



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:31 PM EDT

PDB ID : 3DH4 / pdb_00003dh4
Title : Crystal Structure of Sodium/Sugar symporter with bound Galactose from vibrio parahaemolyticus
Authors : Abramson, J.; Faham, S.; Cascio, D.
Deposited on : 2008-06-16
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

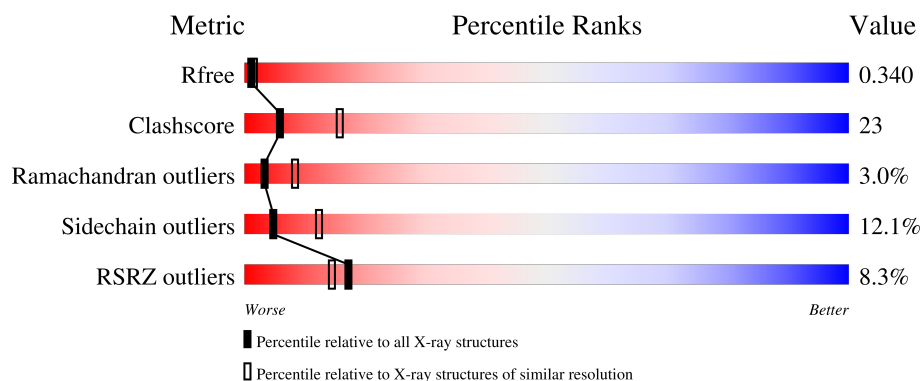
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

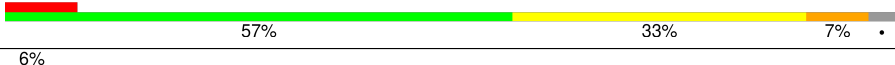
The reported resolution of this entry is 2.70 Å.

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	530	
1	B	530	
1	C	530	
1	D	530	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15472 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 Sodium/glucose cotransporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			3854	2579	580	675	20			
1	B	512	Total	C	N	O	S	0	0	0
			3854	2579	580	675	20			
1	C	512	Total	C	N	O	S	0	0	0
			3854	2579	580	675	20			
1	D	512	Total	C	N	O	S	0	0	0
			3854	2579	580	675	20			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	544	VAL	-	expression tag	UNP P96169
A	545	LEU	-	expression tag	UNP P96169
A	546	TYR	-	expression tag	UNP P96169
A	547	LYS	-	expression tag	UNP P96169
A	548	SER	-	expression tag	UNP P96169
A	549	GLY	-	expression tag	UNP P96169
A	550	GLY	-	expression tag	UNP P96169
A	551	SER	-	expression tag	UNP P96169
A	552	PRO	-	expression tag	UNP P96169
A	553	GLY	-	expression tag	UNP P96169
A	554	HIS	-	expression tag	UNP P96169
A	555	HIS	-	expression tag	UNP P96169
A	556	HIS	-	expression tag	UNP P96169
A	557	HIS	-	expression tag	UNP P96169
A	558	HIS	-	expression tag	UNP P96169
A	559	HIS	-	expression tag	UNP P96169
B	544	VAL	-	expression tag	UNP P96169
B	545	LEU	-	expression tag	UNP P96169
B	546	TYR	-	expression tag	UNP P96169
B	547	LYS	-	expression tag	UNP P96169
B	548	SER	-	expression tag	UNP P96169

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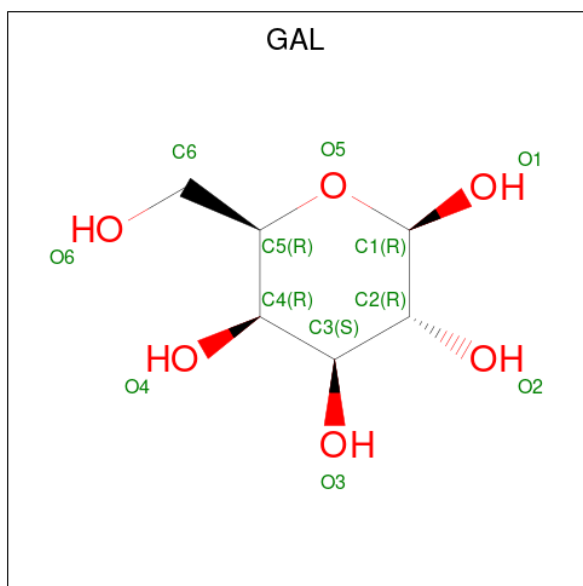
Chain	Residue	Modelled	Actual	Comment	Reference
B	549	GLY	-	expression tag	UNP P96169
B	550	GLY	-	expression tag	UNP P96169
B	551	SER	-	expression tag	UNP P96169
B	552	PRO	-	expression tag	UNP P96169
B	553	GLY	-	expression tag	UNP P96169
B	554	HIS	-	expression tag	UNP P96169
B	555	HIS	-	expression tag	UNP P96169
B	556	HIS	-	expression tag	UNP P96169
B	557	HIS	-	expression tag	UNP P96169
B	558	HIS	-	expression tag	UNP P96169
B	559	HIS	-	expression tag	UNP P96169
C	544	VAL	-	expression tag	UNP P96169
C	545	LEU	-	expression tag	UNP P96169
C	546	TYR	-	expression tag	UNP P96169
C	547	LYS	-	expression tag	UNP P96169
C	548	SER	-	expression tag	UNP P96169
C	549	GLY	-	expression tag	UNP P96169
C	550	GLY	-	expression tag	UNP P96169
C	551	SER	-	expression tag	UNP P96169
C	552	PRO	-	expression tag	UNP P96169
C	553	GLY	-	expression tag	UNP P96169
C	554	HIS	-	expression tag	UNP P96169
C	555	HIS	-	expression tag	UNP P96169
C	556	HIS	-	expression tag	UNP P96169
C	557	HIS	-	expression tag	UNP P96169
C	558	HIS	-	expression tag	UNP P96169
C	559	HIS	-	expression tag	UNP P96169
D	544	VAL	-	expression tag	UNP P96169
D	545	LEU	-	expression tag	UNP P96169
D	546	TYR	-	expression tag	UNP P96169
D	547	LYS	-	expression tag	UNP P96169
D	548	SER	-	expression tag	UNP P96169
D	549	GLY	-	expression tag	UNP P96169
D	550	GLY	-	expression tag	UNP P96169
D	551	SER	-	expression tag	UNP P96169
D	552	PRO	-	expression tag	UNP P96169
D	553	GLY	-	expression tag	UNP P96169
D	554	HIS	-	expression tag	UNP P96169
D	555	HIS	-	expression tag	UNP P96169
D	556	HIS	-	expression tag	UNP P96169
D	557	HIS	-	expression tag	UNP P96169
D	558	HIS	-	expression tag	UNP P96169

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Chain	Residue	Modelled	Actual	Comment	Reference
D	559	HIS	-	expression tag	UNP P96169

- Molecule 2 is beta-D-galactopyranose (CCD ID: GAL) (formula: $C_6H_{12}O_6$).



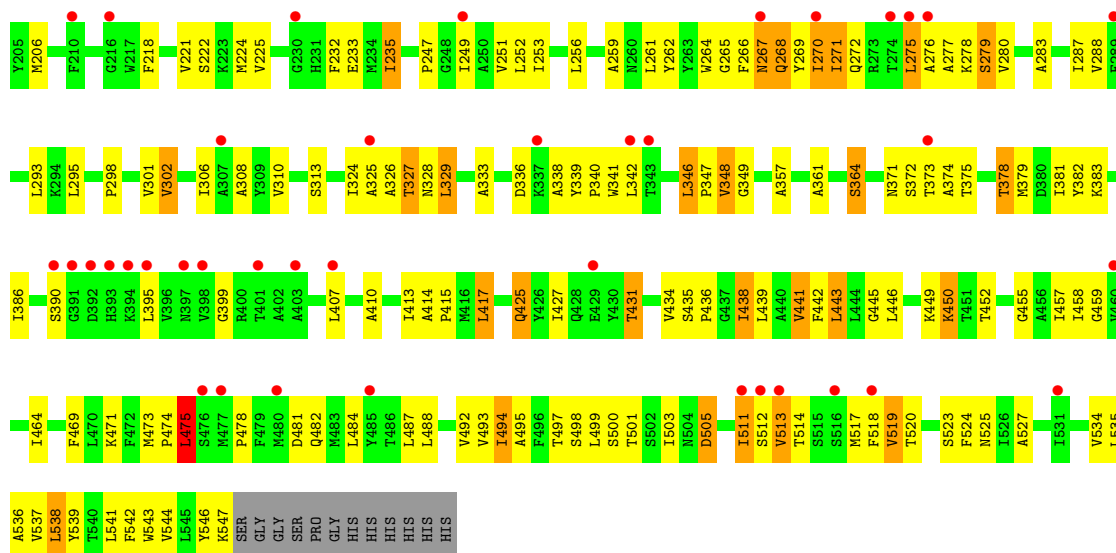
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is ERBIUM (III) ION (CCD ID: ER3) (formula: Er).

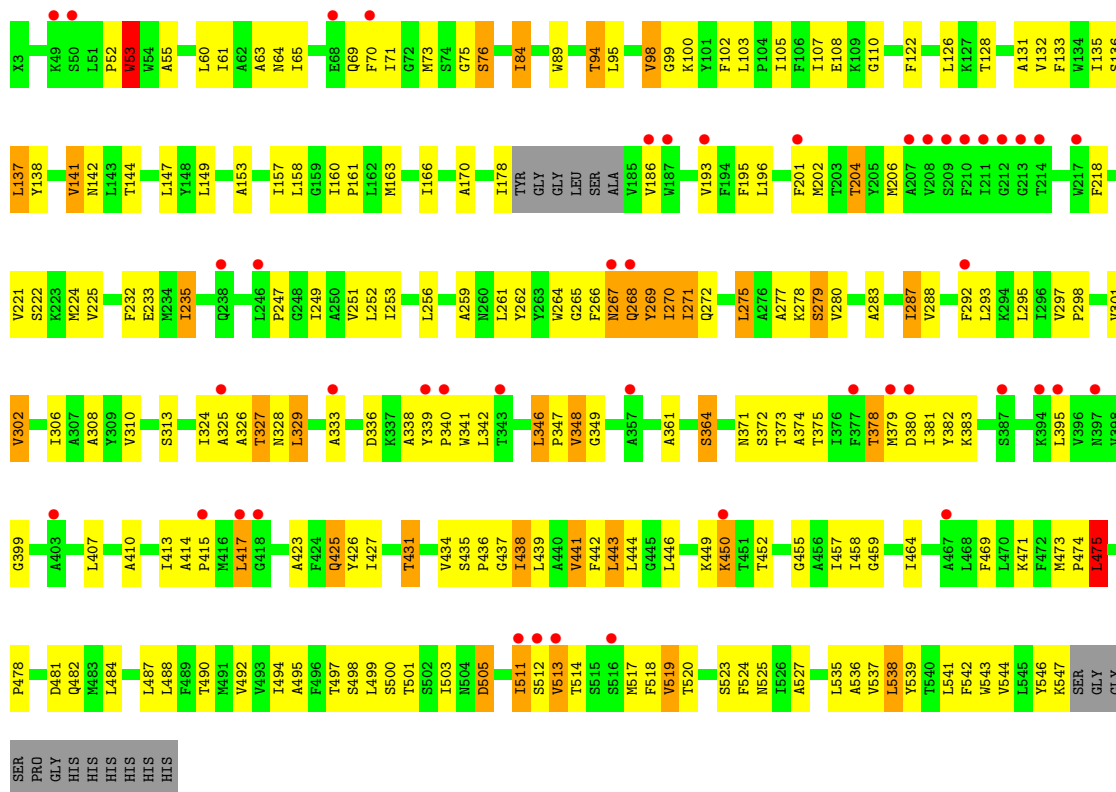
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Er	0	0
			2	2		
3	D	2	Total	Er	0	0
			2	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Na 1	0	0
4	B	1	Total 1	Na 1	0	0
4	C	1	Total 1	Na 1	0	0
4	D	1	Total 1	Na 1	0	0



• Molecule 1: Sodium/glucose cotransporter



• Molecule 1: Sodium/glucose cotransporter





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	83.28Å 109.21Å 127.58Å 109.70° 92.02° 102.11°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	53.3 (30.00-2.70) 91.2 (30.00-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.270 , 0.287 0.330 , 0.340	Depositor DCC
R_{free} test set	5170 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15472	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: GAL, ER3, NA

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	0.61	0/3867	0.88	1/5279 (0.0%)
1	B	0.59	0/3867	0.88	1/5279 (0.0%)
1	C	0.60	0/3867	0.89	1/5279 (0.0%)
1	D	0.59	0/3867	0.88	2/5279 (0.0%)
All	All	0.60	0/15468	0.88	5/21116 (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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	269	TYR	N-CA-C	-6.52	104.17	111.28
1	A	269	TYR	N-CA-C	-6.51	104.18	111.28
1	C	269	TYR	N-CA-C	-5.28	105.53	111.28
1	B	390	SER	N-CA-C	-5.01	105.28	111.40
1	D	390	SER	N-CA-C	-5.01	105.29	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	PHE	Peptide
1	B	122	PHE	Peptide
1	C	122	PHE	Peptide
1	D	122	PHE	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	3854	0	3887	192	0
1	B	3854	0	3887	173	0
1	C	3854	0	3887	177	0
1	D	3854	0	3887	201	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	15472	0	15596	714	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 23.

All (714) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HD11	1:B:275:LEU:HD13	1.36	1.06
1:A:103:LEU:HD11	1:A:275:LEU:HD13	1.42	1.01
1:C:103:LEU:HD11	1:C:275:LEU:HD13	1.39	1.01
1:D:103:LEU:HD11	1:D:275:LEU:HD13	1.42	1.00
1:C:505:ASP:HB2	1:D:513:VAL:HB	1.47	0.96
1:A:50:SER:HB3	1:D:513:VAL:CG1	1.95	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:LEU:HD23	1:B:475:LEU:O	1.68	0.93
1:B:103:LEU:CD1	1:B:275:LEU:HD13	2.00	0.91
1:C:511:ILE:HD13	1:C:512:SER:N	1.86	0.90
1:A:475:LEU:HD23	1:A:475:LEU:O	1.72	0.90
1:D:475:LEU:HD23	1:D:475:LEU:O	1.71	0.90
1:A:511:ILE:HD13	1:A:512:SER:N	1.87	0.89
1:B:446:LEU:O	1:B:511:ILE:HG21	1.72	0.89
1:C:446:LEU:O	1:C:511:ILE:HG21	1.72	0.88
1:C:475:LEU:O	1:C:475:LEU:HD23	1.74	0.88
1:C:505:ASP:OD2	1:D:513:VAL:HG12	1.74	0.88
1:C:103:LEU:CD1	1:C:275:LEU:HD13	2.03	0.87
1:D:446:LEU:O	1:D:511:ILE:HG21	1.75	0.87
1:D:511:ILE:HD13	1:D:512:SER:N	1.90	0.86
1:B:511:ILE:HD13	1:B:512:SER:N	1.91	0.85
1:D:107:ILE:HD13	1:D:280:VAL:HG21	1.59	0.85
1:D:473:MET:HB3	1:D:475:LEU:HD22	1.59	0.85
1:A:103:LEU:CD1	1:A:275:LEU:HD13	2.06	0.85
1:D:275:LEU:HD23	1:D:283:ALA:HB1	1.58	0.84
1:B:107:ILE:HD13	1:B:280:VAL:HG21	1.59	0.84
1:C:275:LEU:HD23	1:C:283:ALA:HB1	1.57	0.84
1:C:505:ASP:CB	1:D:513:VAL:HB	2.08	0.84
1:B:275:LEU:HD23	1:B:283:ALA:HB1	1.57	0.84
1:D:103:LEU:CD1	1:D:275:LEU:HD13	2.07	0.84
1:C:107:ILE:HD13	1:C:280:VAL:HG21	1.58	0.83
1:A:473:MET:HB3	1:A:475:LEU:HD22	1.61	0.83
1:A:47:ALA:HB2	1:D:108:GLU:OE2	1.79	0.82
1:B:473:MET:HB3	1:B:475:LEU:HD22	1.61	0.82
1:A:446:LEU:O	1:A:511:ILE:HG21	1.79	0.81
1:C:473:MET:HB3	1:C:475:LEU:HD22	1.60	0.81
1:A:275:LEU:HD23	1:A:283:ALA:HB1	1.60	0.81
1:D:452:THR:HG23	1:D:498:SER:HB2	1.64	0.79
1:A:107:ILE:HD13	1:A:280:VAL:HG21	1.65	0.79
1:A:50:SER:HB3	1:D:513:VAL:HG13	1.64	0.79
1:A:488:LEU:HD11	1:B:488:LEU:HD11	1.68	0.76
1:A:133:PHE:CZ	1:A:464:ILE:HD11	2.21	0.76
1:A:513:VAL:HB	1:B:505:ASP:HB2	1.68	0.76
1:C:452:THR:HG23	1:C:498:SER:HB2	1.67	0.76
1:B:452:THR:HG23	1:B:498:SER:HB2	1.68	0.76
1:D:268:GLN:HB3	1:D:271:ILE:HB	1.68	0.76
1:B:268:GLN:HB3	1:B:271:ILE:HB	1.69	0.75
1:A:505:ASP:HB2	1:B:513:VAL:HB	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:GLN:HB3	1:C:271:ILE:HB	1.68	0.74
1:D:133:PHE:CZ	1:D:464:ILE:HD11	2.21	0.74
1:A:268:GLN:HB3	1:A:271:ILE:HB	1.69	0.74
1:A:452:THR:HG23	1:A:498:SER:HB2	1.69	0.74
1:A:50:SER:CA	1:D:513:VAL:HG21	2.18	0.74
1:B:133:PHE:CZ	1:B:464:ILE:HD11	2.23	0.73
1:C:133:PHE:CZ	1:C:464:ILE:HD11	2.24	0.73
1:A:153:ALA:O	1:A:157:ILE:HG22	1.89	0.73
1:A:473:MET:HB3	1:A:475:LEU:CD2	2.19	0.73
1:C:473:MET:HB3	1:C:475:LEU:CD2	2.18	0.73
1:D:473:MET:HB3	1:D:475:LEU:CD2	2.19	0.73
1:C:410:ALA:O	1:C:414:ALA:HB2	1.89	0.72
1:A:50:SER:HB3	1:D:513:VAL:HG11	1.72	0.72
1:D:153:ALA:O	1:D:157:ILE:HG22	1.89	0.72
1:A:271:ILE:HG22	1:A:272:GLN:N	2.05	0.72
1:D:170:ALA:HB1	1:D:407:LEU:HD21	1.72	0.71
1:A:206:MET:HE2	1:A:346:LEU:HD12	1.71	0.71
1:D:271:ILE:HG22	1:D:272:GLN:N	2.04	0.71
1:A:511:ILE:HD13	1:A:511:ILE:C	2.14	0.71
1:A:410:ALA:O	1:A:414:ALA:HB2	1.90	0.71
1:B:410:ALA:O	1:B:414:ALA:HB2	1.89	0.71
1:C:170:ALA:HB1	1:C:407:LEU:HD21	1.72	0.71
1:B:153:ALA:O	1:B:157:ILE:HG22	1.90	0.70
1:D:511:ILE:HD13	1:D:511:ILE:C	2.16	0.70
1:D:410:ALA:O	1:D:414:ALA:HB2	1.92	0.70
1:A:50:SER:HA	1:D:513:VAL:HG21	1.73	0.70
1:D:100:LYS:HZ2	1:D:520:THR:HG22	1.57	0.70
1:C:511:ILE:HD13	1:C:511:ILE:C	2.16	0.70
1:B:455:GLY:O	1:B:494:ILE:HG22	1.92	0.70
1:A:170:ALA:HB1	1:A:407:LEU:HD21	1.72	0.69
1:C:488:LEU:HD11	1:D:488:LEU:HD11	1.73	0.69
1:B:206:MET:HE2	1:B:346:LEU:HD12	1.74	0.69
1:B:473:MET:HB3	1:B:475:LEU:CD2	2.20	0.69
1:C:63:ALA:CB	1:C:270:ILE:HG21	2.23	0.69
1:B:170:ALA:HB1	1:B:407:LEU:HD21	1.75	0.69
1:B:511:ILE:HD13	1:B:511:ILE:C	2.18	0.68
1:C:153:ALA:O	1:C:157:ILE:HG22	1.93	0.68
1:A:50:SER:H	1:D:513:VAL:CG2	2.06	0.68
1:C:251:VAL:HG12	1:C:252:LEU:HD23	1.73	0.68
1:B:63:ALA:CB	1:B:270:ILE:HG21	2.24	0.68
1:A:50:SER:N	1:D:513:VAL:CG2	2.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ILE:CG2	1:D:272:GLN:N	2.58	0.67
1:C:206:MET:HE2	1:C:346:LEU:HD12	1.74	0.67
1:C:224:MET:HB2	1:C:310:VAL:HG21	1.77	0.67
1:A:538:LEU:HD12	1:A:538:LEU:C	2.20	0.67
1:D:105:ILE:HG21	1:D:446:LEU:CD2	2.25	0.67
1:C:271:ILE:HG22	1:C:272:GLN:N	2.10	0.67
1:A:327:THR:HA	1:A:329:LEU:HD22	1.77	0.66
1:A:63:ALA:CB	1:A:270:ILE:HG21	2.25	0.66
1:D:308:ALA:HB2	1:D:342:LEU:HD11	1.78	0.66
1:D:251:VAL:HG12	1:D:252:LEU:HD23	1.78	0.66
1:D:224:MET:HB2	1:D:310:VAL:HG21	1.78	0.66
1:A:271:ILE:CG2	1:A:272:GLN:N	2.59	0.66
1:C:105:ILE:HG21	1:C:446:LEU:CD2	2.26	0.65
1:B:222:SER:O	1:B:225:VAL:HG12	1.95	0.65
1:C:513:VAL:HG12	1:D:505:ASP:OD2	1.97	0.65
1:A:288:VAL:HG23	1:A:524:PHE:CD1	2.31	0.65
1:D:206:MET:HE2	1:D:346:LEU:HD12	1.77	0.65
1:B:288:VAL:HG23	1:B:524:PHE:CD1	2.31	0.65
1:C:105:ILE:HD13	1:C:446:LEU:HD22	1.79	0.65
1:B:271:ILE:HG22	1:B:272:GLN:N	2.10	0.65
1:D:100:LYS:NZ	1:D:520:THR:HG22	2.12	0.65
1:C:513:VAL:HB	1:D:505:ASP:HB2	1.78	0.65
1:D:538:LEU:C	1:D:538:LEU:HD12	2.22	0.65
1:C:222:SER:O	1:C:225:VAL:HG12	1.96	0.65
1:D:141:VAL:HG22	1:D:142:ASN:N	2.12	0.64
1:D:63:ALA:CB	1:D:270:ILE:HG21	2.26	0.64
1:A:505:ASP:OD2	1:B:513:VAL:HG12	1.97	0.64
1:A:459:GLY:HA3	1:A:494:ILE:HG23	1.79	0.64
1:B:327:THR:HA	1:B:329:LEU:HD22	1.79	0.64
1:B:224:MET:HB2	1:B:310:VAL:HG21	1.79	0.64
1:D:144:THR:HG23	1:D:414:ALA:HA	1.80	0.64
1:D:327:THR:HA	1:D:329:LEU:HD22	1.79	0.64
1:C:288:VAL:HG23	1:C:524:PHE:CD1	2.33	0.64
1:D:288:VAL:HG23	1:D:524:PHE:CD1	2.32	0.64
1:C:141:VAL:HG22	1:C:142:ASN:N	2.13	0.64
1:B:484:LEU:C	1:B:484:LEU:HD23	2.22	0.64
1:A:63:ALA:HB1	1:A:270:ILE:HD12	1.80	0.63
1:A:224:MET:HB2	1:A:310:VAL:HG21	1.80	0.63
1:C:271:ILE:CG2	1:C:272:GLN:N	2.62	0.63
1:A:455:GLY:O	1:A:494:ILE:HG22	1.98	0.63
1:B:141:VAL:HG22	1:B:142:ASN:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:THR:HA	1:C:329:LEU:HD22	1.79	0.63
1:A:107:ILE:HD12	1:A:108:GLU:N	2.14	0.63
1:C:455:GLY:O	1:C:494:ILE:HG22	1.98	0.63
1:C:484:LEU:HD23	1:C:484:LEU:C	2.23	0.63
1:B:63:ALA:HB1	1:B:270:ILE:HD12	1.81	0.62
1:B:144:THR:HG23	1:B:414:ALA:HA	1.81	0.62
1:C:459:GLY:HA3	1:C:494:ILE:HG23	1.81	0.62
1:A:308:ALA:HB2	1:A:342:LEU:HD11	1.81	0.62
1:B:251:VAL:HG12	1:B:252:LEU:HD23	1.81	0.62
1:D:63:ALA:HB1	1:D:270:ILE:HD12	1.82	0.62
1:D:105:ILE:HD13	1:D:446:LEU:HD22	1.80	0.62
1:D:455:GLY:O	1:D:494:ILE:HG22	2.00	0.62
1:A:202:MET:HE2	1:A:202:MET:HA	1.81	0.62
1:B:308:ALA:HB2	1:B:342:LEU:HD11	1.82	0.62
1:B:459:GLY:HA3	1:B:494:ILE:HG23	1.80	0.62
1:A:513:VAL:HG12	1:B:505:ASP:OD2	2.00	0.62
1:A:144:THR:HG23	1:A:414:ALA:HA	1.80	0.62
1:C:144:THR:HG23	1:C:414:ALA:HA	1.81	0.62
1:A:251:VAL:HG12	1:A:252:LEU:HD23	1.82	0.62
1:B:95:LEU:HA	1:B:98:VAL:HG13	1.82	0.61
1:A:50:SER:CB	1:D:513:VAL:HG11	2.30	0.61
1:B:271:ILE:CG2	1:B:272:GLN:N	2.63	0.61
1:A:100:LYS:NZ	1:A:520:THR:HG22	2.15	0.61
1:C:63:ALA:HB1	1:C:270:ILE:HD12	1.82	0.61
1:B:105:ILE:HG21	1:B:446:LEU:CD2	2.31	0.61
1:C:95:LEU:HA	1:C:98:VAL:HG13	1.83	0.60
1:C:308:ALA:HB2	1:C:342:LEU:HD11	1.81	0.60
1:B:105:ILE:HD13	1:B:446:LEU:HD22	1.81	0.60
1:A:266:PHE:O	1:A:268:GLN:N	2.35	0.60
1:A:105:ILE:HD13	1:A:446:LEU:HD22	1.83	0.60
1:B:538:LEU:C	1:B:538:LEU:HD12	2.25	0.60
1:D:222:SER:O	1:D:225:VAL:HG12	2.01	0.60
1:A:271:ILE:O	1:A:275:LEU:HD12	2.01	0.60
1:B:458:ILE:HD12	1:B:497:THR:HG21	1.84	0.60
1:B:271:ILE:HG23	1:B:275:LEU:CD1	2.32	0.60
1:C:98:VAL:HB	1:C:265:GLY:HA2	1.83	0.60
1:C:100:LYS:NZ	1:C:520:THR:HG22	2.17	0.60
1:D:266:PHE:CE2	1:D:442:PHE:HB3	2.36	0.60
1:D:459:GLY:HA3	1:D:494:ILE:HG23	1.82	0.60
1:A:458:ILE:HD12	1:A:497:THR:HG21	1.84	0.59
1:B:202:MET:HA	1:B:202:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ILE:HG23	1:A:275:LEU:CD1	2.32	0.59
1:A:98:VAL:HB	1:A:265:GLY:HA2	1.85	0.59
1:D:202:MET:HE2	1:D:202:MET:HA	1.84	0.59
1:A:95:LEU:HA	1:A:98:VAL:HG13	1.85	0.59
1:A:141:VAL:HG22	1:A:142:ASN:N	2.17	0.59
1:B:98:VAL:HB	1:B:265:GLY:HA2	1.83	0.59
1:A:222:SER:O	1:A:225:VAL:HG12	2.03	0.59
1:C:459:GLY:HA3	1:C:494:ILE:CG2	2.33	0.59
1:B:100:LYS:NZ	1:B:520:THR:HG22	2.17	0.58
1:B:107:ILE:HD12	1:B:108:GLU:N	2.18	0.58
1:B:474:PRO:O	1:B:475:LEU:C	2.45	0.58
1:C:329:LEU:HD12	1:C:341:TRP:NE1	2.19	0.58
1:D:271:ILE:O	1:D:275:LEU:HD12	2.03	0.58
1:B:329:LEU:HD12	1:B:341:TRP:NE1	2.19	0.58
1:C:202:MET:HE2	1:C:202:MET:HA	1.86	0.58
1:C:206:MET:CE	1:C:346:LEU:HD12	2.34	0.58
1:A:327:THR:O	1:A:329:LEU:HD13	2.04	0.58
1:C:538:LEU:HD12	1:C:538:LEU:C	2.28	0.58
1:D:95:LEU:HA	1:D:98:VAL:HG13	1.84	0.58
1:D:107:ILE:HD12	1:D:108:GLU:N	2.19	0.58
1:A:100:LYS:HZ2	1:A:520:THR:HG22	1.69	0.58
1:A:327:THR:C	1:A:329:LEU:HD13	2.29	0.58
1:C:107:ILE:HD12	1:C:108:GLU:N	2.19	0.58
1:D:206:MET:CE	1:D:346:LEU:HD12	2.33	0.58
1:D:249:ILE:HD12	1:D:253:ILE:HD11	1.86	0.58
1:A:105:ILE:HG21	1:A:446:LEU:CD2	2.34	0.58
1:D:266:PHE:O	1:D:268:GLN:N	2.37	0.58
1:D:271:ILE:HG23	1:D:275:LEU:CD1	2.34	0.58
1:A:50:SER:N	1:D:513:VAL:HG22	2.18	0.57
1:A:249:ILE:HD12	1:A:253:ILE:HD11	1.84	0.57
1:B:379:MET:HE1	1:B:395:LEU:HG	1.87	0.57
1:C:224:MET:HE3	1:C:306:ILE:HG22	1.87	0.57
1:C:327:THR:O	1:C:329:LEU:HD13	2.05	0.57
1:A:379:MET:HE1	1:A:395:LEU:HG	1.87	0.57
1:D:379:MET:HE1	1:D:395:LEU:HG	1.86	0.57
1:A:206:MET:CE	1:A:346:LEU:HD12	2.35	0.57
1:A:459:GLY:HA3	1:A:494:ILE:CG2	2.34	0.57
1:D:459:GLY:HA3	1:D:494:ILE:CG2	2.35	0.57
1:C:427:ILE:O	1:C:431:THR:HG23	2.05	0.56
1:A:266:PHE:CE2	1:A:442:PHE:HB3	2.40	0.56
1:C:266:PHE:CE2	1:C:442:PHE:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:ILE:HD12	1:C:497:THR:HG21	1.87	0.56
1:B:427:ILE:O	1:B:431:THR:HG23	2.06	0.56
1:D:98:VAL:HB	1:D:265:GLY:HA2	1.87	0.56
1:D:484:LEU:C	1:D:484:LEU:HD23	2.30	0.56
1:B:160:ILE:HG23	1:B:161:PRO:HD2	1.88	0.56
1:C:271:ILE:HG23	1:C:275:LEU:CD1	2.36	0.56
1:B:266:PHE:CE2	1:B:442:PHE:HB3	2.40	0.56
1:B:469:PHE:O	1:B:473:MET:HB2	2.06	0.56
1:A:160:ILE:HG23	1:A:161:PRO:HD2	1.88	0.56
1:C:327:THR:C	1:C:329:LEU:HD13	2.30	0.56
1:A:71:ILE:HG22	1:A:149:LEU:HD22	1.88	0.56
1:D:458:ILE:HD12	1:D:497:THR:HG21	1.87	0.56
1:A:329:LEU:HD12	1:A:341:TRP:NE1	2.20	0.56
1:A:484:LEU:C	1:A:484:LEU:HD23	2.31	0.56
1:D:324:ILE:HG22	1:D:324:ILE:O	2.06	0.56
1:B:71:ILE:HG22	1:B:149:LEU:HD22	1.88	0.56
1:B:95:LEU:HD21	1:B:264:TRP:CE3	2.41	0.55
1:A:137:LEU:HD23	1:A:138:TYR:N	2.21	0.55
1:A:275:LEU:HD23	1:A:283:ALA:CB	2.35	0.55
1:C:249:ILE:HD12	1:C:253:ILE:HD11	1.88	0.55
1:C:379:MET:HE1	1:C:395:LEU:HG	1.88	0.55
1:A:50:SER:N	1:D:513:VAL:HG21	2.21	0.55
1:A:474:PRO:O	1:A:475:LEU:C	2.50	0.55
1:D:275:LEU:HD23	1:D:283:ALA:CB	2.34	0.55
1:B:271:ILE:O	1:B:275:LEU:HD12	2.07	0.55
1:B:327:THR:C	1:B:329:LEU:HD13	2.32	0.55
1:A:301:VAL:HG23	1:A:302:VAL:HG13	1.89	0.54
1:B:107:ILE:CD1	1:B:280:VAL:HG21	2.34	0.54
1:C:275:LEU:HD23	1:C:283:ALA:CB	2.34	0.54
1:D:224:MET:HE3	1:D:306:ILE:HG22	1.89	0.54
1:D:327:THR:C	1:D:329:LEU:HD13	2.32	0.54
1:D:427:ILE:O	1:D:431:THR:HG23	2.07	0.54
1:A:371:ASN:OD1	1:A:372:SER:N	2.41	0.54
1:A:511:ILE:C	1:A:511:ILE:CD1	2.81	0.54
1:B:459:GLY:HA3	1:B:494:ILE:CG2	2.37	0.54
1:B:327:THR:O	1:B:329:LEU:HD13	2.07	0.54
1:B:371:ASN:OD1	1:B:372:SER:N	2.40	0.54
1:C:478:PRO:O	1:C:482:GLN:HB2	2.07	0.54
1:D:107:ILE:CD1	1:D:280:VAL:HG21	2.35	0.54
1:B:301:VAL:HG23	1:B:302:VAL:HG13	1.89	0.54
1:D:474:PRO:O	1:D:475:LEU:C	2.49	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:MET:HE3	1:A:306:ILE:HG22	1.89	0.54
1:B:295:LEU:HD22	1:B:535:LEU:HD21	1.89	0.54
1:C:160:ILE:HG23	1:C:161:PRO:HD2	1.88	0.54
1:C:425:GLN:HE21	1:C:425:GLN:HA	1.73	0.54
1:D:478:PRO:O	1:D:482:GLN:HB2	2.07	0.54
1:B:417:LEU:N	1:B:417:LEU:HD23	2.22	0.54
1:D:262:TYR:HB2	1:D:439:LEU:HD22	1.89	0.54
1:D:329:LEU:HD12	1:D:341:TRP:NE1	2.23	0.54
1:D:441:VAL:HG12	1:D:442:PHE:N	2.22	0.54
1:A:95:LEU:HD21	1:A:264:TRP:CE3	2.43	0.54
1:A:417:LEU:HD23	1:A:417:LEU:N	2.23	0.54
1:A:469:PHE:O	1:A:473:MET:HB2	2.07	0.54
1:B:266:PHE:O	1:B:268:GLN:N	2.41	0.54
1:B:395:LEU:HD23	1:B:395:LEU:C	2.33	0.54
1:B:407:LEU:C	1:B:407:LEU:HD23	2.33	0.54
1:A:478:PRO:O	1:A:482:GLN:HB2	2.09	0.53
1:C:266:PHE:O	1:C:268:GLN:N	2.41	0.53
1:C:324:ILE:O	1:C:324:ILE:HG22	2.08	0.53
1:D:98:VAL:HA	1:D:102:PHE:CD1	2.43	0.53
1:D:133:PHE:HB3	1:D:434:VAL:HG21	1.90	0.53
1:A:324:ILE:O	1:A:324:ILE:HG22	2.08	0.53
1:B:439:LEU:HG	1:B:443:LEU:CD2	2.37	0.53
1:C:95:LEU:HD21	1:C:264:TRP:CE3	2.43	0.53
1:B:52:PRO:HD2	1:B:55:ALA:HB3	1.90	0.53
1:C:52:PRO:HD2	1:C:55:ALA:HB3	1.90	0.53
1:C:271:ILE:O	1:C:275:LEU:HD12	2.09	0.53
1:C:439:LEU:HG	1:C:443:LEU:CD2	2.38	0.53
1:C:474:PRO:O	1:C:475:LEU:C	2.51	0.53
1:D:538:LEU:HD12	1:D:539:TYR:N	2.24	0.53
1:A:513:VAL:HB	1:B:505:ASP:CB	2.37	0.53
1:B:133:PHE:HB3	1:B:434:VAL:HG21	1.90	0.53
1:B:478:PRO:O	1:B:482:GLN:HB2	2.09	0.53
1:C:513:VAL:HB	1:D:505:ASP:CB	2.38	0.53
1:D:160:ILE:HG23	1:D:161:PRO:HD2	1.90	0.53
1:D:546:TYR:O	1:D:547:LYS:CB	2.56	0.53
1:C:450:LYS:NZ	1:C:505:ASP:OD1	2.41	0.53
1:D:425:GLN:HA	1:D:425:GLN:HE21	1.74	0.53
1:D:469:PHE:O	1:D:473:MET:HB2	2.08	0.53
1:C:301:VAL:HG23	1:C:302:VAL:HG13	1.89	0.52
1:B:206:MET:CE	1:B:346:LEU:HD12	2.37	0.52
1:C:469:PHE:O	1:C:473:MET:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ILE:HG22	1:D:149:LEU:HD22	1.91	0.52
1:D:235:ILE:H	1:D:235:ILE:HD12	1.74	0.52
1:D:518:PHE:O	1:D:519:VAL:C	2.53	0.52
1:D:417:LEU:N	1:D:417:LEU:HD23	2.24	0.52
1:A:295:LEU:HD22	1:A:535:LEU:HD21	1.91	0.52
1:A:378:THR:C	1:A:379:MET:HE2	2.34	0.52
1:A:407:LEU:C	1:A:407:LEU:HD23	2.35	0.52
1:A:458:ILE:HD12	1:A:497:THR:CG2	2.40	0.52
1:C:511:ILE:C	1:C:511:ILE:CD1	2.82	0.52
1:C:546:TYR:O	1:C:547:LYS:CB	2.56	0.52
1:A:98:VAL:HA	1:A:102:PHE:CD1	2.45	0.52
1:B:378:THR:C	1:B:379:MET:HE2	2.35	0.52
1:C:371:ASN:OD1	1:C:372:SER:N	2.43	0.52
1:C:407:LEU:HD23	1:C:407:LEU:C	2.35	0.52
1:A:538:LEU:HD12	1:A:539:TYR:N	2.25	0.52
1:C:147:LEU:HD12	1:C:410:ALA:HB1	1.92	0.52
1:A:546:TYR:O	1:A:547:LYS:CB	2.56	0.52
1:B:458:ILE:HD12	1:B:497:THR:CG2	2.40	0.52
1:B:546:TYR:O	1:B:547:LYS:CB	2.58	0.52
1:C:417:LEU:HD23	1:C:417:LEU:N	2.24	0.52
1:D:511:ILE:C	1:D:511:ILE:CD1	2.83	0.52
1:C:71:ILE:HG22	1:C:149:LEU:HD22	1.91	0.51
1:C:295:LEU:HD22	1:C:535:LEU:HD21	1.92	0.51
1:B:249:ILE:HD12	1:B:253:ILE:HD11	1.91	0.51
1:D:371:ASN:OD1	1:D:372:SER:N	2.43	0.51
1:D:512:SER:O	1:D:514:THR:N	2.43	0.51
1:B:137:LEU:O	1:B:141:VAL:HG13	2.10	0.51
1:D:196:LEU:HD11	1:D:361:ALA:CB	2.40	0.51
1:A:518:PHE:O	1:A:519:VAL:C	2.53	0.51
1:B:324:ILE:HG22	1:B:324:ILE:O	2.10	0.51
1:A:505:ASP:CB	1:B:513:VAL:HB	2.39	0.51
1:B:518:PHE:O	1:B:519:VAL:C	2.53	0.51
1:C:484:LEU:C	1:C:484:LEU:CD2	2.83	0.51
1:D:295:LEU:HD22	1:D:535:LEU:HD21	1.92	0.51
1:D:301:VAL:HG23	1:D:302:VAL:HG13	1.91	0.51
1:D:407:LEU:C	1:D:407:LEU:HD23	2.35	0.51
1:A:69:GLN:O	1:A:73:MET:HB3	2.10	0.51
1:C:458:ILE:HD12	1:C:497:THR:CG2	2.41	0.51
1:D:327:THR:O	1:D:329:LEU:HD13	2.11	0.51
1:D:537:VAL:HG13	1:D:538:LEU:N	2.26	0.51
1:A:512:SER:O	1:A:514:THR:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LEU:HD11	1:B:361:ALA:CB	2.41	0.51
1:B:275:LEU:HD23	1:B:283:ALA:CB	2.34	0.51
1:C:133:PHE:HB3	1:C:434:VAL:HG21	1.93	0.51
1:C:137:LEU:O	1:C:141:VAL:HG13	2.10	0.51
1:D:69:GLN:O	1:D:73:MET:HB3	2.11	0.50
1:D:196:LEU:HD11	1:D:361:ALA:HB2	1.93	0.50
1:B:137:LEU:HD23	1:B:138:TYR:N	2.25	0.50
1:D:95:LEU:HD21	1:D:264:TRP:CE3	2.46	0.50
1:B:147:LEU:HD12	1:B:410:ALA:HB1	1.94	0.50
1:B:484:LEU:C	1:B:484:LEU:CD2	2.84	0.50
1:A:133:PHE:HB3	1:A:434:VAL:HG21	1.93	0.50
1:A:439:LEU:HG	1:A:443:LEU:CD2	2.41	0.50
1:A:444:LEU:HD12	1:A:494:ILE:HD11	1.93	0.50
1:B:288:VAL:CG2	1:B:524:PHE:CD1	2.95	0.50
1:B:425:GLN:HE21	1:B:425:GLN:HA	1.77	0.50
1:B:69:GLN:O	1:B:73:MET:HB3	2.11	0.50
1:B:98:VAL:HA	1:B:102:PHE:CD1	2.46	0.50
1:C:395:LEU:C	1:C:395:LEU:HD23	2.37	0.50
1:A:288:VAL:CG2	1:A:524:PHE:CD1	2.95	0.50
1:A:378:THR:HB	1:A:379:MET:HE2	1.93	0.50
1:B:262:TYR:HB2	1:B:439:LEU:HD22	1.94	0.50
1:A:262:TYR:HB2	1:A:439:LEU:HD22	1.93	0.50
1:D:137:LEU:HD23	1:D:138:TYR:N	2.27	0.50
1:D:378:THR:C	1:D:379:MET:HE2	2.37	0.50
1:A:271:ILE:HG23	1:A:275:LEU:HD12	1.94	0.49
1:A:450:LYS:NZ	1:A:505:ASP:OD1	2.43	0.49
1:B:327:THR:HG22	1:B:328:ASN:H	1.77	0.49
1:C:327:THR:HG22	1:C:328:ASN:H	1.77	0.49
1:D:395:LEU:HD23	1:D:395:LEU:C	2.37	0.49
1:A:427:ILE:O	1:A:431:THR:HG23	2.11	0.49
1:B:538:LEU:HD12	1:B:539:TYR:N	2.27	0.49
1:A:324:ILE:C	1:A:326:ALA:N	2.70	0.49
1:B:324:ILE:C	1:B:326:ALA:N	2.70	0.49
1:B:224:MET:HE3	1:B:306:ILE:HG22	1.94	0.49
1:D:52:PRO:HD2	1:D:55:ALA:HB3	1.94	0.49
1:C:235:ILE:HD12	1:C:235:ILE:H	1.78	0.49
1:D:458:ILE:HD12	1:D:497:THR:CG2	2.42	0.49
1:B:541:LEU:O	1:B:544:VAL:HG12	2.12	0.49
1:C:378:THR:C	1:C:379:MET:HE2	2.37	0.49
1:B:266:PHE:CZ	1:B:446:LEU:HD12	2.48	0.49
1:C:69:GLN:O	1:C:73:MET:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:SER:O	1:C:514:THR:N	2.46	0.49
1:D:327:THR:HG22	1:D:328:ASN:H	1.77	0.49
1:D:513:VAL:O	1:D:513:VAL:HG23	2.12	0.49
1:A:73:MET:HE1	1:A:88:GLU:HG2	1.94	0.49
1:C:61:ILE:HG13	1:C:293:LEU:HD12	1.94	0.49
1:D:178:ILE:N	1:D:178:ILE:HD12	2.28	0.49
1:A:52:PRO:HD2	1:A:55:ALA:HB3	1.94	0.49
1:C:137:LEU:HD23	1:C:138:TYR:N	2.27	0.49
1:D:325:ALA:O	1:D:329:LEU:HD11	2.13	0.49
1:A:196:LEU:HD11	1:A:361:ALA:CB	2.43	0.48
1:A:534:VAL:O	1:A:537:VAL:HG12	2.13	0.48
1:C:441:VAL:HG12	1:C:442:PHE:N	2.27	0.48
1:D:324:ILE:C	1:D:326:ALA:N	2.71	0.48
1:A:444:LEU:HD12	1:A:494:ILE:CD1	2.43	0.48
1:C:126:LEU:HD12	1:C:457:ILE:HD13	1.96	0.48
1:D:61:ILE:HG13	1:D:293:LEU:HD12	1.95	0.48
1:D:266:PHE:CZ	1:D:442:PHE:HB3	2.48	0.48
1:D:534:VAL:O	1:D:537:VAL:HG12	2.13	0.48
1:B:61:ILE:HG13	1:B:293:LEU:HD12	1.95	0.48
1:B:178:ILE:N	1:B:178:ILE:HD12	2.28	0.48
1:C:100:LYS:HZ2	1:C:520:THR:HG22	1.77	0.48
1:C:348:VAL:HG23	1:C:349:GLY:H	1.78	0.48
1:A:537:VAL:HG13	1:A:538:LEU:N	2.28	0.48
1:A:541:LEU:O	1:A:544:VAL:HG12	2.14	0.48
1:B:100:LYS:HZ3	1:B:520:THR:HG22	1.76	0.48
1:B:271:ILE:C	1:B:275:LEU:HD12	2.38	0.48
1:C:196:LEU:HD11	1:C:361:ALA:CB	2.43	0.48
1:A:378:THR:HG21	1:A:399:GLY:HA2	1.96	0.48
1:B:512:SER:O	1:B:514:THR:N	2.46	0.48
1:C:107:ILE:CD1	1:C:280:VAL:HG21	2.35	0.48
1:C:178:ILE:HD12	1:C:178:ILE:N	2.28	0.48
1:C:339:TYR:N	1:C:340:PRO:HD2	2.29	0.48
1:A:49:LYS:HG2	1:D:512:SER:OG	2.14	0.48
1:A:325:ALA:O	1:A:329:LEU:HD11	2.13	0.48
1:A:425:GLN:HE21	1:A:425:GLN:HA	1.79	0.48
1:A:395:LEU:C	1:A:395:LEU:HD23	2.38	0.48
1:D:541:LEU:O	1:D:544:VAL:HG12	2.14	0.48
1:A:178:ILE:N	1:A:178:ILE:HD12	2.29	0.48
1:A:327:THR:HG22	1:A:328:ASN:H	1.77	0.48
1:B:537:VAL:HG13	1:B:538:LEU:N	2.29	0.48
1:C:518:PHE:O	1:C:519:VAL:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:THR:HB	1:D:379:MET:HE2	1.96	0.48
1:A:196:LEU:HD11	1:A:361:ALA:HB2	1.96	0.48
1:D:348:VAL:HG23	1:D:349:GLY:H	1.79	0.48
1:A:267:ASN:O	1:A:269:TYR:N	2.47	0.47
1:D:132:VAL:O	1:D:136:SER:OG	2.31	0.47
1:D:225:VAL:HG23	1:D:232:PHE:CD1	2.49	0.47
1:A:271:ILE:C	1:A:275:LEU:HD12	2.39	0.47
1:B:379:MET:O	1:B:383:LYS:HB3	2.13	0.47
1:B:196:LEU:HD11	1:B:361:ALA:HB2	1.95	0.47
1:C:98:VAL:HA	1:C:102:PHE:CD1	2.48	0.47
1:A:107:ILE:CD1	1:A:280:VAL:HG21	2.40	0.47
1:C:378:THR:HG21	1:C:399:GLY:HA2	1.97	0.47
1:C:379:MET:O	1:C:383:LYS:HB3	2.14	0.47
1:D:271:ILE:C	1:D:275:LEU:HD12	2.39	0.47
1:A:147:LEU:HD12	1:A:410:ALA:HB1	1.97	0.47
1:D:271:ILE:HG23	1:D:275:LEU:HD12	1.96	0.47
1:D:278:LYS:O	1:D:279:SER:C	2.57	0.47
1:D:288:VAL:CG2	1:D:524:PHE:CD1	2.97	0.47
1:A:75:GLY:HA3	1:A:336:ASP:HA	1.96	0.47
1:A:128:THR:O	1:A:131:ALA:HB3	2.14	0.47
1:A:379:MET:O	1:A:383:LYS:HB3	2.15	0.47
1:A:535:LEU:O	1:A:536:ALA:C	2.58	0.47
1:B:201:PHE:HA	1:B:204:THR:HG22	1.95	0.47
1:C:262:TYR:HB2	1:C:439:LEU:HD22	1.97	0.47
1:C:266:PHE:CZ	1:C:446:LEU:HD12	2.49	0.47
1:D:71:ILE:HD11	1:D:153:ALA:HB2	1.97	0.47
1:A:201:PHE:HA	1:A:204:THR:HG22	1.97	0.47
1:B:535:LEU:O	1:B:536:ALA:C	2.58	0.47
1:C:324:ILE:C	1:C:326:ALA:N	2.70	0.47
1:D:126:LEU:HD12	1:D:457:ILE:HD13	1.97	0.47
1:D:137:LEU:O	1:D:141:VAL:HG13	2.15	0.47
1:A:71:ILE:CG2	1:A:149:LEU:HD22	2.44	0.47
1:A:278:LYS:O	1:A:279:SER:C	2.58	0.47
1:B:271:ILE:HG23	1:B:275:LEU:HD12	1.96	0.47
1:A:266:PHE:O	1:A:267:ASN:C	2.58	0.47
1:A:348:VAL:HG23	1:A:349:GLY:H	1.80	0.47
1:A:441:VAL:HG12	1:A:442:PHE:N	2.29	0.47
1:B:126:LEU:HD12	1:B:457:ILE:HD13	1.97	0.47
1:C:196:LEU:HD11	1:C:361:ALA:HB2	1.96	0.47
1:C:278:LYS:O	1:C:279:SER:C	2.58	0.47
1:D:201:PHE:HA	1:D:204:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:THR:O	1:B:131:ALA:HB3	2.15	0.46
1:C:105:ILE:CD1	1:C:446:LEU:HD22	2.44	0.46
1:D:147:LEU:HD12	1:D:410:ALA:HB1	1.97	0.46
1:B:71:ILE:CG2	1:B:149:LEU:HD22	2.44	0.46
1:B:378:THR:HB	1:B:379:MET:HE2	1.97	0.46
1:B:75:GLY:HA3	1:B:336:ASP:HA	1.97	0.46
1:B:325:ALA:O	1:B:329:LEU:HD11	2.15	0.46
1:C:201:PHE:HA	1:C:204:THR:HG22	1.97	0.46
1:C:271:ILE:C	1:C:275:LEU:HD12	2.40	0.46
1:A:50:SER:HB3	1:D:513:VAL:CG2	2.46	0.46
1:B:256:LEU:O	1:B:259:ALA:HB3	2.14	0.46
1:C:288:VAL:CG2	1:C:524:PHE:CD1	2.98	0.46
1:C:538:LEU:HD12	1:C:539:TYR:N	2.30	0.46
1:D:94:THR:HG22	1:D:95:LEU:N	2.31	0.46
1:D:439:LEU:HG	1:D:443:LEU:CD2	2.45	0.46
1:B:339:TYR:N	1:B:340:PRO:HD2	2.30	0.46
1:C:374:ALA:HB1	1:C:399:GLY:O	2.16	0.46
1:D:339:TYR:N	1:D:340:PRO:HD2	2.30	0.46
1:A:50:SER:CA	1:D:513:VAL:CG2	2.90	0.46
1:B:71:ILE:HD11	1:B:153:ALA:HB2	1.98	0.46
1:B:534:VAL:O	1:B:537:VAL:HG12	2.16	0.46
1:C:435:SER:N	1:C:436:PRO:CD	2.79	0.46
1:B:94:THR:HG22	1:B:95:LEU:N	2.31	0.46
1:D:266:PHE:O	1:D:267:ASN:C	2.59	0.46
1:D:379:MET:O	1:D:383:LYS:HB3	2.15	0.46
1:A:61:ILE:HG13	1:A:293:LEU:HD12	1.98	0.46
1:B:278:LYS:O	1:B:279:SER:C	2.59	0.46
1:B:374:ALA:HB1	1:B:399:GLY:O	2.15	0.46
1:C:541:LEU:O	1:C:544:VAL:HG12	2.15	0.46
1:C:542:PHE:O	1:C:543:TRP:C	2.59	0.46
1:D:128:THR:O	1:D:131:ALA:HB3	2.15	0.46
1:D:444:LEU:HD12	1:D:494:ILE:HD11	1.98	0.46
1:D:542:PHE:O	1:D:543:TRP:C	2.59	0.46
1:B:128:THR:O	1:B:132:VAL:HG23	2.16	0.45
1:C:266:PHE:CZ	1:C:442:PHE:HB3	2.51	0.45
1:A:52:PRO:O	1:A:53:TRP:C	2.59	0.45
1:C:128:THR:O	1:C:131:ALA:HB3	2.17	0.45
1:D:267:ASN:O	1:D:269:TYR:N	2.49	0.45
1:A:128:THR:O	1:A:132:VAL:HG23	2.16	0.45
1:A:137:LEU:O	1:A:141:VAL:HG13	2.16	0.45
1:A:339:TYR:N	1:A:340:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:VAL:HG23	1:B:232:PHE:CD1	2.52	0.45
1:A:235:ILE:HD12	1:A:235:ILE:H	1.82	0.45
1:A:266:PHE:CZ	1:A:442:PHE:HB3	2.51	0.45
1:A:275:LEU:C	1:A:277:ALA:H	2.24	0.45
1:A:495:ALA:O	1:A:499:LEU:HB2	2.17	0.45
1:A:542:PHE:O	1:A:543:TRP:C	2.58	0.45
1:B:94:THR:CG2	1:B:95:LEU:N	2.80	0.45
1:A:225:VAL:HG23	1:A:232:PHE:CD1	2.52	0.45
1:B:348:VAL:HG23	1:B:349:GLY:H	1.80	0.45
1:D:437:GLY:HA2	1:D:490:THR:HG21	1.97	0.45
1:B:378:THR:HG21	1:B:399:GLY:HA2	1.99	0.45
1:D:535:LEU:O	1:D:536:ALA:C	2.60	0.45
1:B:235:ILE:HD12	1:B:235:ILE:H	1.82	0.45
1:B:371:ASN:O	1:B:375:THR:HG23	2.17	0.45
1:A:437:GLY:HA2	1:A:490:THR:HG21	1.99	0.45
1:B:266:PHE:CZ	1:B:442:PHE:HB3	2.51	0.45
1:B:450:LYS:NZ	1:B:505:ASP:OD1	2.41	0.45
1:B:511:ILE:C	1:B:511:ILE:CD1	2.85	0.45
1:C:75:GLY:HA3	1:C:336:ASP:HA	1.99	0.45
1:B:295:LEU:CD2	1:B:535:LEU:HD21	2.47	0.45
1:C:128:THR:O	1:C:132:VAL:HG23	2.17	0.45
1:A:266:PHE:CZ	1:A:446:LEU:HD12	2.52	0.45
1:D:89:TRP:NE1	1:D:298:PRO:HG2	2.32	0.45
1:D:374:ALA:HB1	1:D:399:GLY:O	2.17	0.45
1:D:378:THR:HG21	1:D:399:GLY:HA2	1.97	0.45
1:C:71:ILE:HD11	1:C:153:ALA:HB2	1.98	0.44
1:C:256:LEU:O	1:C:259:ALA:HB3	2.17	0.44
1:C:271:ILE:HG23	1:C:275:LEU:HD12	1.99	0.44
1:A:71:ILE:HD11	1:A:153:ALA:HB2	1.98	0.44
1:D:414:ALA:N	1:D:415:PRO:HD2	2.32	0.44
1:B:288:VAL:HG11	1:B:527:ALA:CB	2.47	0.44
1:C:89:TRP:NE1	1:C:298:PRO:HG2	2.33	0.44
1:C:94:THR:CG2	1:C:95:LEU:N	2.81	0.44
1:C:94:THR:HG22	1:C:95:LEU:N	2.32	0.44
1:D:382:TYR:HA	1:D:386:ILE:HD12	2.00	0.44
1:D:450:LYS:NZ	1:D:505:ASP:OD1	2.41	0.44
1:C:535:LEU:O	1:C:536:ALA:C	2.59	0.44
1:B:103:LEU:CG	1:B:275:LEU:HD13	2.47	0.44
1:C:325:ALA:O	1:C:329:LEU:HD11	2.17	0.44
1:A:89:TRP:NE1	1:A:298:PRO:HG2	2.33	0.44
1:B:542:PHE:O	1:B:543:TRP:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:ALA:O	1:C:499:LEU:HB2	2.18	0.44
1:D:75:GLY:HA3	1:D:336:ASP:HA	1.99	0.44
1:A:76:SER:HB3	1:A:84:ILE:HD13	2.00	0.44
1:C:163:MET:SD	1:C:166:ILE:HD11	2.58	0.44
1:C:225:VAL:HG23	1:C:232:PHE:CD1	2.53	0.44
1:D:275:LEU:C	1:D:277:ALA:H	2.26	0.44
1:A:414:ALA:N	1:A:415:PRO:HD2	2.32	0.44
1:B:439:LEU:HG	1:B:443:LEU:HD21	2.00	0.44
1:B:441:VAL:HG12	1:B:442:PHE:N	2.31	0.44
1:C:132:VAL:O	1:C:136:SER:OG	2.33	0.44
1:C:371:ASN:O	1:C:375:THR:HG23	2.17	0.44
1:D:71:ILE:CG2	1:D:149:LEU:HD22	2.48	0.44
1:D:145:SER:HB2	1:D:427:ILE:HD11	1.99	0.44
1:A:301:VAL:HG23	1:A:302:VAL:N	2.33	0.43
1:C:71:ILE:CG2	1:C:149:LEU:HD22	2.48	0.43
1:C:103:LEU:CG	1:C:275:LEU:HD13	2.48	0.43
1:C:537:VAL:HG13	1:C:538:LEU:N	2.32	0.43
1:D:435:SER:N	1:D:436:PRO:CD	2.81	0.43
1:B:434:VAL:O	1:B:438:ILE:HG23	2.18	0.43
1:D:94:THR:CG2	1:D:95:LEU:N	2.80	0.43
1:A:278:LYS:CG	1:A:279:SER:N	2.81	0.43
1:A:374:ALA:HB1	1:A:399:GLY:O	2.17	0.43
1:A:382:TYR:HA	1:A:386:ILE:HD12	2.00	0.43
1:B:121:ARG:NH1	1:B:445:GLY:O	2.51	0.43
1:C:63:ALA:HB1	1:C:270:ILE:CD1	2.48	0.43
1:C:135:ILE:HA	1:C:373:THR:HG23	2.00	0.43
1:D:65:ILE:HA	1:D:69:GLN:HG3	2.00	0.43
1:A:224:MET:CE	1:A:306:ILE:HG22	2.48	0.43
1:A:367:ALA:HA	1:A:370:LEU:HD12	2.01	0.43
1:B:414:ALA:N	1:B:415:PRO:HD2	2.33	0.43
1:C:157:ILE:HG23	1:C:158:LEU:HG	2.00	0.43
1:C:434:VAL:O	1:C:438:ILE:HG23	2.19	0.43
1:D:295:LEU:CD2	1:D:535:LEU:HD21	2.48	0.43
1:D:301:VAL:HG23	1:D:302:VAL:N	2.33	0.43
1:D:484:LEU:C	1:D:484:LEU:CD2	2.91	0.43
1:A:65:ILE:HA	1:A:69:GLN:HG3	2.00	0.43
1:A:94:THR:HG22	1:A:95:LEU:N	2.34	0.43
1:A:145:SER:HB2	1:A:427:ILE:HD11	2.01	0.43
1:A:414:ALA:HB3	1:A:415:PRO:HD3	2.01	0.43
1:A:484:LEU:C	1:A:484:LEU:CD2	2.90	0.43
1:B:145:SER:HB2	1:B:427:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:LEU:HD13	1:C:272:GLN:HE22	1.82	0.43
1:A:121:ARG:NH1	1:A:445:GLY:O	2.52	0.43
1:A:128:THR:HG23	1:A:381:ILE:HD13	2.01	0.43
1:A:435:SER:N	1:A:436:PRO:CD	2.82	0.43
1:B:65:ILE:HA	1:B:69:GLN:HG3	2.00	0.43
1:C:414:ALA:N	1:C:415:PRO:HD2	2.33	0.43
1:D:141:VAL:CG2	1:D:142:ASN:N	2.79	0.43
1:D:327:THR:CA	1:D:329:LEU:HD13	2.49	0.43
1:D:444:LEU:HD12	1:D:494:ILE:CD1	2.47	0.43
1:A:135:ILE:HA	1:A:373:THR:HG23	2.01	0.43
1:D:103:LEU:CG	1:D:275:LEU:HD13	2.48	0.43
1:B:495:ALA:O	1:B:499:LEU:HB2	2.19	0.43
1:C:437:GLY:HA2	1:C:490:THR:HG21	2.00	0.43
1:D:128:THR:O	1:D:132:VAL:HG23	2.19	0.43
1:A:103:LEU:O	1:A:104:PRO:C	2.62	0.43
1:A:126:LEU:HD12	1:A:457:ILE:HD13	2.00	0.43
1:B:52:PRO:O	1:B:53:TRP:C	2.61	0.43
1:B:275:LEU:C	1:B:277:ALA:H	2.27	0.43
1:D:103:LEU:O	1:D:104:PRO:C	2.62	0.43
1:D:266:PHE:CZ	1:D:446:LEU:HD12	2.54	0.43
1:B:128:THR:HG23	1:B:381:ILE:HD13	2.01	0.42
1:B:501:THR:O	1:B:503:ILE:HD12	2.19	0.42
1:C:224:MET:CE	1:C:306:ILE:HG22	2.49	0.42
1:D:52:PRO:O	1:D:53:TRP:C	2.61	0.42
1:D:121:ARG:NH1	1:D:445:GLY:O	2.52	0.42
1:D:414:ALA:HB3	1:D:415:PRO:HD3	2.00	0.42
1:A:327:THR:CA	1:A:329:LEU:HD13	2.50	0.42
1:B:63:ALA:HB1	1:B:270:ILE:CD1	2.47	0.42
1:B:89:TRP:NE1	1:B:298:PRO:HG2	2.34	0.42
1:B:288:VAL:HG23	1:B:524:PHE:CE1	2.53	0.42
1:C:52:PRO:O	1:C:53:TRP:C	2.62	0.42
1:C:267:ASN:O	1:C:269:TYR:N	2.52	0.42
1:D:111:ILE:HG21	1:D:117:PHE:HB2	2.01	0.42
1:D:170:ALA:HB2	1:D:411:CYS:SG	2.59	0.42
1:D:196:LEU:HD21	1:D:357:ALA:C	2.44	0.42
1:B:435:SER:N	1:B:436:PRO:CD	2.81	0.42
1:B:493:VAL:HG12	1:B:494:ILE:N	2.34	0.42
1:C:65:ILE:HA	1:C:69:GLN:HG3	2.01	0.42
1:C:271:ILE:O	1:C:275:LEU:N	2.50	0.42
1:C:444:LEU:HD12	1:C:494:ILE:HD11	2.02	0.42
1:D:475:LEU:O	1:D:475:LEU:CD2	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:HG23	1:A:524:PHE:CE1	2.54	0.42
1:B:135:ILE:HA	1:B:373:THR:HG23	2.00	0.42
1:B:141:VAL:CG2	1:B:142:ASN:N	2.80	0.42
1:C:295:LEU:CD2	1:C:535:LEU:HD21	2.49	0.42
1:D:157:ILE:HG23	1:D:158:LEU:HG	2.02	0.42
1:A:423:ALA:O	1:A:426:TYR:HB3	2.19	0.42
1:C:76:SER:HB3	1:C:84:ILE:HD13	2.02	0.42
1:D:73:MET:HE1	1:D:88:GLU:HG2	2.01	0.42
1:D:423:ALA:O	1:D:426:TYR:HB3	2.19	0.42
1:B:247:PRO:HG3	1:B:478:PRO:HB3	2.00	0.42
1:C:346:LEU:HG	1:C:347:PRO:CD	2.49	0.42
1:C:378:THR:HB	1:C:379:MET:HE2	2.00	0.42
1:D:224:MET:CE	1:D:306:ILE:HG22	2.49	0.42
1:D:367:ALA:HA	1:D:370:LEU:HD12	2.01	0.42
1:D:379:MET:HE1	1:D:395:LEU:CG	2.49	0.42
1:C:99:GLY:HA2	1:C:287:ILE:HD13	2.01	0.42
1:C:247:PRO:HG3	1:C:478:PRO:HB3	2.00	0.42
1:C:292:PHE:CD2	1:C:292:PHE:C	2.98	0.42
1:C:414:ALA:HB3	1:C:415:PRO:HD3	2.01	0.42
1:D:105:ILE:CD1	1:D:446:LEU:HD22	2.47	0.42
1:A:256:LEU:O	1:A:259:ALA:HB3	2.19	0.42
1:A:111:ILE:HG21	1:A:117:PHE:HB2	2.01	0.42
1:B:266:PHE:O	1:B:267:ASN:C	2.63	0.42
1:D:76:SER:HB3	1:D:84:ILE:HD13	2.02	0.42
1:A:297:VAL:HB	1:A:298:PRO:HD3	2.01	0.42
1:A:346:LEU:HG	1:A:347:PRO:CD	2.50	0.42
1:C:288:VAL:HG11	1:C:527:ALA:CB	2.50	0.42
1:C:439:LEU:HG	1:C:443:LEU:HD21	2.02	0.42
1:D:103:LEU:HD13	1:D:272:GLN:HE22	1.83	0.42
1:D:288:VAL:HG23	1:D:524:PHE:CE1	2.55	0.42
1:A:63:ALA:HB1	1:A:270:ILE:CD1	2.47	0.41
1:A:295:LEU:CD2	1:A:535:LEU:HD21	2.50	0.41
1:B:157:ILE:HG23	1:B:158:LEU:HG	2.01	0.41
1:A:94:THR:CG2	1:A:95:LEU:N	2.83	0.41
1:A:292:PHE:CD2	1:A:292:PHE:C	2.98	0.41
1:B:327:THR:CA	1:B:329:LEU:HD13	2.51	0.41
1:B:414:ALA:HB3	1:B:415:PRO:HD3	2.01	0.41
1:D:128:THR:HG23	1:D:381:ILE:HD13	2.01	0.41
1:A:103:LEU:CG	1:A:275:LEU:HD13	2.50	0.41
1:C:501:THR:O	1:C:503:ILE:HD12	2.20	0.41
1:D:249:ILE:HD12	1:D:253:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PHE:HB3	1:B:357:ALA:HB1	2.03	0.41
1:C:297:VAL:HB	1:C:298:PRO:HD3	2.01	0.41
1:D:63:ALA:HB1	1:D:270:ILE:CD1	2.47	0.41
1:D:346:LEU:HG	1:D:347:PRO:CD	2.50	0.41
1:C:301:VAL:HG23	1:C:302:VAL:N	2.35	0.41
1:D:195:PHE:HB3	1:D:357:ALA:HB1	2.01	0.41
1:D:256:LEU:O	1:D:259:ALA:HB3	2.20	0.41
1:C:327:THR:CA	1:C:329:LEU:HD13	2.50	0.41
1:D:158:LEU:HB2	1:D:160:ILE:HD12	2.03	0.41
1:D:495:ALA:O	1:D:499:LEU:HB2	2.20	0.41
1:B:218:PHE:O	1:B:221:VAL:HB	2.20	0.41
1:B:346:LEU:HG	1:B:347:PRO:CD	2.50	0.41
1:C:141:VAL:CG2	1:C:142:ASN:N	2.80	0.41
1:C:266:PHE:O	1:C:267:ASN:C	2.63	0.41
1:B:267:ASN:O	1:B:269:TYR:N	2.54	0.41
1:A:288:VAL:HG11	1:A:527:ALA:CB	2.51	0.41
1:A:488:LEU:HD23	1:A:488:LEU:HA	1.96	0.41
1:B:271:ILE:O	1:B:275:LEU:N	2.51	0.41
1:B:382:TYR:HA	1:B:386:ILE:HD12	2.03	0.41
1:D:135:ILE:HA	1:D:373:THR:HG23	2.02	0.41
1:D:292:PHE:CD2	1:D:292:PHE:C	2.98	0.41
1:A:524:PHE:CD2	1:A:524:PHE:C	2.98	0.41
1:B:76:SER:HB3	1:B:84:ILE:HD13	2.01	0.41
1:C:275:LEU:C	1:C:277:ALA:H	2.28	0.41
1:D:247:PRO:HG3	1:D:478:PRO:HB3	2.02	0.41
1:B:158:LEU:HB2	1:B:160:ILE:HD12	2.04	0.40
1:C:505:ASP:CG	1:D:513:VAL:HG12	2.45	0.40
1:C:524:PHE:CD2	1:C:524:PHE:C	2.99	0.40
1:D:262:TYR:HA	1:D:439:LEU:HD13	2.03	0.40
1:D:297:VAL:HB	1:D:298:PRO:HD3	2.03	0.40
1:D:524:PHE:CD2	1:D:524:PHE:C	2.99	0.40
1:A:196:LEU:HD21	1:A:357:ALA:C	2.46	0.40
1:C:128:THR:HG23	1:C:381:ILE:HD13	2.02	0.40
1:D:278:LYS:CG	1:D:279:SER:N	2.83	0.40
1:A:157:ILE:HG23	1:A:158:LEU:HG	2.04	0.40
1:A:301:VAL:HG23	1:A:302:VAL:H	1.86	0.40
1:A:501:THR:O	1:A:503:ILE:HD12	2.22	0.40
1:B:105:ILE:CD1	1:B:446:LEU:HD22	2.49	0.40
1:B:379:MET:HE2	1:B:379:MET:N	2.36	0.40
1:B:475:LEU:O	1:B:475:LEU:CD2	2.55	0.40
1:C:379:MET:HE2	1:C:379:MET:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:PRO:HA	1:D:302:VAL:HG13	2.03	0.40
1:D:525:ASN:HD22	1:D:525:ASN:HA	1.68	0.40
1:B:163:MET:SD	1:B:166:ILE:HD11	2.62	0.40
1:B:196:LEU:HD21	1:B:357:ALA:C	2.46	0.40
1:C:378:THR:O	1:C:382:TYR:HB3	2.22	0.40
1:C:423:ALA:O	1:C:426:TYR:HB3	2.22	0.40
1:A:218:PHE:O	1:A:221:VAL:HB	2.21	0.40
1:A:327:THR:C	1:A:329:LEU:N	2.78	0.40
1:A:479:PHE:HA	1:A:482:GLN:HB2	2.02	0.40
1:C:218:PHE:O	1:C:221:VAL:HB	2.22	0.40
1:C:288:VAL:HG23	1:C:524:PHE:CE1	2.56	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	491/530 (93%)	424 (86%)	53 (11%)	14 (3%)	3	9
1	B	491/530 (93%)	417 (85%)	59 (12%)	15 (3%)	3	8
1	C	491/530 (93%)	418 (85%)	59 (12%)	14 (3%)	3	9
1	D	491/530 (93%)	421 (86%)	54 (11%)	16 (3%)	3	7
All	All	1964/2120 (93%)	1680 (86%)	225 (12%)	59 (3%)	3	8

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	TRP
1	A	110	GLY
1	A	268	GLN
1	A	348	VAL

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Mol	Chain	Res	Type
1	A	513	VAL
1	A	519	VAL
1	B	53	TRP
1	B	110	GLY
1	B	268	GLN
1	B	348	VAL
1	B	513	VAL
1	B	519	VAL
1	C	53	TRP
1	C	110	GLY
1	C	268	GLN
1	C	348	VAL
1	C	513	VAL
1	C	519	VAL
1	D	53	TRP
1	D	110	GLY
1	D	268	GLN
1	D	348	VAL
1	D	513	VAL
1	D	519	VAL
1	A	279	SER
1	A	475	LEU
1	A	523	SER
1	B	279	SER
1	B	475	LEU
1	B	505	ASP
1	B	523	SER
1	C	279	SER
1	C	475	LEU
1	C	505	ASP
1	C	523	SER
1	D	279	SER
1	D	475	LEU
1	D	523	SER
1	A	267	ASN
1	A	505	ASP
1	B	267	ASN
1	C	267	ASN
1	D	267	ASN
1	D	505	ASP
1	A	333	ALA
1	A	364	SER

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Mol	Chain	Res	Type
1	B	333	ALA
1	B	338	ALA
1	C	333	ALA
1	C	338	ALA
1	C	364	SER
1	D	333	ALA
1	D	364	SER
1	A	338	ALA
1	B	364	SER
1	D	327	THR
1	D	338	ALA
1	B	276	ALA
1	D	493	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	396/413 (96%)	348 (88%)	48 (12%)	5	12
1	B	396/413 (96%)	348 (88%)	48 (12%)	5	12
1	C	396/413 (96%)	348 (88%)	48 (12%)	5	12
1	D	396/413 (96%)	349 (88%)	47 (12%)	5	13
All	All	1584/1652 (96%)	1393 (88%)	191 (12%)	5	12

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	TRP
1	A	60	LEU
1	A	64	ASN
1	A	70	PHE
1	A	76	SER
1	A	84	ILE
1	A	94	THR
1	A	98	VAL

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Mol	Chain	Res	Type
1	A	137	LEU
1	A	141	VAL
1	A	155	GLU
1	A	186	VAL
1	A	193	VAL
1	A	195	PHE
1	A	204	THR
1	A	233	GLU
1	A	235	ILE
1	A	261	LEU
1	A	270	ILE
1	A	271	ILE
1	A	275	LEU
1	A	287	ILE
1	A	302	VAL
1	A	313	SER
1	A	327	THR
1	A	329	LEU
1	A	346	LEU
1	A	364	SER
1	A	378	THR
1	A	380	ASP
1	A	413	ILE
1	A	417	LEU
1	A	431	THR
1	A	438	ILE
1	A	441	VAL
1	A	443	LEU
1	A	449	LYS
1	A	450	LYS
1	A	471	LYS
1	A	475	LEU
1	A	481	ASP
1	A	487	LEU
1	A	492	VAL
1	A	500	SER
1	A	511	ILE
1	A	517	MET
1	A	525	ASN
1	A	538	LEU
1	B	53	TRP
1	B	60	LEU

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Mol	Chain	Res	Type
1	B	64	ASN
1	B	70	PHE
1	B	76	SER
1	B	84	ILE
1	B	94	THR
1	B	98	VAL
1	B	137	LEU
1	B	141	VAL
1	B	186	VAL
1	B	193	VAL
1	B	195	PHE
1	B	204	THR
1	B	233	GLU
1	B	235	ILE
1	B	261	LEU
1	B	270	ILE
1	B	271	ILE
1	B	275	LEU
1	B	287	ILE
1	B	302	VAL
1	B	313	SER
1	B	327	THR
1	B	329	LEU
1	B	346	LEU
1	B	364	SER
1	B	378	THR
1	B	413	ILE
1	B	417	LEU
1	B	425	GLN
1	B	431	THR
1	B	438	ILE
1	B	441	VAL
1	B	443	LEU
1	B	449	LYS
1	B	450	LYS
1	B	471	LYS
1	B	475	LEU
1	B	481	ASP
1	B	487	LEU
1	B	492	VAL
1	B	494	ILE
1	B	500	SER

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Mol	Chain	Res	Type
1	B	511	ILE
1	B	517	MET
1	B	525	ASN
1	B	538	LEU
1	C	53	TRP
1	C	60	LEU
1	C	64	ASN
1	C	70	PHE
1	C	76	SER
1	C	84	ILE
1	C	94	THR
1	C	98	VAL
1	C	137	LEU
1	C	141	VAL
1	C	186	VAL
1	C	193	VAL
1	C	195	PHE
1	C	204	THR
1	C	233	GLU
1	C	235	ILE
1	C	261	LEU
1	C	270	ILE
1	C	271	ILE
1	C	275	LEU
1	C	287	ILE
1	C	302	VAL
1	C	313	SER
1	C	327	THR
1	C	329	LEU
1	C	346	LEU
1	C	364	SER
1	C	378	THR
1	C	380	ASP
1	C	413	ILE
1	C	417	LEU
1	C	425	GLN
1	C	431	THR
1	C	438	ILE
1	C	441	VAL
1	C	443	LEU
1	C	449	LYS
1	C	450	LYS

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Mol	Chain	Res	Type
1	C	471	LYS
1	C	475	LEU
1	C	481	ASP
1	C	487	LEU
1	C	492	VAL
1	C	500	SER
1	C	511	ILE
1	C	517	MET
1	C	525	ASN
1	C	538	LEU
1	D	53	TRP
1	D	60	LEU
1	D	64	ASN
1	D	70	PHE
1	D	76	SER
1	D	84	ILE
1	D	94	THR
1	D	98	VAL
1	D	137	LEU
1	D	141	VAL
1	D	186	VAL
1	D	193	VAL
1	D	195	PHE
1	D	204	THR
1	D	233	GLU
1	D	235	ILE
1	D	261	LEU
1	D	270	ILE
1	D	271	ILE
1	D	275	LEU
1	D	287	ILE
1	D	302	VAL
1	D	313	SER
1	D	327	THR
1	D	329	LEU
1	D	346	LEU
1	D	378	THR
1	D	380	ASP
1	D	413	ILE
1	D	417	LEU
1	D	431	THR
1	D	438	ILE

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Mol	Chain	Res	Type
1	D	441	VAL
1	D	443	LEU
1	D	449	LYS
1	D	450	LYS
1	D	471	LYS
1	D	475	LEU
1	D	481	ASP
1	D	487	LEU
1	D	492	VAL
1	D	494	ILE
1	D	500	SER
1	D	511	ILE
1	D	517	MET
1	D	525	ASN
1	D	538	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	142	ASN
1	A	245	ASN
1	A	260	ASN
1	A	272	GLN
1	A	397	ASN
1	A	425	GLN
1	A	525	ASN
1	B	64	ASN
1	B	142	ASN
1	B	245	ASN
1	B	260	ASN
1	B	272	GLN
1	B	334	ASN
1	B	397	ASN
1	B	425	GLN
1	B	525	ASN
1	C	142	ASN
1	C	245	ASN
1	C	260	ASN
1	C	272	GLN
1	C	397	ASN
1	C	425	GLN

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Mol	Chain	Res	Type
1	C	525	ASN
1	D	64	ASN
1	D	142	ASN
1	D	245	ASN
1	D	260	ASN
1	D	272	GLN
1	D	334	ASN
1	D	397	ASN
1	D	425	GLN
1	D	525	ASN

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z > 2$
2	GAL	B	701	-	12,12,12	0.54	0	17,17,17	0.57	0
2	GAL	D	701	-	12,12,12	0.54	0	17,17,17	0.61	0
2	GAL	C	701	-	12,12,12	0.54	0	17,17,17	0.63	0
2	GAL	A	701	-	12,12,12	0.54	0	17,17,17	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	B	701	-	-	0/2/22/22	0/1/1/1
2	GAL	D	701	-	-	0/2/22/22	0/1/1/1
2	GAL	C	701	-	-	0/2/22/22	0/1/1/1
2	GAL	A	701	-	-	0/2/22/22	0/1/1/1

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](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	19:UNK	C	47:ALA	N	17.80
1	C	19:UNK	C	47:ALA	N	17.80
1	A	19:UNK	C	47:ALA	N	17.79
1	D	19:UNK	C	47:ALA	N	17.78

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	495/530 (93%)	0.48	30 (6%) 27 24	10, 47, 74, 91	0
1	B	495/530 (93%)	0.69	59 (11%) 9 7	10, 47, 74, 92	0
1	C	495/530 (93%)	0.61	45 (9%) 15 12	10, 47, 75, 92	0
1	D	495/530 (93%)	0.41	30 (6%) 27 24	10, 47, 74, 92	0
All	All	1980/2120 (93%)	0.55	164 (8%) 17 14	10, 47, 75, 92	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	513	VAL	9.5
1	B	274	THR	8.5
1	C	209	SER	7.4
1	C	238	GLN	7.0
1	C	187	TRP	6.6
1	C	395	LEU	6.6
1	B	175	VAL	6.5
1	A	513	VAL	6.3
1	A	321	LEU	6.1
1	A	508	PRO	6.0
1	B	511	ILE	5.9
1	A	503	ILE	5.7
1	C	68	GLU	5.6
1	D	108	GLU	5.3
1	C	394	LYS	5.1
1	B	403	ALA	5.0
1	D	399	GLY	5.0
1	B	49	LYS	5.0
1	C	213	GLY	5.0
1	C	70	PHE	4.9
1	C	210	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	267	ASN	4.8
1	B	343	THR	4.7
1	C	207	ALA	4.7
1	C	268	GLN	4.7
1	A	47	ALA	4.6
1	D	403	ALA	4.6
1	C	208	VAL	4.6
1	A	217	TRP	4.6
1	B	58	ALA	4.6
1	D	388	PRO	4.5
1	C	212	GLY	4.4
1	C	511	ILE	4.4
1	B	186	VAL	4.3
1	B	394	LYS	4.3
1	A	277	ALA	4.3
1	D	187	TRP	4.0
1	D	178	ILE	3.9
1	C	380	ASP	3.9
1	B	392	ASP	3.8
1	B	460	VAL	3.8
1	C	513	VAL	3.8
1	A	420	ILE	3.7
1	B	395	LEU	3.7
1	B	48	GLY	3.6
1	A	214	THR	3.6
1	B	50	SER	3.6
1	D	514	THR	3.6
1	B	398	VAL	3.6
1	C	418	GLY	3.5
1	B	62	ALA	3.5
1	B	107	ILE	3.4
1	C	325	ALA	3.3
1	B	275	LEU	3.2
1	B	54	TRP	3.1
1	C	467	ALA	3.1
1	C	417	LEU	3.1
1	A	48	GLY	3.1
1	D	244	MET	3.1
1	B	230	GLY	3.0
1	B	401	THR	3.0
1	C	267	ASN	3.0
1	B	162	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	278	LYS	2.9
1	B	210	PHE	2.9
1	C	357	ALA	2.9
1	B	342	LEU	2.9
1	C	387	SER	2.9
1	B	270	ILE	2.9
1	D	402	ALA	2.9
1	C	193	VAL	2.9
1	C	512	SER	2.9
1	D	393	HIS	2.9
1	B	476	SER	2.8
1	A	525	ASN	2.8
1	B	189	ASP	2.8
1	C	340	PRO	2.8
1	B	114	ILE	2.8
1	B	393	HIS	2.8
1	B	118	VAL	2.8
1	B	518	PHE	2.8
1	D	51	LEU	2.7
1	D	267	ASN	2.7
1	B	407	LEU	2.7
1	B	373	THR	2.7
1	D	515	SER	2.7
1	B	513	VAL	2.7
1	C	214	THR	2.7
1	B	64	ASN	2.6
1	B	390	SER	2.6
1	B	325	ALA	2.6
1	A	177	SER	2.6
1	B	477	MET	2.6
1	D	249	ILE	2.6
1	B	391	GLY	2.6
1	C	217	TRP	2.5
1	D	511	ILE	2.5
1	A	185	VAL	2.5
1	D	215	ASP	2.5
1	C	50	SER	2.5
1	B	429	GLU	2.5
1	A	49	LYS	2.4
1	B	512	SER	2.4
1	D	476	SER	2.4
1	A	104	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	369	MET	2.4
1	C	379	MET	2.4
1	C	343	THR	2.3
1	D	214	THR	2.3
1	C	339	TYR	2.3
1	A	50	SER	2.3
1	A	507	ASP	2.3
1	B	187	TRP	2.3
1	C	186	VAL	2.3
1	A	158	LEU	2.3
1	B	276	ALA	2.3
1	D	104	PRO	2.3
1	D	275	LEU	2.3
1	C	403	ALA	2.3
1	A	187	TRP	2.3
1	B	70	PHE	2.3
1	B	531	ILE	2.2
1	D	270	ILE	2.2
1	C	49	LYS	2.2
1	A	388	PRO	2.2
1	D	348	VAL	2.2
1	D	49	LYS	2.2
1	D	119	GLU	2.2
1	C	516	SER	2.2
1	B	178	ILE	2.2
1	B	289	PHE	2.2
1	B	516	SER	2.2
1	A	350	VAL	2.2
1	B	480	MET	2.2
1	B	249	ILE	2.2
1	B	176	TYR	2.2
1	C	415	PRO	2.2
1	A	433	LEU	2.2
1	A	330	PRO	2.1
1	C	211	ILE	2.1
1	C	201	PHE	2.1
1	B	47	ALA	2.1
1	B	397	ASN	2.1
1	C	397	ASN	2.1
1	A	159	GLY	2.1
1	A	526	ILE	2.1
1	D	105	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	345	PHE	2.1
1	D	272	GLN	2.1
1	B	65	ILE	2.1
1	D	347	PRO	2.1
1	B	485	TYR	2.1
1	D	291	ALA	2.0
1	B	267	ASN	2.0
1	B	216	GLY	2.0
1	A	176	TYR	2.0
1	C	292	PHE	2.0
1	C	377	PHE	2.0
1	B	307	ALA	2.0
1	B	337	LYS	2.0
1	C	333	ALA	2.0
1	C	450	LYS	2.0
1	C	246	LEU	2.0
1	A	393	HIS	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
4	NA	C	801	1/1	0.59	0.13	43,43,43,43	0
4	NA	D	801	1/1	0.68	0.07	42,42,42,42	0
4	NA	B	801	1/1	0.69	0.08	41,41,41,41	0
4	NA	A	801	1/1	0.85	0.05	42,42,42,42	0
2	GAL	D	701	12/12	0.88	0.16	24,25,26,27	0
2	GAL	A	701	12/12	0.89	0.09	24,25,26,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	B	701	12/12	0.90	0.10	24,25,27,27	0
2	GAL	C	701	12/12	0.91	0.09	24,25,26,27	0
3	ER3	A	702	1/1	0.94	0.05	54,54,54,54	0
3	ER3	D	703	1/1	0.96	0.07	53,53,53,53	0
3	ER3	A	704	1/1	0.98	0.10	93,93,93,93	0
3	ER3	D	705	1/1	0.98	0.15	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.