



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:52 AM GMT

PDB ID : 3NAZ
Title : Basal state form of Yeast Glycogen Synthase
Authors : Baskaran, S.; Hurley, T.D.
Deposited on : 2010-06-02
Resolution : 3.00 Å(reported)

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

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

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

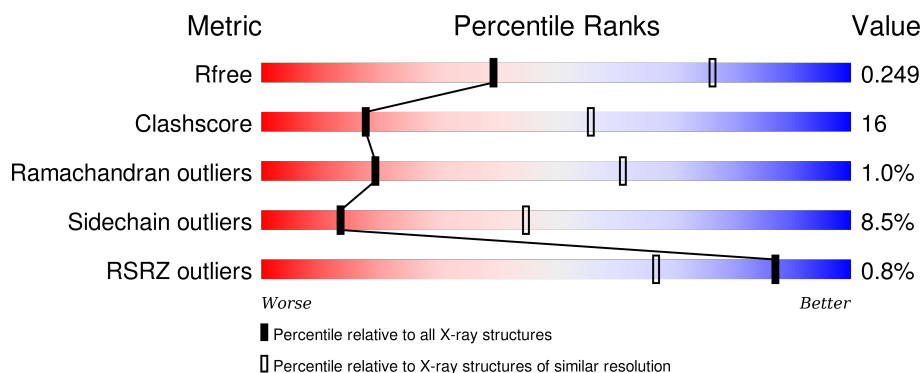
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	725	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 55%, green 26%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 55% 26% • 16% </div> </div>
1	B	725	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 53%, green 27%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 53% 27% • 16% </div> </div>
1	C	725	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 57%, green 24%, orange 1%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 57% 24% • 15% </div> </div>
1	D	725	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 57%, green 23%, orange 1%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 57% 23% • 15% </div> </div>
2	E	6	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 83%, grey 17%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 83% 17% </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	6	 <div>83%17%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	D	801	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19851 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 Glycogen [starch] synthase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4923	3148	857	899	19			
1	B	611	Total	C	N	O	S	0	0	0
			4923	3148	857	899	19			
1	C	613	Total	C	N	O	S	0	0	0
			4935	3154	860	902	19			
1	D	613	Total	C	N	O	S	0	0	0
			4935	3154	860	902	19			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P27472
A	-18	GLY	-	EXPRESSION TAG	UNP P27472
A	-17	SER	-	EXPRESSION TAG	UNP P27472
A	-16	SER	-	EXPRESSION TAG	UNP P27472
A	-15	HIS	-	EXPRESSION TAG	UNP P27472
A	-14	HIS	-	EXPRESSION TAG	UNP P27472
A	-13	HIS	-	EXPRESSION TAG	UNP P27472
A	-12	HIS	-	EXPRESSION TAG	UNP P27472
A	-11	HIS	-	EXPRESSION TAG	UNP P27472
A	-10	HIS	-	EXPRESSION TAG	UNP P27472
A	-9	SER	-	EXPRESSION TAG	UNP P27472
A	-8	SER	-	EXPRESSION TAG	UNP P27472
A	-7	GLY	-	EXPRESSION TAG	UNP P27472
A	-6	LEU	-	EXPRESSION TAG	UNP P27472
A	-5	VAL	-	EXPRESSION TAG	UNP P27472
A	-4	PRO	-	EXPRESSION TAG	UNP P27472
A	-3	ARG	-	EXPRESSION TAG	UNP P27472
A	-2	GLY	-	EXPRESSION TAG	UNP P27472
A	-1	SER	-	EXPRESSION TAG	UNP P27472
A	0	HIS	-	EXPRESSION TAG	UNP P27472
A	535	SER	ALA	SEE REMARK 999	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
A	580	ALA	ARG	ENGINEERED MUTATION	UNP P27472
A	581	ALA	ARG	ENGINEERED MUTATION	UNP P27472
A	583	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	-19	MET	-	EXPRESSION TAG	UNP P27472
B	-18	GLY	-	EXPRESSION TAG	UNP P27472
B	-17	SER	-	EXPRESSION TAG	UNP P27472
B	-16	SER	-	EXPRESSION TAG	UNP P27472
B	-15	HIS	-	EXPRESSION TAG	UNP P27472
B	-14	HIS	-	EXPRESSION TAG	UNP P27472
B	-13	HIS	-	EXPRESSION TAG	UNP P27472
B	-12	HIS	-	EXPRESSION TAG	UNP P27472
B	-11	HIS	-	EXPRESSION TAG	UNP P27472
B	-10	HIS	-	EXPRESSION TAG	UNP P27472
B	-9	SER	-	EXPRESSION TAG	UNP P27472
B	-8	SER	-	EXPRESSION TAG	UNP P27472
B	-7	GLY	-	EXPRESSION TAG	UNP P27472
B	-6	LEU	-	EXPRESSION TAG	UNP P27472
B	-5	VAL	-	EXPRESSION TAG	UNP P27472
B	-4	PRO	-	EXPRESSION TAG	UNP P27472
B	-3	ARG	-	EXPRESSION TAG	UNP P27472
B	-2	GLY	-	EXPRESSION TAG	UNP P27472
B	-1	SER	-	EXPRESSION TAG	UNP P27472
B	0	HIS	-	EXPRESSION TAG	UNP P27472
B	535	SER	ALA	SEE REMARK 999	UNP P27472
B	580	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	581	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	583	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	-19	MET	-	EXPRESSION TAG	UNP P27472
C	-18	GLY	-	EXPRESSION TAG	UNP P27472
C	-17	SER	-	EXPRESSION TAG	UNP P27472
C	-16	SER	-	EXPRESSION TAG	UNP P27472
C	-15	HIS	-	EXPRESSION TAG	UNP P27472
C	-14	HIS	-	EXPRESSION TAG	UNP P27472
C	-13	HIS	-	EXPRESSION TAG	UNP P27472
C	-12	HIS	-	EXPRESSION TAG	UNP P27472
C	-11	HIS	-	EXPRESSION TAG	UNP P27472
C	-10	HIS	-	EXPRESSION TAG	UNP P27472
C	-9	SER	-	EXPRESSION TAG	UNP P27472
C	-8	SER	-	EXPRESSION TAG	UNP P27472
C	-7	GLY	-	EXPRESSION TAG	UNP P27472
C	-6	LEU	-	EXPRESSION TAG	UNP P27472
C	-5	VAL	-	EXPRESSION TAG	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	EXPRESSION TAG	UNP P27472
C	-3	ARG	-	EXPRESSION TAG	UNP P27472
C	-2	GLY	-	EXPRESSION TAG	UNP P27472
C	-1	SER	-	EXPRESSION TAG	UNP P27472
C	0	HIS	-	EXPRESSION TAG	UNP P27472
C	535	SER	ALA	SEE REMARK 999	UNP P27472
C	580	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	581	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	583	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	-19	MET	-	EXPRESSION TAG	UNP P27472
D	-18	GLY	-	EXPRESSION TAG	UNP P27472
D	-17	SER	-	EXPRESSION TAG	UNP P27472
D	-16	SER	-	EXPRESSION TAG	UNP P27472
D	-15	HIS	-	EXPRESSION TAG	UNP P27472
D	-14	HIS	-	EXPRESSION TAG	UNP P27472
D	-13	HIS	-	EXPRESSION TAG	UNP P27472
D	-12	HIS	-	EXPRESSION TAG	UNP P27472
D	-11	HIS	-	EXPRESSION TAG	UNP P27472
D	-10	HIS	-	EXPRESSION TAG	UNP P27472
D	-9	SER	-	EXPRESSION TAG	UNP P27472
D	-8	SER	-	EXPRESSION TAG	UNP P27472
D	-7	GLY	-	EXPRESSION TAG	UNP P27472
D	-6	LEU	-	EXPRESSION TAG	UNP P27472
D	-5	VAL	-	EXPRESSION TAG	UNP P27472
D	-4	PRO	-	EXPRESSION TAG	UNP P27472
D	-3	ARG	-	EXPRESSION TAG	UNP P27472
D	-2	GLY	-	EXPRESSION TAG	UNP P27472
D	-1	SER	-	EXPRESSION TAG	UNP P27472
D	0	HIS	-	EXPRESSION TAG	UNP P27472
D	535	SER	ALA	SEE REMARK 999	UNP P27472
D	580	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	581	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	583	ALA	ARG	ENGINEERED MUTATION	UNP P27472

- Molecule 2 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	F	6	Total	C	N	O	0	0	0
			30	18	6	6			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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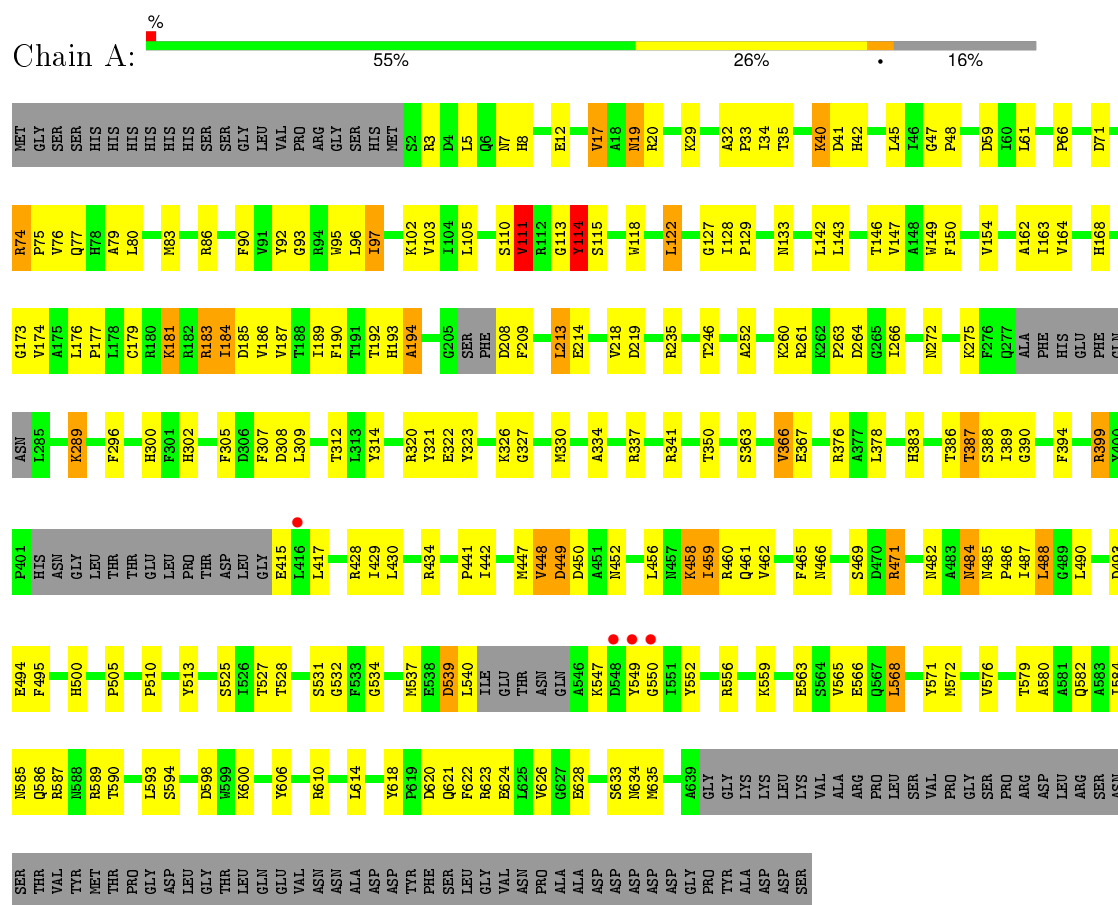
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

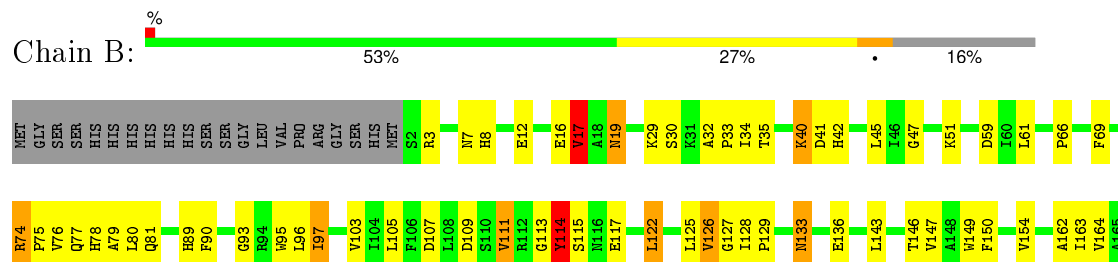
3 Residue-property plots

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

• Molecule 1: Glycogen [starch] synthase isoform 2



• Molecule 1: Glycogen [starch] synthase isoform 2



15%

17%

17%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.53Å 166.15Å 121.03Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	48.03 – 3.00 48.03 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.03-3.00) 99.1 (48.03-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.203 , 0.254 0.197 , 0.249	Depositor DCC
R_{free} test set	3715 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 73751 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19851	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.41	0/5038	0.55	0/6819
1	B	0.40	0/5038	0.54	0/6819
1	C	0.38	0/5050	0.55	0/6835
1	D	0.40	0/5050	0.55	0/6835
All	All	0.39	0/20176	0.55	0/27308

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4923	0	4850	162	0
1	B	4923	0	4850	170	0
1	C	4935	0	4859	163	0
1	D	4935	0	4859	148	0
2	E	25	0	7	0	0
2	F	30	0	8	1	0
3	A	20	0	0	1	0
3	B	20	0	0	0	0
3	C	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	20	0	0	1	0
All	All	19851	0	19433	626	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 16.

All (626) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:THR:HG22	1:C:350:THR:HB	1.35	1.06
1:D:314:TYR:H	1:D:500:HIS:HD2	1.03	1.00
1:C:29:LYS:HG3	1:C:97:ILE:HG21	1.45	0.98
1:B:29:LYS:HG3	1:B:97:ILE:HG21	1.46	0.98
1:D:332:ILE:HD13	1:D:459:ILE:HG22	1.47	0.95
1:A:235:ARG:HH21	1:A:260:LYS:HG3	1.35	0.92
1:B:484:ASN:H	1:B:484:ASN:HD22	1.17	0.91
1:C:442:ILE:HD12	1:C:459:ILE:HD11	1.53	0.90
1:C:550:GLY:HA3	1:C:590:THR:HG22	1.53	0.89
1:D:442:ILE:HD12	1:D:459:ILE:HD11	1.55	0.88
1:B:192:THR:HG22	1:B:246:THR:HG22	1.55	0.87
1:A:29:LYS:HG3	1:A:97:ILE:HG21	1.56	0.87
1:B:482:ASN:HB3	1:B:484:ASN:ND2	1.89	0.87
1:A:550:GLY:HA3	1:A:590:THR:HG22	1.57	0.85
1:C:443:VAL:CG2	1:C:456:LEU:HD21	2.05	0.85
1:C:284:ASN:N	1:C:284:ASN:HD22	1.75	0.84
1:D:29:LYS:HG3	1:D:97:ILE:HG21	1.57	0.84
1:A:482:ASN:HB3	1:A:484:ASN:HD21	1.42	0.84
1:B:266:ILE:HG22	1:B:268:PRO:HD3	1.60	0.83
1:C:484:ASN:H	1:C:484:ASN:HD22	1.20	0.82
1:B:314:TYR:H	1:B:500:HIS:HD2	1.29	0.81
1:A:552:TYR:HD1	1:A:571:TYR:CD2	1.98	0.81
1:D:314:TYR:H	1:D:500:HIS:CD2	1.95	0.80
1:A:95:TRP:CE3	1:A:97:ILE:HD11	2.16	0.80
1:B:95:TRP:CE3	1:B:97:ILE:HD11	2.17	0.80
1:C:133:ASN:HD22	1:C:133:ASN:H	1.28	0.80
1:A:17:VAL:HG21	1:A:47:GLY:HA3	1.65	0.79
1:A:95:TRP:CD2	1:A:97:ILE:HD11	2.17	0.79
1:C:95:TRP:CD2	1:C:97:ILE:HD11	2.18	0.79
1:C:443:VAL:HG21	1:C:456:LEU:HD21	1.63	0.79
1:A:550:GLY:HA3	1:A:590:THR:CG2	2.13	0.79
1:B:442:ILE:HD12	1:B:459:ILE:HD11	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ILE:HD12	1:A:459:ILE:HD11	1.64	0.78
1:B:448:VAL:O	1:B:449:ASP:HB2	1.84	0.78
1:C:550:GLY:HA3	1:C:590:THR:CG2	2.13	0.77
1:D:579:THR:HG23	1:D:582:GLN:OE1	1.85	0.77
1:C:484:ASN:ND2	1:C:484:ASN:H	1.82	0.77
1:C:122:LEU:HD13	1:C:128:ILE:HB	1.67	0.76
1:C:54:TYR:HE1	1:C:60:ILE:HD11	1.48	0.76
1:B:528:THR:HG22	1:B:530:VAL:H	1.51	0.76
1:B:549:TYR:O	1:B:590:THR:HG22	1.86	0.76
1:D:484:ASN:HD22	1:D:484:ASN:H	1.33	0.75
1:D:17:VAL:HG23	1:D:18:ALA:H	1.51	0.75
1:B:484:ASN:ND2	1:B:484:ASN:H	1.84	0.75
1:A:74:ARG:NH1	1:A:77:GLN:OE1	2.20	0.75
1:A:482:ASN:HB3	1:A:484:ASN:ND2	2.00	0.74
1:A:549:TYR:O	1:A:590:THR:HG22	1.87	0.74
1:A:308:ASP:O	1:A:312:THR:HG23	1.86	0.74
1:C:95:TRP:CE3	1:C:97:ILE:HD11	2.22	0.74
1:A:487:ILE:HG22	1:A:488:LEU:N	2.02	0.74
1:A:484:ASN:ND2	1:A:484:ASN:H	1.85	0.74
1:A:122:LEU:HD13	1:A:128:ILE:HB	1.70	0.74
1:A:12:GLU:HB3	1:A:45:LEU:HD23	1.70	0.74
1:A:383:HIS:O	1:A:387:THR:HG23	1.88	0.74
1:B:59:ASP:HB2	1:B:96:LEU:HD21	1.68	0.73
1:C:314:TYR:H	1:C:500:HIS:HD2	1.33	0.73
1:A:386:THR:HG21	1:C:390:GLY:HA2	1.70	0.73
1:A:484:ASN:H	1:A:484:ASN:HD22	1.35	0.73
1:D:264:ASP:O	1:D:635:MET:HG3	1.88	0.73
1:D:550:GLY:HA3	1:D:590:THR:CG2	2.18	0.73
1:D:448:VAL:O	1:D:449:ASP:HB2	1.90	0.72
1:A:623:ARG:HG3	1:A:628:GLU:O	1.89	0.72
1:B:235:ARG:HH21	1:B:260:LYS:HG3	1.54	0.72
1:B:528:THR:CG2	1:B:530:VAL:HG22	2.20	0.72
1:B:17:VAL:HG21	1:B:47:GLY:HA3	1.72	0.71
1:B:311:ASN:HD21	1:B:348:LYS:HD2	1.55	0.71
1:D:192:THR:HG22	1:D:246:THR:HG22	1.71	0.71
1:B:482:ASN:HB3	1:B:484:ASN:HD21	1.53	0.70
1:A:32:ALA:HB3	1:A:33:PRO:HD3	1.72	0.70
1:C:448:VAL:O	1:C:449:ASP:HB2	1.92	0.69
1:D:133:ASN:H	1:D:133:ASN:HD22	1.38	0.69
1:B:32:ALA:HB3	1:B:33:PRO:HD3	1.71	0.69
1:C:163:ILE:HB	1:C:186:VAL:HG12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:VAL:O	1:A:177:PRO:HD2	1.93	0.69
1:A:323:TYR:OH	1:A:458:LYS:HG3	1.93	0.69
1:D:550:GLY:HA3	1:D:590:THR:HG22	1.73	0.69
1:B:299:GLY:HA2	1:B:375:VAL:HG21	1.74	0.69
1:B:351:VAL:HB	1:B:472:VAL:HG12	1.75	0.69
1:A:59:ASP:HB2	1:A:96:LEU:HD21	1.76	0.68
1:A:314:TYR:H	1:A:500:HIS:HD2	1.41	0.68
1:B:254:GLU:HG3	1:B:258:LEU:HD12	1.73	0.68
1:C:192:THR:HG22	1:C:246:THR:HG22	1.73	0.68
1:A:17:VAL:CG2	1:A:47:GLY:HA3	2.24	0.68
1:B:567:GLN:HG2	1:B:571:TYR:CE1	2.30	0.67
1:C:17:VAL:HG23	1:C:18:ALA:H	1.57	0.67
1:C:383:HIS:O	1:C:387:THR:HG23	1.94	0.67
1:C:174:VAL:O	1:C:177:PRO:HD2	1.94	0.67
1:B:550:GLY:HA3	1:B:590:THR:HG22	1.76	0.67
1:A:3:ARG:NH1	1:A:185:ASP:OD2	2.26	0.67
1:A:320:ARG:NH1	1:A:322:GLU:OE2	2.27	0.67
1:C:484:ASN:HD22	1:C:484:ASN:N	1.92	0.67
1:C:443:VAL:HG12	1:C:445:HIS:H	1.60	0.66
1:D:549:TYR:O	1:D:590:THR:HG22	1.95	0.66
1:A:127:GLY:O	1:A:129:PRO:HD3	1.94	0.66
1:B:447:MET:HG3	1:B:456:LEU:HD11	1.78	0.66
1:B:17:VAL:CG2	1:B:47:GLY:HA3	2.27	0.65
1:A:80:LEU:HD22	1:A:90:PHE:CZ	2.31	0.65
1:B:264:ASP:O	1:B:635:MET:HG3	1.96	0.65
1:C:579:THR:HG23	1:C:582:GLN:OE1	1.97	0.65
1:B:586:GLN:O	1:B:590:THR:HG23	1.97	0.65
1:B:320:ARG:NH1	1:B:322:GLU:OE2	2.30	0.65
1:C:299:GLY:HA2	1:C:375:VAL:HG21	1.77	0.64
1:D:484:ASN:H	1:D:484:ASN:ND2	1.94	0.64
1:A:181:LYS:HD3	1:A:181:LYS:C	2.17	0.64
1:A:114:TYR:HD1	1:A:114:TYR:H	1.43	0.64
1:B:552:TYR:HD1	1:B:571:TYR:CD2	2.15	0.64
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.33	0.64
1:B:133:ASN:ND2	1:B:133:ASN:H	1.96	0.64
1:D:122:LEU:HD13	1:D:128:ILE:HB	1.78	0.64
1:D:74:ARG:NH1	1:D:77:GLN:OE1	2.30	0.63
1:A:429:ILE:HG12	1:C:397:ALA:HB1	1.80	0.63
1:B:133:ASN:HD22	1:B:133:ASN:H	1.47	0.63
1:D:59:ASP:HB2	1:D:96:LEU:HD21	1.81	0.63
1:D:271:LEU:HD13	1:D:520:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:ILE:HG22	1:B:488:LEU:N	2.13	0.63
1:C:549:TYR:O	1:C:590:THR:HG22	1.98	0.63
1:A:618:TYR:HB3	1:A:621:GLN:HG3	1.80	0.63
1:C:181:LYS:HD3	1:C:181:LYS:O	1.99	0.63
1:A:66:PRO:O	1:A:74:ARG:NH2	2.32	0.62
1:A:192:THR:CG2	1:A:246:THR:HG22	2.29	0.62
1:A:314:TYR:H	1:A:500:HIS:CD2	2.16	0.62
1:D:180:ARG:HH11	1:D:180:ARG:CG	2.12	0.62
1:D:383:HIS:O	1:D:387:THR:HG23	1.97	0.62
1:B:8:HIS:HB2	1:B:162:ALA:O	1.99	0.62
1:C:447:MET:HG3	1:C:456:LEU:HD11	1.81	0.62
1:D:198:GLY:HA3	1:D:254:GLU:OE1	2.00	0.62
1:C:32:ALA:HB3	1:C:33:PRO:HD3	1.81	0.62
1:B:252:ALA:HB2	1:B:266:ILE:HD11	1.79	0.62
1:A:192:THR:HG22	1:A:246:THR:HG22	1.82	0.62
1:C:572:MET:O	1:C:576:VAL:HG23	2.00	0.62
1:D:168:HIS:HD2	1:D:193:HIS:NE2	1.97	0.62
1:D:314:TYR:N	1:D:500:HIS:HD2	1.87	0.61
1:C:322:GLU:HB2	1:C:326:LYS:HG2	1.81	0.61
1:D:585:ASN:HB3	1:D:589:ARG:NH2	2.15	0.61
1:C:284:ASN:N	1:C:284:ASN:ND2	2.45	0.61
1:A:580:ALA:O	1:A:584:ILE:HG13	2.01	0.61
1:D:213:LEU:C	1:D:213:LEU:HD12	2.22	0.61
1:B:80:LEU:HB3	1:B:90:PHE:CZ	2.36	0.60
1:D:634:ASN:HB2	1:D:637:ALA:H	1.66	0.60
1:D:299:GLY:HA2	1:D:375:VAL:HG21	1.82	0.60
1:B:550:GLY:HA3	1:B:590:THR:CG2	2.31	0.60
1:B:528:THR:HG22	1:B:530:VAL:HG22	1.82	0.60
1:D:79:ALA:O	1:D:83:MET:HG2	2.02	0.60
1:C:482:ASN:HB3	1:C:484:ASN:ND2	2.16	0.59
1:A:320:ARG:NH2	3:A:802:SO4:O1	2.35	0.59
1:D:455:ILE:O	1:D:459:ILE:HG23	2.02	0.59
1:C:19:ASN:N	1:C:19:ASN:HD22	2.00	0.59
1:C:442:ILE:HG13	1:C:443:VAL:HG23	1.85	0.59
1:C:425:LEU:O	1:C:429:ILE:HG13	2.03	0.59
1:A:252:ALA:HB2	1:A:266:ILE:HD11	1.85	0.59
1:A:448:VAL:O	1:A:449:ASP:HB2	2.02	0.59
1:C:458:LYS:HE3	1:C:461:GLN:OE1	2.03	0.59
1:B:213:LEU:HD21	1:B:253:PHE:CE1	2.37	0.59
1:B:309:LEU:HA	1:B:312:THR:HG23	1.84	0.59
1:C:612:LEU:HD21	1:C:616:ARG:HH21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:HD22	1:A:90:PHE:CE1	2.38	0.58
1:C:389:ILE:HD11	1:C:417:LEU:HD21	1.83	0.58
1:A:307:PHE:O	1:C:399:ARG:NH2	2.36	0.58
1:A:235:ARG:HH21	1:A:260:LYS:CG	2.14	0.58
1:B:626:VAL:HG12	1:B:628:GLU:HG2	1.86	0.58
1:B:390:GLY:HA2	1:D:386:THR:HG21	1.85	0.58
1:C:54:TYR:CE1	1:C:60:ILE:HD11	2.35	0.58
1:D:180:ARG:HH11	1:D:180:ARG:HG3	1.69	0.58
1:A:213:LEU:C	1:A:213:LEU:HD12	2.24	0.58
1:B:193:HIS:O	1:B:194:ALA:HB2	2.03	0.58
1:A:19:ASN:N	1:A:19:ASN:HD22	2.01	0.58
1:D:448:VAL:O	1:D:449:ASP:CB	2.52	0.58
1:A:181:LYS:HD3	1:A:181:LYS:O	2.04	0.58
1:A:447:MET:HG3	1:A:456:LEU:HD11	1.84	0.58
1:C:176:LEU:HB2	1:C:177:PRO:HD3	1.85	0.57
1:C:487:ILE:HG22	1:C:488:LEU:N	2.20	0.57
1:A:606:TYR:O	1:A:610:ARG:HG3	2.04	0.57
1:B:323:TYR:OH	1:B:458:LYS:HG3	2.04	0.57
1:B:181:LYS:HD3	1:B:181:LYS:O	2.04	0.57
1:A:302:HIS:O	1:A:434:ARG:HD2	2.05	0.57
1:C:210:TYR:CE1	1:C:250:ILE:HD11	2.39	0.57
1:D:54:TYR:HE1	1:D:60:ILE:HD11	1.70	0.57
1:C:134:ASP:OD2	1:C:137:THR:HG23	2.03	0.57
1:D:181:LYS:C	1:D:181:LYS:HD3	2.25	0.57
1:B:122:LEU:HD13	1:B:128:ILE:HB	1.86	0.57
1:C:314:TYR:H	1:C:500:HIS:CD2	2.19	0.57
1:A:585:ASN:HB3	1:A:589:ARG:NH2	2.19	0.57
1:B:80:LEU:HD22	1:B:90:PHE:CE1	2.40	0.57
1:B:439:LEU:HD22	1:B:467:SER:HA	1.87	0.56
1:B:78:HIS:O	1:B:81:GLN:HB2	2.05	0.56
1:C:612:LEU:HD21	1:C:616:ARG:NH2	2.20	0.56
1:A:386:THR:HG21	1:C:390:GLY:CA	2.35	0.56
1:D:12:GLU:HB3	1:D:45:LEU:HD23	1.87	0.56
1:D:12:GLU:OE2	1:D:168:HIS:HE1	1.87	0.56
1:B:213:LEU:HD21	1:B:253:PHE:HE1	1.69	0.56
1:A:163:ILE:HB	1:A:186:VAL:HG12	1.88	0.56
1:D:309:LEU:HA	1:D:312:THR:HG23	1.88	0.56
1:D:227:ILE:HD12	1:D:230:ARG:HD2	1.87	0.56
1:A:208:ASP:OD1	1:A:209:PHE:N	2.38	0.56
1:B:580:ALA:O	1:B:584:ILE:HG13	2.06	0.56
1:D:95:TRP:CE3	1:D:97:ILE:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:VAL:HG23	1:C:219:ASP:N	2.20	0.56
1:A:168:HIS:HD2	1:A:193:HIS:NE2	2.04	0.56
1:A:305:PHE:HZ	1:A:309:LEU:HG	1.71	0.55
1:B:399:ARG:NH2	1:D:308:ASP:HA	2.21	0.55
1:B:3:ARG:NH1	1:B:185:ASP:OD2	2.39	0.55
1:B:623:ARG:HG3	1:B:628:GLU:O	2.07	0.55
1:D:176:LEU:HD12	1:D:237:ALA:HB1	1.88	0.55
1:C:338:LEU:HD22	1:C:338:LEU:O	2.07	0.55
1:B:383:HIS:O	1:B:387:THR:HG23	2.07	0.55
1:D:448:VAL:O	1:D:448:VAL:HG12	2.07	0.55
1:B:305:PHE:HZ	1:B:309:LEU:HG	1.72	0.55
1:A:487:ILE:CG2	1:A:488:LEU:N	2.69	0.55
1:B:386:THR:HG21	1:D:390:GLY:CA	2.37	0.55
1:A:92:TYR:OH	1:A:102:LYS:HD3	2.07	0.55
1:B:181:LYS:HD3	1:B:181:LYS:C	2.26	0.55
1:C:59:ASP:HB2	1:C:96:LEU:HD21	1.89	0.55
1:C:149:TRP:HD1	1:C:149:TRP:O	1.89	0.55
1:B:12:GLU:HB3	1:B:45:LEU:HD23	1.88	0.55
1:B:127:GLY:O	1:B:129:PRO:HD3	2.06	0.55
1:B:471:ARG:HA	1:B:471:ARG:NE	2.22	0.54
1:A:113:GLY:C	1:A:115:SER:H	2.11	0.54
1:D:32:ALA:HB3	1:D:33:PRO:HD3	1.88	0.54
1:B:447:MET:HG3	1:B:456:LEU:CD1	2.36	0.54
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.90	0.54
1:A:146:THR:O	1:A:149:TRP:HB3	2.06	0.54
1:A:296:PHE:CE1	1:A:487:ILE:HG23	2.42	0.54
1:C:458:LYS:O	1:C:458:LYS:HD3	2.07	0.54
1:A:179:CYS:HA	1:A:184:ILE:HG13	1.88	0.54
1:C:3:ARG:NH1	1:C:185:ASP:OD2	2.39	0.54
1:C:504:PHE:CD2	1:C:515:PRO:HB3	2.43	0.54
1:C:218:VAL:HG23	1:C:219:ASP:H	1.74	0.53
1:A:622:PHE:CE1	1:A:626:VAL:HG21	2.43	0.53
1:C:254:GLU:HG3	1:C:258:LEU:HD12	1.89	0.53
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.90	0.53
1:D:181:LYS:HD3	1:D:181:LYS:O	2.08	0.53
1:D:252:ALA:HB2	1:D:266:ILE:HD11	1.90	0.53
1:D:459:ILE:HA	1:D:462:VAL:HG22	1.91	0.53
1:A:307:PHE:HD1	1:A:312:THR:HG21	1.73	0.53
1:D:565:VAL:O	1:D:569:VAL:HG23	2.09	0.53
1:D:208:ASP:OD2	1:D:209:PHE:N	2.42	0.53
1:A:449:ASP:OD2	1:A:452:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLY:C	1:B:115:SER:H	2.12	0.53
1:C:112:ARG:O	1:C:115:SER:HB2	2.09	0.53
1:B:314:TYR:H	1:B:500:HIS:CD2	2.19	0.53
1:A:552:TYR:N	1:A:552:TYR:CD2	2.77	0.53
1:A:114:TYR:CD1	1:A:114:TYR:N	2.77	0.53
1:C:490:LEU:HD13	1:C:495:PHE:HA	1.90	0.53
1:D:482:ASN:HB3	1:D:484:ASN:ND2	2.23	0.53
1:C:181:LYS:C	1:C:181:LYS:HD3	2.29	0.53
1:D:17:VAL:HG23	1:D:18:ALA:N	2.23	0.53
1:B:146:THR:O	1:B:149:TRP:HB3	2.09	0.53
1:B:338:LEU:O	1:B:338:LEU:HD22	2.08	0.53
1:B:528:THR:HG21	1:B:530:VAL:HG22	1.90	0.53
1:D:322:GLU:HB2	1:D:326:LYS:HG2	1.90	0.53
1:C:266:ILE:HG22	1:C:268:PRO:HG3	1.91	0.53
1:B:66:PRO:O	1:B:74:ARG:NH2	2.41	0.53
1:B:311:ASN:ND2	1:B:348:LYS:HD2	2.22	0.52
1:D:180:ARG:HG3	1:D:180:ARG:NH1	2.23	0.52
1:C:330:MET:CE	1:C:568:LEU:HD12	2.39	0.52
1:D:323:TYR:OH	1:D:458:LYS:HG3	2.10	0.52
1:A:150:PHE:O	1:A:154:VAL:HG23	2.09	0.52
1:C:361:ASN:HA	1:C:448:VAL:HG23	1.92	0.52
1:D:490:LEU:HD22	1:D:494:GLU:HB3	1.91	0.52
1:A:218:VAL:HG23	1:A:219:ASP:N	2.24	0.52
1:C:17:VAL:HG23	1:C:18:ALA:N	2.23	0.52
1:A:189:ILE:HD11	1:A:610:ARG:HA	1.92	0.52
1:B:61:LEU:HG	1:B:93:GLY:HA2	1.92	0.52
1:A:527:THR:OG1	1:A:528:THR:N	2.39	0.52
1:A:341:ARG:NH2	1:A:566:GLU:OE1	2.43	0.52
1:B:443:VAL:HG22	1:B:445:HIS:H	1.74	0.52
1:C:5:LEU:HD21	1:C:618:TYR:CD1	2.45	0.52
1:D:174:VAL:O	1:D:177:PRO:HD2	2.09	0.52
1:D:552:TYR:HD1	1:D:571:TYR:CD2	2.28	0.52
1:C:213:LEU:O	1:C:216:VAL:HG22	2.08	0.52
1:D:449:ASP:OD2	1:D:452:ASN:HB2	2.09	0.52
1:C:315:PHE:CE2	1:C:572:MET:HG2	2.45	0.52
1:C:264:ASP:O	1:C:635:MET:HG3	2.10	0.52
1:D:20:ARG:NH1	3:D:802:SO4:O3	2.43	0.52
1:B:449:ASP:OD1	1:B:452:ASN:HB2	2.10	0.51
1:D:180:ARG:HH11	1:D:180:ARG:CB	2.23	0.51
1:D:14:ALA:HB2	1:D:168:HIS:HB2	1.92	0.51
1:D:382:VAL:O	1:D:386:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:HIS:O	1:C:194:ALA:HB2	2.11	0.51
1:C:332:ILE:HD13	1:C:459:ILE:HG22	1.91	0.51
1:A:389:ILE:HD11	1:A:417:LEU:HD21	1.93	0.51
1:D:550:GLY:HA3	1:D:590:THR:HG21	1.91	0.51
1:C:74:ARG:N	1:C:75:PRO:CD	2.73	0.51
1:A:264:ASP:O	1:A:635:MET:HG3	2.10	0.51
1:D:51:LYS:HE3	1:D:107:ASP:OD1	2.11	0.51
1:B:333:GLU:OE2	1:B:337:ARG:HD2	2.10	0.51
1:A:598:ASP:OD2	1:A:600:LYS:HD2	2.10	0.51
1:C:565:VAL:O	1:C:569:VAL:HG23	2.11	0.51
1:A:549:TYR:HB3	1:A:593:LEU:HD11	1.90	0.51
1:C:113:GLY:C	1:C:115:SER:H	2.14	0.51
1:C:378:LEU:HD22	1:C:382:VAL:HG23	1.92	0.51
1:C:16:GLU:O	1:C:17:VAL:C	2.49	0.51
1:C:123:TRP:O	1:C:127:GLY:HA2	2.11	0.51
1:C:103:VAL:HG13	1:C:105:LEU:HG	1.92	0.51
1:D:351:VAL:HB	1:D:472:VAL:HG12	1.93	0.51
1:B:213:LEU:C	1:B:213:LEU:HD12	2.32	0.51
1:B:499:CYS:O	1:B:587:ARG:NH2	2.44	0.51
1:B:29:LYS:HE3	1:B:97:ILE:CG2	2.41	0.50
1:C:389:ILE:HD11	1:C:417:LEU:CD2	2.42	0.50
1:C:372:GLN:O	1:C:376:ARG:HB2	2.12	0.50
1:A:143:LEU:O	1:A:147:VAL:HG23	2.10	0.50
1:B:133:ASN:HD22	1:B:133:ASN:N	2.08	0.50
1:A:447:MET:HG3	1:A:456:LEU:CD1	2.41	0.50
1:C:235:ARG:HH21	1:C:260:LYS:HG3	1.76	0.50
1:A:289:LYS:HZ3	1:A:494:GLU:HG2	1.76	0.50
1:B:250:ILE:HG12	1:B:530:VAL:HA	1.92	0.50
1:B:114:TYR:HD1	1:B:114:TYR:H	1.59	0.50
1:A:430:LEU:HD13	1:D:55:GLN:O	2.12	0.50
1:A:330:MET:HE3	1:A:568:LEU:HD12	1.94	0.50
1:B:361:ASN:HA	1:B:448:VAL:HG23	1.93	0.50
1:D:458:LYS:HD3	1:D:458:LYS:O	2.11	0.50
1:C:560:ALA:HB1	1:C:561:PRO:HD2	1.93	0.50
1:C:88:VAL:HG22	1:C:111:VAL:HG23	1.94	0.50
1:A:399:ARG:NH2	1:C:307:PHE:O	2.45	0.50
1:B:266:ILE:HG22	1:B:268:PRO:CD	2.38	0.50
1:A:312:THR:HG22	1:A:350:THR:HB	1.93	0.50
1:D:487:ILE:HG22	1:D:488:LEU:N	2.26	0.50
1:D:447:MET:HG3	1:D:456:LEU:HD11	1.93	0.50
1:A:111:VAL:HG12	1:A:142:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:TYR:OH	1:C:458:LYS:HG3	2.11	0.50
1:A:394:PHE:HE1	1:C:379:GLU:HG3	1.76	0.50
1:D:442:ILE:CD1	1:D:459:ILE:HD11	2.36	0.50
1:C:286:HIS:ND1	1:C:587:ARG:NH2	2.60	0.50
1:D:305:PHE:HZ	1:D:309:LEU:HG	1.76	0.49
1:B:179:CYS:HA	1:B:184:ILE:HG13	1.93	0.49
1:C:320:ARG:NH1	1:C:320:ARG:HB2	2.27	0.49
1:B:307:PHE:O	1:D:399:ARG:NH2	2.44	0.49
1:D:134:ASP:CG	1:D:137:THR:HG23	2.32	0.49
1:A:61:LEU:HG	1:A:93:GLY:HA2	1.93	0.49
1:B:150:PHE:O	1:B:154:VAL:HG23	2.11	0.49
1:D:31:LYS:O	1:D:35:THR:HG23	2.12	0.49
1:A:399:ARG:NH2	1:C:308:ASP:HA	2.26	0.49
1:C:321:TYR:C	1:C:321:TYR:CD1	2.86	0.49
1:A:552:TYR:CD1	1:A:571:TYR:CD2	2.90	0.49
1:A:450:ASP:OD1	1:A:460:ARG:NH2	2.37	0.49
1:D:317:ILE:HG13	1:D:503:VAL:O	2.12	0.49
1:B:296:PHE:CE1	1:B:487:ILE:HG23	2.48	0.49
1:B:337:ARG:O	1:B:341:ARG:HG3	2.12	0.49
1:D:300:HIS:CE1	1:D:475:ILE:CD1	2.96	0.49
1:B:30:SER:O	1:B:599:TRP:CD1	2.66	0.49
1:A:113:GLY:O	1:A:115:SER:N	2.45	0.49
1:C:235:ARG:HG2	1:C:239:HIS:HD2	1.77	0.49
1:B:143:LEU:O	1:B:147:VAL:HG23	2.13	0.49
1:C:12:GLU:HB3	1:C:45:LEU:HD23	1.95	0.49
1:A:484:ASN:HD22	1:A:484:ASN:N	2.08	0.49
1:A:487:ILE:HG22	1:A:488:LEU:H	1.74	0.49
1:A:327:GLY:HA3	1:A:505:PRO:O	2.12	0.49
1:C:252:ALA:HB2	1:C:266:ILE:HD11	1.95	0.48
1:A:572:MET:O	1:A:576:VAL:HG23	2.12	0.48
1:B:385:VAL:CG1	1:B:417:LEU:HD21	2.43	0.48
1:D:19:ASN:HD22	1:D:19:ASN:N	2.11	0.48
1:A:133:ASN:ND2	1:A:133:ASN:H	2.11	0.48
1:D:29:LYS:HE3	1:D:97:ILE:CG2	2.43	0.48
1:C:75:PRO:CB	1:C:158:ASP:HB2	2.42	0.48
1:C:490:LEU:HD22	1:C:494:GLU:HB3	1.95	0.48
1:B:514:THR:OG1	1:B:515:PRO:CD	2.61	0.48
1:C:482:ASN:HB3	1:C:484:ASN:HD21	1.79	0.48
1:A:289:LYS:NZ	1:A:494:GLU:HG2	2.29	0.48
1:A:307:PHE:CD1	1:A:312:THR:HG21	2.49	0.48
1:B:133:ASN:ND2	1:B:133:ASN:N	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ARG:N	1:B:75:PRO:CD	2.77	0.48
1:C:34:ILE:HD12	1:C:34:ILE:HA	1.66	0.48
1:B:322:GLU:HB2	1:B:326:LYS:HG2	1.95	0.48
1:C:176:LEU:HD12	1:C:237:ALA:HB1	1.96	0.48
1:B:34:ILE:HD11	1:B:600:LYS:HG3	1.95	0.48
1:D:180:ARG:HH11	1:D:180:ARG:HB2	1.79	0.48
1:A:111:VAL:HG13	1:A:118:TRP:CZ3	2.49	0.48
1:A:458:LYS:HE3	1:A:461:GLN:OE1	2.14	0.47
1:B:125:LEU:O	1:B:126:VAL:HG22	2.14	0.47
1:D:308:ASP:O	1:D:312:THR:HG23	2.14	0.47
1:D:48:PRO:HD3	1:D:143:LEU:HD22	1.96	0.47
1:D:442:ILE:HD12	1:D:459:ILE:CD1	2.33	0.47
1:C:146:THR:O	1:C:149:TRP:HB3	2.14	0.47
1:C:30:SER:O	1:C:599:TRP:CD1	2.67	0.47
1:B:117:GLU:O	1:B:117:GLU:HG2	2.14	0.47
1:D:189:ILE:HD11	1:D:610:ARG:HA	1.96	0.47
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.50	0.47
1:B:572:MET:O	1:B:576:VAL:HG23	2.13	0.47
1:C:442:ILE:HD12	1:C:459:ILE:CD1	2.36	0.47
1:D:29:LYS:CG	1:D:97:ILE:HG21	2.38	0.47
1:C:296:PHE:CE1	1:C:487:ILE:HG23	2.49	0.47
1:B:386:THR:HG21	1:D:390:GLY:HA2	1.95	0.47
1:A:29:LYS:HE3	1:A:97:ILE:CG2	2.45	0.47
1:A:176:LEU:CD1	1:A:190:PHE:HB2	2.44	0.47
1:D:6:GLN:HE21	1:D:625:LEU:HD11	1.80	0.47
1:C:321:TYR:C	1:C:321:TYR:HD1	2.18	0.47
1:C:561:PRO:O	1:C:565:VAL:HG23	2.15	0.47
1:C:88:VAL:HG22	1:C:111:VAL:CG2	2.45	0.47
1:D:527:THR:HG21	1:D:534:GLY:HA2	1.97	0.47
1:A:550:GLY:CA	1:A:590:THR:HG22	2.39	0.47
1:D:578:LYS:HG2	1:D:582:GLN:HB3	1.97	0.47
1:D:3:ARG:NH1	1:D:185:ASP:OD2	2.48	0.47
1:B:32:ALA:HB3	1:B:33:PRO:CD	2.43	0.47
1:D:180:ARG:CG	1:D:180:ARG:NH1	2.76	0.47
1:B:12:GLU:HG3	1:B:166:HIS:HB3	1.95	0.46
1:A:176:LEU:HD11	1:A:190:PHE:HB2	1.96	0.46
1:B:163:ILE:HB	1:B:186:VAL:HG12	1.96	0.46
1:A:183:ARG:HE	1:A:183:ARG:HB2	1.58	0.46
1:B:579:THR:HG23	1:B:582:GLN:OE1	2.16	0.46
1:A:334:ALA:CB	1:A:568:LEU:HD13	2.45	0.46
1:A:300:HIS:HE1	1:A:441:PRO:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:VAL:HG21	1:A:614:LEU:HD23	1.97	0.46
1:C:40:LYS:HB3	1:C:41:ASP:H	1.47	0.46
1:A:390:GLY:HA2	1:C:386:THR:HG21	1.97	0.46
1:B:484:ASN:HD22	1:B:484:ASN:N	1.98	0.46
1:A:484:ASN:ND2	1:A:484:ASN:N	2.59	0.46
1:B:308:ASP:O	1:B:312:THR:HG23	2.15	0.46
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.37	0.46
1:A:76:VAL:O	1:A:79:ALA:HB3	2.15	0.46
1:D:193:HIS:HA	1:D:247:VAL:HG22	1.97	0.46
1:C:442:ILE:CD1	1:C:459:ILE:HD11	2.35	0.46
1:C:482:ASN:O	1:C:484:ASN:N	2.48	0.46
1:A:448:VAL:O	1:A:448:VAL:HG12	2.16	0.46
1:B:272:ASN:O	1:B:275:LYS:HB3	2.15	0.46
1:A:163:ILE:CG2	1:A:186:VAL:HG12	2.45	0.46
1:D:338:LEU:O	1:D:338:LEU:HD22	2.14	0.46
1:C:455:ILE:O	1:C:459:ILE:HG23	2.16	0.46
1:D:323:TYR:CE1	1:D:329:ASP:HB3	2.51	0.46
1:B:265:GLY:O	1:B:266:ILE:HD13	2.16	0.46
1:B:335:LEU:HA	1:B:335:LEU:HD12	1.76	0.46
1:B:103:VAL:CG1	1:B:105:LEU:HG	2.46	0.45
1:A:48:PRO:HD3	1:A:143:LEU:HD22	1.98	0.45
1:A:103:VAL:CG1	1:A:105:LEU:HG	2.46	0.45
1:B:449:ASP:CG	1:B:452:ASN:HB2	2.35	0.45
1:C:265:GLY:HA3	1:C:635:MET:SD	2.55	0.45
1:A:510:PRO:O	1:A:532:GLY:HA3	2.16	0.45
1:A:539:ASP:N	1:A:539:ASP:OD1	2.49	0.45
1:C:333:GLU:OE2	1:C:337:ARG:HD2	2.17	0.45
1:B:95:TRP:CD2	1:B:97:ILE:HD11	2.52	0.45
1:B:448:VAL:O	1:B:448:VAL:HG12	2.17	0.45
1:D:439:LEU:HD22	1:D:467:SER:HA	1.97	0.45
1:C:131:PRO:HD2	1:C:229:HIS:CD2	2.52	0.45
1:A:40:LYS:HB3	1:A:41:ASP:H	1.62	0.45
1:B:136:GLU:OE1	1:B:136:GLU:N	2.46	0.45
1:C:300:HIS:CE1	1:C:475:ILE:CD1	2.99	0.45
1:A:442:ILE:HD12	1:A:459:ILE:CD1	2.40	0.45
1:A:74:ARG:N	1:A:75:PRO:CD	2.79	0.45
1:B:634:ASN:HB2	1:B:637:ALA:H	1.81	0.45
1:B:547:LYS:HD2	1:B:571:TYR:HE2	1.82	0.45
1:C:330:MET:HE3	1:C:568:LEU:HD12	1.99	0.45
1:A:330:MET:CE	1:A:568:LEU:HD12	2.47	0.45
1:A:394:PHE:CE1	1:C:379:GLU:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:PHE:O	1:B:537:MET:HB2	2.17	0.45
1:D:95:TRP:CD2	1:D:97:ILE:HD11	2.52	0.45
1:D:344:VAL:C	1:D:346:GLY:H	2.19	0.45
1:D:112:ARG:NH2	1:D:139:ASP:OD1	2.50	0.44
1:D:218:VAL:HG23	1:D:219:ASP:H	1.81	0.44
1:C:25:TYR:CD2	1:C:25:TYR:C	2.91	0.44
1:C:315:PHE:HE2	1:C:572:MET:HG2	1.80	0.44
1:D:146:THR:O	1:D:149:TRP:HB3	2.18	0.44
1:A:471:ARG:NE	1:A:471:ARG:HA	2.32	0.44
1:C:133:ASN:H	1:C:133:ASN:ND2	2.06	0.44
1:D:176:LEU:HB2	1:D:177:PRO:HD3	1.98	0.44
1:A:289:LYS:N	1:A:289:LYS:HD2	2.31	0.44
1:A:465:PHE:O	1:A:466:ASN:HB2	2.16	0.44
1:B:463:GLN:HA	1:B:465:PHE:CE2	2.52	0.44
1:C:539:ASP:O	1:C:540:LEU:HD23	2.18	0.44
1:B:555:ASP:OD1	1:B:555:ASP:C	2.56	0.44
1:B:598:ASP:OD2	1:B:600:LYS:HB2	2.18	0.44
1:A:8:HIS:HB2	1:A:162:ALA:O	2.17	0.44
1:D:425:LEU:HD23	1:D:425:LEU:HA	1.80	0.44
1:A:173:GLY:O	1:A:176:LEU:HB2	2.17	0.44
1:C:305:PHE:HZ	1:C:309:LEU:HG	1.82	0.44
1:B:374:GLU:HA	1:B:374:GLU:OE1	2.17	0.44
1:A:3:ARG:HH12	1:A:185:ASP:HB3	1.81	0.44
1:B:113:GLY:O	1:B:115:SER:N	2.50	0.44
1:B:334:ALA:CB	1:B:568:LEU:HD13	2.47	0.44
1:A:547:LYS:HD2	1:A:571:TYR:CE2	2.53	0.44
1:D:6:GLN:NE2	1:D:625:LEU:HD21	2.33	0.44
1:C:526:ILE:HG12	1:C:552:TYR:HB2	2.00	0.44
1:B:449:ASP:OD2	1:B:452:ASN:HB2	2.18	0.44
1:D:213:LEU:HD12	1:D:214:GLU:N	2.33	0.44
1:B:307:PHE:HD1	1:B:312:THR:HG21	1.83	0.44
1:A:559:LYS:HB3	1:A:563:GLU:HB2	1.99	0.44
1:C:312:THR:HA	1:C:350:THR:O	2.18	0.44
1:D:218:VAL:HG23	1:D:219:ASP:N	2.32	0.44
1:B:173:GLY:O	1:B:176:LEU:HB2	2.18	0.43
1:A:34:ILE:HA	1:A:34:ILE:HD12	1.77	0.43
1:D:36:VAL:CG2	1:D:101:PRO:HB3	2.48	0.43
1:A:366:VAL:HG12	1:A:367:GLU:N	2.33	0.43
1:C:443:VAL:HG12	1:C:444:THR:N	2.33	0.43
1:B:311:ASN:HD21	1:B:348:LYS:CD	2.28	0.43
1:D:54:TYR:CE1	1:D:60:ILE:HD11	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:TYR:HD1	1:C:571:TYR:CD2	2.36	0.43
1:C:183:ARG:HB2	1:C:183:ARG:HE	1.63	0.43
1:D:235:ARG:HG2	1:D:239:HIS:HD2	1.83	0.43
1:B:342:LEU:HA	1:B:342:LEU:HD23	1.76	0.43
1:D:514:THR:OG1	1:D:515:PRO:CD	2.66	0.43
1:D:372:GLN:O	1:D:376:ARG:HB2	2.19	0.43
1:C:447:MET:HG3	1:C:456:LEU:CD1	2.47	0.43
1:B:210:TYR:CZ	1:B:530:VAL:HB	2.54	0.43
1:A:322:GLU:HB2	1:A:326:LYS:HG2	2.01	0.43
1:B:296:PHE:HE1	1:B:487:ILE:HG23	1.83	0.43
1:B:193:HIS:O	1:B:194:ALA:CB	2.65	0.43
1:D:323:TYR:CZ	1:D:329:ASP:HB3	2.53	0.43
1:B:109:ASP:C	1:B:111:VAL:H	2.22	0.43
1:D:560:ALA:HB1	1:D:561:PRO:CD	2.49	0.43
1:A:235:ARG:NH2	1:A:260:LYS:HG3	2.18	0.43
1:C:608:LYS:HB2	1:C:635:MET:HE3	1.99	0.43
1:D:320:ARG:HA	2:F:5:UNK:O	2.18	0.43
1:D:624:GLU:H	1:D:624:GLU:HG2	1.60	0.43
1:C:63:TRP:HZ3	1:C:81:GLN:HG2	1.83	0.43
1:A:459:ILE:HA	1:A:462:VAL:HG22	2.00	0.43
1:B:529:ASN:HD21	1:B:557:ARG:HB3	1.84	0.43
1:C:344:VAL:C	1:C:346:GLY:H	2.22	0.43
1:B:560:ALA:HB1	1:B:561:PRO:HD2	2.01	0.43
1:B:302:HIS:CD2	1:B:371:GLY:HA2	2.53	0.43
1:D:77:GLN:O	1:D:81:GLN:HG3	2.18	0.43
1:A:272:ASN:O	1:A:275:LYS:HB3	2.19	0.43
1:C:537:MET:CG	1:C:551:ILE:HD13	2.49	0.43
1:D:626:VAL:HG11	1:D:630:LEU:HD11	1.99	0.43
1:D:183:ARG:HB2	1:D:183:ARG:HE	1.59	0.43
1:B:19:ASN:N	1:B:19:ASN:HD22	2.16	0.43
1:D:549:TYR:C	1:D:590:THR:HG22	2.38	0.43
1:A:485:ASN:HA	1:A:486:PRO:HD3	1.81	0.43
1:A:579:THR:HG23	1:A:582:GLN:OE1	2.19	0.43
1:D:74:ARG:HA	1:D:74:ARG:HD3	1.67	0.42
1:A:449:ASP:CG	1:A:452:ASN:HB2	2.39	0.42
1:C:210:TYR:CZ	1:C:530:VAL:HB	2.54	0.42
1:B:126:VAL:HG11	1:B:128:ILE:HD11	2.01	0.42
1:B:398:ILE:HA	1:B:398:ILE:HD12	1.90	0.42
1:C:425:LEU:HD23	1:C:425:LEU:HA	1.77	0.42
1:A:547:LYS:HD2	1:A:571:TYR:HE2	1.84	0.42
1:A:261:ARG:O	1:A:263:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:TRP:O	1:D:127:GLY:HA2	2.19	0.42
1:A:5:LEU:HD21	1:A:618:TYR:CD1	2.54	0.42
1:B:390:GLY:CA	1:D:386:THR:HG21	2.48	0.42
1:B:126:VAL:O	1:B:126:VAL:HG12	2.19	0.42
1:C:149:TRP:C	1:C:149:TRP:CD1	2.92	0.42
1:B:180:ARG:HH11	1:B:180:ARG:HG3	1.84	0.42
1:B:425:LEU:O	1:B:429:ILE:HG13	2.18	0.42
1:B:76:VAL:O	1:B:79:ALA:HB3	2.18	0.42
1:D:504:PHE:CD2	1:D:515:PRO:HB3	2.54	0.42
1:D:88:VAL:HG22	1:D:111:VAL:HG23	2.02	0.42
1:A:330:MET:HE2	1:A:505:PRO:HB3	2.01	0.42
1:D:350:THR:OG1	1:D:471:ARG:NH1	2.52	0.42
1:C:176:LEU:HD11	1:C:190:PHE:HB2	2.02	0.42
1:B:350:THR:OG1	1:B:471:ARG:NH1	2.53	0.42
1:C:552:TYR:CD2	1:C:552:TYR:N	2.88	0.42
1:B:89:HIS:O	1:B:107:ASP:HB3	2.20	0.42
1:A:490:LEU:HD13	1:A:495:PHE:HA	2.01	0.42
1:C:227:ILE:HG22	1:C:227:ILE:O	2.19	0.42
1:A:399:ARG:HH22	1:C:308:ASP:HA	1.84	0.42
1:C:326:LYS:NZ	3:C:706:SO4:O1	2.53	0.42
1:A:330:MET:HG2	1:A:565:VAL:HG22	2.01	0.42
1:B:300:HIS:HE1	1:B:441:PRO:O	2.03	0.42
1:D:321:TYR:C	1:D:321:TYR:CD1	2.92	0.41
1:A:71:ASP:HA	1:A:74:ARG:HG2	2.00	0.41
1:B:3:ARG:HD3	1:B:162:ALA:HA	2.03	0.41
1:D:213:LEU:O	1:D:216:VAL:HG22	2.20	0.41
1:B:114:TYR:N	1:B:114:TYR:CD1	2.88	0.41
1:C:472:VAL:HG23	1:C:472:VAL:O	2.20	0.41
1:C:8:HIS:CE1	1:C:39:TYR:HE1	2.37	0.41
1:D:208:ASP:OD2	1:D:208:ASP:C	2.58	0.41
1:D:487:ILE:HD12	1:D:487:ILE:HA	1.82	0.41
1:B:448:VAL:O	1:B:449:ASP:CB	2.58	0.41
1:B:125:LEU:C	1:B:126:VAL:CG2	2.88	0.41
1:A:142:LEU:HA	1:A:142:LEU:HD23	1.81	0.41
1:D:485:ASN:HA	1:D:486:PRO:HD3	1.83	0.41
1:C:7:ASN:O	1:C:7:ASN:CG	2.59	0.41
1:B:316:PHE:CZ	1:B:496:VAL:HG22	2.56	0.41
1:C:332:ILE:HG21	1:C:459:ILE:HG22	2.02	0.41
1:C:448:VAL:O	1:C:448:VAL:HG12	2.20	0.41
1:C:210:TYR:HE1	1:C:250:ILE:HD11	1.82	0.41
1:B:341:ARG:NH2	1:B:566:GLU:OE1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:LEU:HD23	1:A:490:LEU:HA	1.83	0.41
1:D:103:VAL:CG1	1:D:105:LEU:HG	2.50	0.41
1:D:34:ILE:HA	1:D:34:ILE:HD12	1.74	0.41
1:C:184:ILE:HG12	1:C:184:ILE:H	1.73	0.41
1:D:590:THR:O	1:D:593:LEU:HB2	2.21	0.41
1:D:144:GLY:HA3	1:D:174:VAL:HB	2.02	0.41
1:C:149:TRP:O	1:C:149:TRP:CD1	2.71	0.41
1:D:456:LEU:HA	1:D:456:LEU:HD23	1.89	0.41
1:B:180:ARG:HG3	1:B:180:ARG:NH1	2.35	0.41
1:D:25:TYR:C	1:D:25:TYR:CD2	2.94	0.41
1:C:459:ILE:HA	1:C:462:VAL:HG22	2.03	0.41
1:B:51:LYS:HE3	1:B:107:ASP:OD1	2.20	0.41
1:B:423:VAL:HG12	1:B:424:MET:N	2.35	0.41
1:A:586:GLN:O	1:A:587:ARG:C	2.59	0.41
1:D:285:LEU:HA	1:D:285:LEU:HD23	1.57	0.41
1:A:623:ARG:HG3	1:A:628:GLU:C	2.41	0.41
1:D:198:GLY:HA2	1:D:209:PHE:CZ	2.56	0.41
1:A:193:HIS:O	1:A:194:ALA:HB2	2.21	0.41
1:C:3:ARG:NH2	1:C:158:ASP:O	2.53	0.41
1:A:415:GLU:HG2	1:A:417:LEU:O	2.21	0.41
1:C:564:SER:O	1:C:565:VAL:C	2.59	0.41
1:A:79:ALA:O	1:A:83:MET:HG2	2.21	0.41
1:C:537:MET:HG2	1:C:551:ILE:HD13	2.03	0.41
1:D:111:VAL:HG13	1:D:118:TRP:CZ3	2.54	0.41
1:D:389:ILE:HG23	1:D:416:LEU:HD13	2.03	0.41
1:B:331:PHE:CE1	1:B:503:VAL:HB	2.56	0.41
1:B:40:LYS:HB3	1:B:41:ASP:H	1.64	0.41
1:D:615:ARG:CZ	1:D:632:ASP:HB3	2.51	0.41
1:A:620:ASP:O	1:A:624:GLU:HG2	2.21	0.41
1:B:528:THR:O	1:B:534:GLY:HA3	2.21	0.40
1:A:74:ARG:HB2	1:A:75:PRO:HD3	2.03	0.40
1:A:337:ARG:O	1:A:341:ARG:HG3	2.20	0.40
1:C:111:VAL:HG13	1:C:118:TRP:CZ3	2.56	0.40
1:B:174:VAL:O	1:B:177:PRO:HD2	2.21	0.40
1:B:69:PHE:CE2	1:B:77:GLN:HG3	2.56	0.40
1:D:133:ASN:H	1:D:133:ASN:ND2	2.14	0.40
1:D:447:MET:HG3	1:D:456:LEU:CD1	2.51	0.40
1:B:289:LYS:N	1:B:289:LYS:HD2	2.36	0.40
1:C:307:PHE:CD1	1:C:312:THR:HG21	2.56	0.40
1:B:125:LEU:O	1:B:126:VAL:CG2	2.69	0.40
1:A:528:THR:O	1:A:534:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:HIS:HA	1:C:247:VAL:HG22	2.03	0.40
1:D:296:PHE:CE1	1:D:487:ILE:HG23	2.57	0.40
1:C:320:ARG:HB2	1:C:320:ARG:HH11	1.87	0.40
1:D:527:THR:OG1	1:D:528:THR:N	2.51	0.40
1:A:539:ASP:O	1:A:540:LEU:HD23	2.22	0.40
1:C:31:LYS:HE2	1:C:606:TYR:CE1	2.56	0.40
1:B:227:ILE:HA	1:B:227:ILE:HD13	1.87	0.40
1:C:321:TYR:OH	1:C:455:ILE:HG12	2.21	0.40
1:B:16:GLU:O	1:B:17:VAL:C	2.60	0.40
1:B:472:VAL:HG23	1:B:472:VAL:O	2.22	0.40
1:B:526:ILE:HG12	1:B:552:TYR:HB2	2.03	0.40
1:A:19:ASN:N	1:A:19:ASN:ND2	2.68	0.40
1:B:66:PRO:HA	1:B:74:ARG:HH22	1.86	0.40
1:C:12:GLU:HG3	1:C:166:HIS:HB3	2.02	0.40
1:B:357:MET:HA	1:B:358:PRO:HD3	1.89	0.40
1:B:623:ARG:HE	1:B:623:ARG:HB2	1.68	0.40
1:C:227:ILE:O	1:C:227:ILE:CG2	2.69	0.40
1:D:75:PRO:CB	1:D:158:ASP:HB2	2.52	0.40
1:C:255:ALA:O	1:C:259:LEU:HB2	2.22	0.40
1:D:348:LYS:HD3	1:D:348:LYS:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	601/725 (83%)	548 (91%)	47 (8%)	6 (1%)	19	61
1	B	601/725 (83%)	543 (90%)	52 (9%)	6 (1%)	19	61
1	C	603/725 (83%)	553 (92%)	43 (7%)	7 (1%)	16	56
1	D	603/725 (83%)	561 (93%)	38 (6%)	4 (1%)	26	70
All	All	2408/2900 (83%)	2205 (92%)	180 (8%)	23 (1%)	19	61

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	TYR
1	A	449	ASP
1	B	114	TYR
1	B	126	VAL
1	B	449	ASP
1	C	285	LEU
1	C	415	GLU
1	C	449	ASP
1	D	17	VAL
1	D	285	LEU
1	D	449	ASP
1	A	20	ARG
1	B	194	ALA
1	C	17	VAL
1	C	194	ALA
1	D	415	GLU
1	C	114	TYR
1	A	194	ALA
1	A	448	VAL
1	B	210	TYR
1	B	17	VAL
1	C	448	VAL
1	A	111	VAL

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	526/622 (85%)	480 (91%)	46 (9%)	13	43
1	B	526/622 (85%)	481 (91%)	45 (9%)	13	44
1	C	527/622 (85%)	487 (92%)	40 (8%)	16	51
1	D	527/622 (85%)	478 (91%)	49 (9%)	11	39
All	All	2106/2488 (85%)	1926 (92%)	180 (8%)	13	45

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	17	VAL
1	A	19	ASN
1	A	35	THR
1	A	40	LYS
1	A	42	HIS
1	A	74	ARG
1	A	86	ARG
1	A	97	ILE
1	A	110	SER
1	A	111	VAL
1	A	114	TYR
1	A	122	LEU
1	A	164	VAL
1	A	181	LYS
1	A	183	ARG
1	A	184	ILE
1	A	213	LEU
1	A	214	GLU
1	A	289	LYS
1	A	321	TYR
1	A	363	SER
1	A	366	VAL
1	A	376	ARG
1	A	378	LEU
1	A	387	THR
1	A	388	SER
1	A	399	ARG
1	A	428	ARG
1	A	458	LYS
1	A	459	ILE
1	A	469	SER
1	A	471	ARG
1	A	484	ASN
1	A	488	LEU
1	A	493	ASP
1	A	513	TYR
1	A	525	SER
1	A	531	SER
1	A	537	MET
1	A	539	ASP
1	A	556	ARG

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Mol	Chain	Res	Type
1	A	568	LEU
1	A	594	SER
1	A	633	SER
1	A	634	ASN
1	B	7	ASN
1	B	17	VAL
1	B	19	ASN
1	B	35	THR
1	B	40	LYS
1	B	42	HIS
1	B	74	ARG
1	B	97	ILE
1	B	111	VAL
1	B	114	TYR
1	B	122	LEU
1	B	133	ASN
1	B	164	VAL
1	B	181	LYS
1	B	183	ARG
1	B	192	THR
1	B	213	LEU
1	B	214	GLU
1	B	249	GLN
1	B	289	LYS
1	B	312	THR
1	B	321	TYR
1	B	335	LEU
1	B	338	LEU
1	B	363	SER
1	B	376	ARG
1	B	378	LEU
1	B	388	SER
1	B	399	ARG
1	B	423	VAL
1	B	427	ARG
1	B	428	ARG
1	B	450	ASP
1	B	455	ILE
1	B	458	LYS
1	B	459	ILE
1	B	469	SER
1	B	471	ARG

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Mol	Chain	Res	Type
1	B	484	ASN
1	B	488	LEU
1	B	513	TYR
1	B	537	MET
1	B	556	ARG
1	B	568	LEU
1	B	633	SER
1	C	7	ASN
1	C	19	ASN
1	C	34	ILE
1	C	40	LYS
1	C	53	THR
1	C	86	ARG
1	C	97	ILE
1	C	103	VAL
1	C	111	VAL
1	C	122	LEU
1	C	133	ASN
1	C	180	ARG
1	C	181	LYS
1	C	183	ARG
1	C	247	VAL
1	C	249	GLN
1	C	284	ASN
1	C	289	LYS
1	C	321	TYR
1	C	335	LEU
1	C	338	LEU
1	C	348	LYS
1	C	363	SER
1	C	376	ARG
1	C	378	LEU
1	C	388	SER
1	C	399	ARG
1	C	428	ARG
1	C	458	LYS
1	C	459	ILE
1	C	469	SER
1	C	471	ARG
1	C	484	ASN
1	C	513	TYR
1	C	537	MET

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Mol	Chain	Res	Type
1	C	556	ARG
1	C	568	LEU
1	C	590	THR
1	C	594	SER
1	C	635	MET
1	D	2	SER
1	D	7	ASN
1	D	17	VAL
1	D	19	ASN
1	D	35	THR
1	D	40	LYS
1	D	42	HIS
1	D	72	GLU
1	D	74	ARG
1	D	97	ILE
1	D	111	VAL
1	D	122	LEU
1	D	133	ASN
1	D	164	VAL
1	D	180	ARG
1	D	181	LYS
1	D	183	ARG
1	D	208	ASP
1	D	213	LEU
1	D	214	GLU
1	D	216	VAL
1	D	227	ILE
1	D	247	VAL
1	D	249	GLN
1	D	289	LYS
1	D	321	TYR
1	D	338	LEU
1	D	348	LYS
1	D	363	SER
1	D	376	ARG
1	D	378	LEU
1	D	388	SER
1	D	399	ARG
1	D	428	ARG
1	D	458	LYS
1	D	459	ILE
1	D	469	SER

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Mol	Chain	Res	Type
1	D	471	ARG
1	D	484	ASN
1	D	487	ILE
1	D	488	LEU
1	D	513	TYR
1	D	537	MET
1	D	556	ARG
1	D	568	LEU
1	D	579	THR
1	D	594	SER
1	D	624	GLU
1	D	635	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	8	HIS
1	A	19	ASN
1	A	78	HIS
1	A	133	ASN
1	A	168	HIS
1	A	300	HIS
1	A	484	ASN
1	A	500	HIS
1	A	621	GLN
1	B	6	GLN
1	B	8	HIS
1	B	19	ASN
1	B	78	HIS
1	B	133	ASN
1	B	168	HIS
1	B	239	HIS
1	B	300	HIS
1	B	311	ASN
1	B	362	ASN
1	B	484	ASN
1	B	500	HIS
1	B	621	GLN
1	C	6	GLN
1	C	8	HIS
1	C	19	ASN

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Mol	Chain	Res	Type
1	C	78	HIS
1	C	81	GLN
1	C	133	ASN
1	C	239	HIS
1	C	300	HIS
1	C	484	ASN
1	C	500	HIS
1	D	6	GLN
1	D	8	HIS
1	D	19	ASN
1	D	133	ASN
1	D	168	HIS
1	D	239	HIS
1	D	300	HIS
1	D	362	ASN
1	D	484	ASN
1	D	500	HIS
1	D	621	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
3	SO4	A	801	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	A	802	-	4,4,4	0.21	0	6,6,6	0.40	0
3	SO4	A	803	-	4,4,4	0.13	0	6,6,6	0.17	0
3	SO4	A	804	-	4,4,4	0.94	0	6,6,6	0.79	0
3	SO4	B	706	-	4,4,4	0.09	0	6,6,6	0.20	0
3	SO4	B	801	-	4,4,4	0.12	0	6,6,6	0.25	0
3	SO4	B	802	-	4,4,4	0.23	0	6,6,6	0.26	0
3	SO4	B	804	-	4,4,4	1.26	0	6,6,6	0.63	0
3	SO4	C	706	-	4,4,4	0.11	0	6,6,6	0.22	0
3	SO4	C	801	-	4,4,4	0.14	0	6,6,6	0.18	0
3	SO4	C	803	-	4,4,4	0.12	0	6,6,6	0.20	0
3	SO4	C	804	-	4,4,4	1.01	0	6,6,6	0.78	0
3	SO4	D	801	-	4,4,4	0.27	0	6,6,6	0.24	0
3	SO4	D	802	-	4,4,4	0.12	0	6,6,6	0.23	0
3	SO4	D	803	-	4,4,4	0.06	0	6,6,6	0.22	0
3	SO4	D	804	-	4,4,4	1.01	0	6,6,6	0.99	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	801	-	-	0/0/0/0	0/0/0/0
3	SO4	A	802	-	-	0/0/0/0	0/0/0/0
3	SO4	A	803	-	-	0/0/0/0	0/0/0/0
3	SO4	A	804	-	-	0/0/0/0	0/0/0/0
3	SO4	B	706	-	-	0/0/0/0	0/0/0/0
3	SO4	B	801	-	-	0/0/0/0	0/0/0/0
3	SO4	B	802	-	-	0/0/0/0	0/0/0/0
3	SO4	B	804	-	-	0/0/0/0	0/0/0/0
3	SO4	C	706	-	-	0/0/0/0	0/0/0/0
3	SO4	C	801	-	-	0/0/0/0	0/0/0/0
3	SO4	C	803	-	-	0/0/0/0	0/0/0/0
3	SO4	C	804	-	-	0/0/0/0	0/0/0/0
3	SO4	D	801	-	-	0/0/0/0	0/0/0/0
3	SO4	D	802	-	-	0/0/0/0	0/0/0/0
3	SO4	D	803	-	-	0/0/0/0	0/0/0/0
3	SO4	D	804	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	D	804	SO4	O4-S-O3	2.12	117.60	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	SO4	1	0
3	C	706	SO4	1	0
3	D	802	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	611/725 (84%)	-0.25	4 (0%) 89 70	39, 61, 87, 120	0
1	B	611/725 (84%)	-0.20	10 (1%) 74 47	48, 66, 91, 124	0
1	C	613/725 (84%)	-0.32	3 (0%) 91 76	38, 63, 88, 116	0
1	D	613/725 (84%)	-0.33	2 (0%) 94 84	36, 58, 85, 115	0
2	E	0/6	-	-	-	-
2	F	0/6	-	-	-	-
All	All	2448/2912 (84%)	-0.27	19 (0%) 87 67	36, 62, 88, 124	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	549	TYR	3.7
1	A	549	TYR	3.3
1	B	437	GLY	3.0
1	A	416	LEU	3.0
1	C	548	ASP	2.8
1	C	625	LEU	2.6
1	D	548	ASP	2.6
1	B	631	ASN	2.4
1	B	629	GLU	2.4
1	A	550	GLY	2.4
1	B	585	ASN	2.3
1	B	622	PHE	2.3
1	D	415	GLU	2.3
1	A	548	ASP	2.2
1	B	626	VAL	2.2
1	B	624	GLU	2.2
1	B	620	ASP	2.1
1	C	628	GLU	2.1
1	B	625	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	D	801	5/5	0.72	0.28	3.06	73,76,89,97	0
3	SO4	C	706	5/5	0.86	0.26	1.87	82,84,95,102	0
3	SO4	B	802	5/5	0.86	0.23	0.93	73,75,86,93	0
3	SO4	D	804	5/5	0.92	0.29	0.42	98,100,102,114	0
3	SO4	A	802	5/5	0.90	0.19	-0.90	67,72,82,91	0
3	SO4	D	802	5/5	0.93	0.17	-	69,74,85,86	0
3	SO4	C	801	5/5	0.97	0.15	-	74,81,89,91	0
3	SO4	D	803	5/5	0.87	0.24	-	91,92,97,101	0
3	SO4	B	804	5/5	0.91	0.23	-	99,99,102,118	0
3	SO4	B	706	5/5	0.90	0.20	-	81,84,93,95	0
3	SO4	A	801	5/5	0.95	0.12	-	71,75,81,84	0
3	SO4	A	803	5/5	0.95	0.15	-	81,85,98,98	0
3	SO4	B	801	5/5	0.92	0.17	-	79,80,88,91	0
3	SO4	C	803	5/5	0.89	0.22	-	91,92,99,104	0
3	SO4	A	804	5/5	0.92	0.24	-	97,99,103,107	0
3	SO4	C	804	5/5	0.95	0.17	-	95,95,101,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.