG2	2.44	0.44
3:F:49:ASP:OD1	3:F:65:LYS:HB2	2.18	0.44
3:C:96:ARG:HB2	3:C:119:ILE:HB	1.99	0.44
1:A:146:ILE:O	1:A:146:ILE:HG22	2.17	0.44
1:A:317:HIS:HB2	1:A:717:MET:SD	2.58	0.44
2:B:282:ILE:HG23	2:B:283:VAL:HG13	1.99	0.44
1:D:620:ASN:OD1	1:D:622:MET:HE1	2.18	0.44
2:E:310:ILE:H	2:E:472:GLY:HA3	1.82	0.44
2:E:571:MET:HE2	2:E:621:TYR:CD2	2.53	0.44
2:E:98:VAL:O	2:E:143:GLY:HA2	2.17	0.44
2:B:511:GLU:HA	2:B:630:GLY:O	2.17	0.44
2:E:310:ILE:HB	2:E:475:GLY:HA2	1.98	0.44
3:F:70:TRP:CD1	3:F:165:ARG:HG3	2.53	0.44
1:A:199:TYR:CE1	1:A:223:MET:HG3	2.52	0.44
2:B:591:THR:O	2:B:593:ALA:N	2.50	0.44
1:D:519:GLY:HA3	1:D:622:MET:O	2.17	0.44
2:E:222:ARG:O	2:E:223:LYS:HB2	2.18	0.44
1:A:610:GLU:O	1:A:612:PHE:HD1	2.01	0.44
1:D:381:ARG:C	1:D:382:LEU:HD23	2.42	0.44
1:D:467:ALA:HA	1:D:628:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:MET:HB2	1:D:440:GLN:HE22	1.83	0.44
1:D:401:TRP:O	1:D:405:VAL:HG22	2.18	0.44
1:A:761:ASP:OD2	1:A:763:SER:OG	2.28	0.43
1:D:144:SER:HB3	1:D:397:PHE:CD2	2.53	0.43
2:E:522:MET:HG3	2:E:595:TRP:CZ2	2.53	0.43
1:A:194:ARG:N	1:A:394:ARG:O	2.46	0.43
2:B:261:PHE:O	2:B:273:TRP:HD1	2.01	0.43
2:B:678:ARG:HD3	2:B:678:ARG:HA	1.65	0.43
1:D:181:ALA:O	1:D:225:ARG:NH1	2.51	0.43
1:D:316:MET:CE	1:D:406:SER:HB2	2.38	0.43
1:D:754:TYR:N	7:D:913:HOH:O	2.51	0.43
2:E:96:LEU:O	2:E:141:THR:HA	2.18	0.43
2:E:395:MET:HE1	2:E:402:PRO:HB3	2.00	0.43
3:C:88:LYS:NZ	3:C:132:ASP:OD2	2.52	0.43
2:E:516:LYS:HB3	2:E:545:LEU:HD11	2.01	0.43
1:A:392:ASP:HA	1:A:760:MET:O	2.18	0.43
2:B:377:GLY:HA2	2:B:385:ILE:HG21	2.00	0.43
1:D:466:THR:HG22	1:D:467:ALA:N	2.33	0.43
2:E:122:ASP:CB	2:E:128:THR:HG21	2.46	0.43
2:E:315:PHE:O	2:E:347:SER:HA	2.18	0.43
2:E:517:SER:HA	2:E:625:GLY:HA2	2.00	0.43
1:A:275:LEU:HD22	1:A:374:ALA:HB1	2.00	0.43
2:B:299:VAL:HG12	2:B:300:LEU:HD23	1.99	0.43
2:B:310:ILE:H	2:B:472:GLY:CA	2.32	0.43
2:B:390:ILE:CD1	2:B:444:LEU:HD22	2.46	0.43
2:B:589:ALA:O	2:B:590:HIS:HB2	2.18	0.43
1:D:503:GLN:O	1:D:520:PHE:HB2	2.19	0.43
1:A:598:GLN:NE2	1:A:600:LYS:HE2	2.33	0.43
2:B:571:MET:HE3	2:B:621:TYR:HB3	2.01	0.43
1:D:89:GLU:HG3	1:D:456:PHE:CE2	2.54	0.43
2:E:249:SER:OG	2:E:253:LYS:NZ	2.51	0.43
2:E:565:LEU:HB3	2:E:628:MET:CE	2.49	0.43
2:E:631:MET:HB3	2:E:631:MET:HE3	1.63	0.43
2:E:651:GLU:OE1	2:E:654:LYS:HD2	2.18	0.43
1:A:357:TRP:HA	1:A:360:MET:HE3	2.00	0.43
1:A:364:LEU:HD23	1:A:364:LEU:HA	1.81	0.43
1:A:460:ALA:O	1:A:474:HIS:HA	2.19	0.43
2:B:266:THR:HG22	2:B:283:VAL:HG22	2.00	0.43
2:B:486:LEU:HD23	2:B:486:LEU:HA	1.75	0.43
1:D:283:THR:CG2	1:D:284:ILE:N	2.76	0.43
2:E:480:TYR:CG	2:E:481:GLY:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:SER:O	1:A:371:ASN:HB2	2.19	0.43
1:A:111:HIS:HA	1:A:114:THR:OG1	2.19	0.43
2:B:184:HIS:HA	2:B:186:TYR:CE2	2.54	0.43
2:B:394:HIS:CB	2:B:400:LEU:HG	2.39	0.43
3:C:5:ARG:NH1	3:C:40:ILE:HG13	2.34	0.43
1:D:184:PRO:HD2	1:D:535:PHE:CE1	2.54	0.43
2:E:179:VAL:HG21	2:E:232:ILE:HA	2.00	0.43
2:E:550:LEU:O	2:E:554:LYS:HG3	2.19	0.43
1:A:288:TYR:CD1	1:A:322:MET:HE2	2.54	0.43
1:A:558:TYR:OH	1:A:582:ASP:OD2	2.32	0.43
2:B:304:ASN:HB3	2:B:466:PHE:HD1	1.84	0.43
2:B:661:TYR:CZ	2:B:664:LYS:HA	2.53	0.43
1:D:560:PHE:HA	1:D:600:LYS:O	2.18	0.43
1:D:746:GLU:O	1:D:749:ILE:HG13	2.18	0.43
2:E:696:PHE:CE2	2:E:704:THR:HG21	2.51	0.43
2:B:424:GLN:O	2:B:428:PRO:HG2	2.19	0.43
2:B:490:ASP:OD2	2:B:713:HIS:ND1	2.48	0.43
2:B:565:LEU:HD22	2:B:628:MET:HE2	2.01	0.42
2:E:250:ASN:O	2:E:254:GLU:HB2	2.18	0.42
2:E:531:LYS:HG3	2:E:595:TRP:CD1	2.54	0.42
2:E:574:ARG:HG3	2:E:620:GLY:C	2.44	0.42
1:A:285:PRO:HD3	3:C:157:TRP:CE3	2.54	0.42
2:B:147:ARG:HD2	2:B:147:ARG:HA	1.61	0.42
2:B:370:ASP:OD1	2:B:370:ASP:N	2.53	0.42
1:D:187:MET:HB2	1:D:440:GLN:NE2	2.34	0.42
1:D:399:TYR:CD2	1:D:537:MET:HE2	2.54	0.42
1:A:40:ARG:NH1	1:A:45:LYS:HD3	2.34	0.42
1:A:466:THR:HG22	1:A:468:VAL:N	2.34	0.42
1:D:285:PRO:HD3	3:F:157:TRP:CZ3	2.55	0.42
1:A:199:TYR:CD1	1:A:223:MET:HG3	2.54	0.42
1:A:651:ARG:HD2	1:A:652:PHE:CE1	2.54	0.42
1:D:208:ALA:O	1:D:209:ASN:C	2.62	0.42
1:D:445:ASN:ND2	1:D:451:HIS:HB2	2.34	0.42
3:F:72:VAL:HG11	3:F:87:TRP:HB3	2.02	0.42
1:D:121:TYR:O	1:D:125:ASN:ND2	2.35	0.42
2:E:147:ARG:HD2	2:E:147:ARG:HA	1.50	0.42
2:E:657:THR:HG22	2:E:670:GLN:HA	2.00	0.42
1:A:73:GLU:O	1:A:76:LYS:HG2	2.20	0.42
1:A:192:VAL:HG13	1:A:342:TRP:HB3	2.02	0.42
1:A:216:TRP:O	1:A:220:SER:OG	2.23	0.42
1:A:230:TRP:CD1	1:A:230:TRP:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:TYR:CE1	1:A:401:TRP:HB2	2.55	0.42
1:A:439:LEU:O	1:A:454:ASN:HA	2.20	0.42
2:B:704:THR:CG2	2:B:712:PHE:HB3	2.49	0.42
1:D:73:GLU:O	1:D:76:LYS:HG2	2.18	0.42
1:D:297:PRO:HB3	3:F:116:TRP:CH2	2.54	0.42
2:B:110:ARG:O	2:B:111:ALA:HB3	2.20	0.42
2:B:234:GLU:O	2:B:239:GLU:HG2	2.20	0.42
1:D:136:LYS:HG3	1:D:210:ASP:OD1	2.20	0.42
1:D:275:LEU:HD22	1:D:374:ALA:HB1	2.02	0.42
1:D:389:ASN:N	1:D:390:PRO:HD3	2.35	0.42
2:E:315:PHE:HB3	2:E:348:VAL:CG1	2.49	0.42
2:E:567:PRO:HG2	2:E:584:SER:HB3	2.01	0.42
1:A:294:VAL:HG12	1:A:316:MET:HE3	2.01	0.42
1:A:453:VAL:HG13	1:A:495:GLU:HG2	2.02	0.42
2:B:74:THR:HG21	2:B:634:ILE:CD1	2.50	0.42
1:A:316:MET:HE3	1:A:316:MET:HB3	1.76	0.42
1:A:94:LEU:HD12	1:A:169:TRP:O	2.19	0.42
1:A:288:TYR:CG	1:A:322:MET:HE2	2.55	0.42
1:D:147:GLY:HA2	1:D:348:HIS:CG	2.55	0.42
1:D:303:VAL:HA	1:D:608:THR:HG23	2.01	0.42
1:D:314:THR:C	1:D:315:ILE:HG13	2.45	0.42
2:B:21:THR:HG22	2:B:22:MET:HG2	2.01	0.41
2:B:142:ARG:NE	2:B:169:ASP:OD2	2.49	0.41
2:B:523:PRO:HA	2:B:574:ARG:NH1	2.35	0.41
2:B:266:THR:HG23	2:B:280:ARG:O	2.19	0.41
2:B:337:VAL:O	2:B:338:LEU:HD23	2.20	0.41
2:B:471:TYR:HA	2:B:497:ALA:HB1	2.02	0.41
1:D:651:ARG:NH1	7:D:904:HOH:O	2.53	0.41
2:B:571:MET:HE2	2:B:621:TYR:CD2	2.55	0.41
1:D:210:ASP:OD2	1:D:245:ARG:NH2	2.42	0.41
2:E:561:ASP:OD1	2:E:561:ASP:N	2.52	0.41
3:C:118:VAL:O	3:C:135:ALA:HA	2.21	0.41
1:D:96:ASN:OD1	1:D:98:ALA:N	2.53	0.41
1:D:102:LEU:CD2	1:D:264:ALA:HA	2.50	0.41
1:D:146:ILE:HG21	1:D:146:ILE:HD13	1.62	0.41
1:D:433:ALA:HB2	1:D:462:GLY:O	2.20	0.41
2:E:264:MET:HE2	2:E:264:MET:HB2	1.87	0.41
2:E:661:TYR:HB2	2:E:666:TRP:CZ3	2.56	0.41
3:C:70:TRP:CE2	3:C:165:ARG:HG3	2.56	0.41
1:D:384:LYS:HD2	1:D:391:ASP:HB3	2.01	0.41
1:A:184:PRO:O	1:A:535:PHE:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:ASP:CG	3:C:130:LEU:HB3	2.45	0.41
2:B:356:ILE:HB	2:B:388:VAL:HG23	2.03	0.41
2:E:147:ARG:NH1	2:E:148:THR:O	2.54	0.41
2:E:523:PRO:HA	2:E:574:ARG:NH1	2.32	0.41
2:B:245:LEU:HD23	2:B:245:LEU:HA	1.94	0.41
2:E:304:ASN:HB3	2:E:466:PHE:CE1	2.55	0.41
1:A:334:PHE:CE2	1:A:352:PHE:HE2	2.38	0.41
2:B:160:GLU:OE2	2:B:194:ARG:NE	2.35	0.41
2:B:310:ILE:HD12	2:B:475:GLY:HA2	2.02	0.41
1:D:285:PRO:HD3	3:F:157:TRP:CE3	2.56	0.41
2:E:110:ARG:HB2	2:E:225:THR:HG21	2.02	0.41
2:E:480:TYR:HE2	2:E:662:ARG:HH21	1.68	0.41
3:F:67:SER:O	3:F:68:LYS:HB2	2.21	0.41
1:A:533:THR:OG1	1:A:609:GLU:HG2	2.21	0.41
2:B:574:ARG:HH11	2:B:620:GLY:HA3	1.84	0.41
2:E:126:LEU:C	2:E:128:THR:H	2.29	0.41
1:A:614:ASP:O	1:A:615:TYR:HB2	2.21	0.40
2:B:472:GLY:HA3	2:B:475:GLY:H	1.86	0.40
1:D:41:TYR:OH	1:D:100:ASP:OD2	2.35	0.40
2:E:29:ASP:OD1	2:E:33:ASP:N	2.54	0.40
1:A:688:LEU:HD23	1:A:688:LEU:HA	1.90	0.40
2:B:22:MET:HE1	2:B:406:LEU:HD21	2.02	0.40
2:B:195:VAL:O	2:B:199:VAL:HG23	2.21	0.40
2:B:414:ARG:O	2:B:418:VAL:HG23	2.21	0.40
2:E:591:THR:O	2:E:591:THR:OG1	2.23	0.40
1:A:63:ARG:HH12	1:A:254:GLU:CD	2.30	0.40
1:A:345:TYR:CD1	1:A:345:TYR:N	2.83	0.40
1:A:617:LEU:HD23	1:A:617:LEU:HA	1.89	0.40
2:B:119:ALA:O	2:B:120:TYR:C	2.64	0.40
2:B:550:LEU:O	2:B:554:LYS:HG3	2.21	0.40
3:F:108:ARG:O	3:F:109:LEU:HB2	2.21	0.40
3:F:114:PRO:HA	3:F:117:GLN:O	2.22	0.40
2:B:34:PHE:CD1	2:B:34:PHE:C	2.99	0.40
1:D:578:PRO:HB3	1:D:590:TRP:CD1	2.56	0.40
1:A:412:TRP:CG	1:A:431:GLY:HA2	2.56	0.40
1:A:694:VAL:HG22	3:C:93:VAL:HB	2.03	0.40
2:B:13:VAL:HB	2:B:28:VAL:HB	2.03	0.40
2:B:449:ARG:HH11	2:B:449:ARG:HD2	1.78	0.40
3:C:76:CYS:SG	3:C:77:GLY:N	2.94	0.40
1:D:438:TRP:CD2	1:D:458:CYS:SG	3.15	0.40
1:D:762:ILE:CD1	1:D:765:LEU:HD12	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:68:LYS:HG2	3:F:164:GLU:CD	2.46	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	761/776 (98%)	719 (94%)	39 (5%)	3 (0%)	30	54
1	D	761/776 (98%)	717 (94%)	40 (5%)	4 (0%)	24	48
2	B	708/727 (97%)	664 (94%)	42 (6%)	2 (0%)	36	60
2	E	708/727 (97%)	665 (94%)	40 (6%)	3 (0%)	30	54
3	C	164/168 (98%)	157 (96%)	7 (4%)	0	100	100
3	F	164/168 (98%)	158 (96%)	6 (4%)	0	100	100
All	All	3266/3342 (98%)	3080 (94%)	174 (5%)	12 (0%)	30	54

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	ASN
1	D	437	ASN
1	A	551	GLY
2	B	112	VAL
2	B	592	ALA
2	E	112	VAL
2	E	592	ALA
1	D	551	GLY
2	E	590	HIS
1	A	454	ASN
1	D	454	ASN
1	D	609	GLU

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	612/622 (98%)	593 (97%)	19 (3%)	35	65
1	D	612/622 (98%)	593 (97%)	19 (3%)	35	65
2	B	574/589 (98%)	553 (96%)	21 (4%)	30	59
2	E	573/589 (97%)	550 (96%)	23 (4%)	28	56
3	C	155/156 (99%)	152 (98%)	3 (2%)	50	77
3	F	155/156 (99%)	153 (99%)	2 (1%)	61	83
All	All	2681/2734 (98%)	2594 (97%)	87 (3%)	34	64

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

Mol	Chain	Res	Type
1	A	22	GLU
1	A	38	THR
1	A	62	SER
1	A	176	VAL
1	A	179	THR
1	A	192	VAL
1	A	201	ILE
1	A	206	VAL
1	A	247	LEU
1	A	290	GLN
1	A	294	VAL
1	A	354	SER
1	A	454	ASN
1	A	461	ASN
1	A	495	GLU
1	A	497	LEU
1	A	559	ARG
1	A	770	THR
1	A	774	VAL
2	B	88	GLN
2	B	121	GLU
2	B	128	THR

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Mol	Chain	Res	Type
2	B	155	VAL
2	B	328	LYS
2	B	339	SER
2	B	340	LEU
2	B	421	ILE
2	B	429	LEU
2	B	454	SER
2	B	516	LYS
2	B	524	THR
2	B	561	ASP
2	B	588	GLN
2	B	622	SER
2	B	631	MET
2	B	634	ILE
2	B	652	SER
2	B	655	ILE
2	B	694	THR
2	B	714	LEU
3	C	69	LYS
3	C	90	SER
3	C	118	VAL
1	D	22	GLU
1	D	38	THR
1	D	104	THR
1	D	136	LYS
1	D	176	VAL
1	D	179	THR
1	D	192	VAL
1	D	206	VAL
1	D	247	LEU
1	D	314	THR
1	D	354	SER
1	D	359	MET
1	D	454	ASN
1	D	495	GLU
1	D	497	LEU
1	D	559	ARG
1	D	567	LEU
1	D	620	ASN
1	D	774	VAL
2	E	88	GLN
2	E	121	GLU

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Mol	Chain	Res	Type
2	E	128	THR
2	E	155	VAL
2	E	317	VAL
2	E	321	THR
2	E	328	LYS
2	E	339	SER
2	E	340	LEU
2	E	391	SER
2	E	421	ILE
2	E	429	LEU
2	E	454	SER
2	E	526	THR
2	E	561	ASP
2	E	586	LEU
2	E	588	GLN
2	E	622	SER
2	E	627	ILE
2	E	631	MET
2	E	634	ILE
2	E	652	SER
2	E	655	ILE
3	F	90	SER
3	F	118	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	ASN
1	A	445	ASN
1	A	587	ASN
2	B	12	GLN
2	B	129	HIS
2	B	154	GLN
2	B	578	ASN
1	D	432	ASN
1	D	437	ASN
1	D	440	GLN
1	D	445	ASN
1	D	587	ASN
1	D	620	ASN
1	D	682	GLN
2	E	521	ASN

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Mol	Chain	Res	Type
2	E	572	GLN
2	E	578	ASN
2	E	603	ASN
3	F	78	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	E	801	-	4,4,4	0.28	0	6,6,6	0.48	0
5	SO4	B	801	-	4,4,4	0.29	0	6,6,6	0.53	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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, 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	763/776 (98%)	0.09	5 (0%)	84 83	27, 45, 63, 108	0
1	D	763/776 (98%)	0.11	2 (0%)	90 89	32, 46, 65, 97	0
2	B	710/727 (97%)	0.39	17 (2%)	59 56	35, 65, 98, 123	0
2	E	710/727 (97%)	0.50	34 (4%)	35 32	34, 64, 108, 134	0
3	C	166/168 (98%)	0.14	1 (0%)	85 85	33, 49, 67, 84	0
3	F	166/168 (98%)	0.17	2 (1%)	76 75	38, 53, 70, 92	0
All	All	3278/3342 (98%)	0.26	61 (1%)	66 63	27, 52, 94, 134	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	8	LEU	4.8
2	B	411	LYS	4.3
2	E	411	LYS	3.8
2	E	655	ILE	3.6
2	E	694	THR	3.6
2	E	660	PHE	3.5
2	E	400	LEU	3.4
2	B	472	GLY	3.3
2	E	472	GLY	3.1
2	B	643	PRO	3.1
2	B	243	GLN	3.0
2	E	717	VAL	3.0
2	E	8	LEU	3.0
3	C	2	ALA	3.0
2	B	660	PHE	3.0
2	E	473	GLY	2.9
2	E	643	PRO	2.9
2	B	693	ALA	2.9
2	E	51	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	555	LEU	2.6
2	E	479	THR	2.6
2	E	697	VAL	2.6
2	E	474	ALA	2.6
3	F	2	ALA	2.5
2	E	648	THR	2.5
2	E	663	LYS	2.5
2	B	410	VAL	2.5
2	E	433	VAL	2.5
2	E	79	GLY	2.5
2	E	699	PRO	2.5
2	B	400	LEU	2.4
1	D	297	PRO	2.4
3	F	93	VAL	2.4
2	E	241	SER	2.4
2	E	313	THR	2.4
1	A	665	ALA	2.4
2	E	437	ALA	2.3
2	E	243	GLN	2.3
2	E	436	ALA	2.3
2	B	366	LYS	2.3
2	B	24	ASP	2.3
2	E	703	GLU	2.2
2	B	75	GLY	2.2
2	E	662	ARG	2.2
2	E	444	LEU	2.2
1	D	656	VAL	2.2
2	E	642	GLU	2.2
2	B	694	THR	2.2
2	E	408	GLY	2.2
2	B	592	ALA	2.1
1	A	662	ARG	2.1
2	E	410	VAL	2.1
1	A	14	THR	2.1
2	E	398	GLY	2.1
2	B	479	THR	2.1
2	B	684	MET	2.1
1	A	146	ILE	2.1
2	B	361	TYR	2.1
2	E	365	ILE	2.1
1	A	304	ARG	2.0
2	E	399	TYR	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 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($\text{\AA}^2$)	Q<0.9
5	SO4	E	801	5/5	0.79	0.19	97,104,106,113	0
5	SO4	B	801	5/5	0.81	0.13	73,75,88,89	0
4	MN	A	801	1/1	0.99	0.02	31,31,31,31	0
4	MN	D	801	1/1	0.99	0.03	28,28,28,28	0
6	ZN	C	201	1/1	0.99	0.03	53,53,53,53	1
6	ZN	F	201	1/1	0.99	0.02	52,52,52,52	1

6.5 Other polymers [i](#)

There are no such residues in this entry.