



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 10:57 AM BST

PDB ID : 3DH4
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

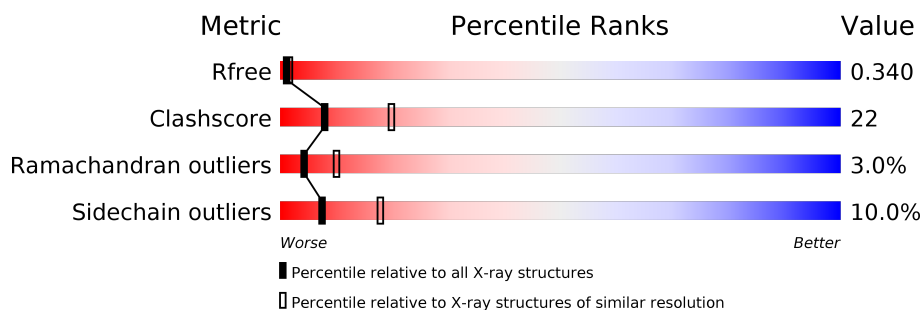
1 Overall quality at a glance

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 on 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	530	
1	B	530	
1	C	530	
1	D	530	

2 Entry composition

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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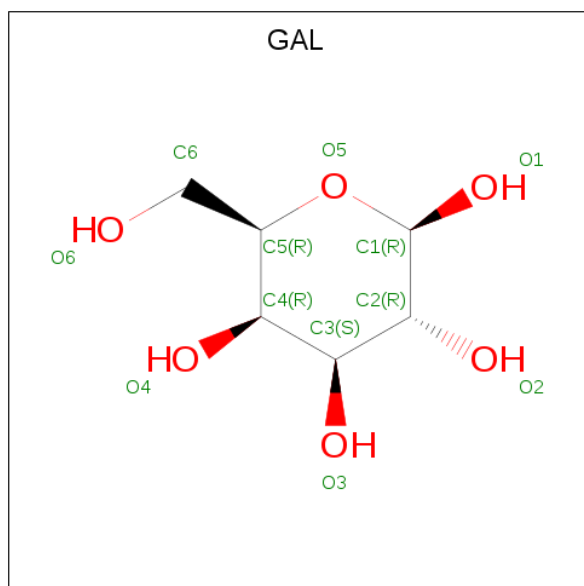
Chain	Residue	Modelled	Actual	Comment	Reference
B	549	GLY	-	expression tag	UNP P96169
B	550	GLY	-	expression tag	UNP P96169
B	551	SER	-	expression tag	UNP P96169
B	552	PRO	-	expression tag	UNP P96169
B	553	GLY	-	expression tag	UNP P96169
B	554	HIS	-	expression tag	UNP P96169
B	555	HIS	-	expression tag	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 (three-letter code: GAL) (formula: C₆H₁₂O₆).



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 (three-letter code: 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		

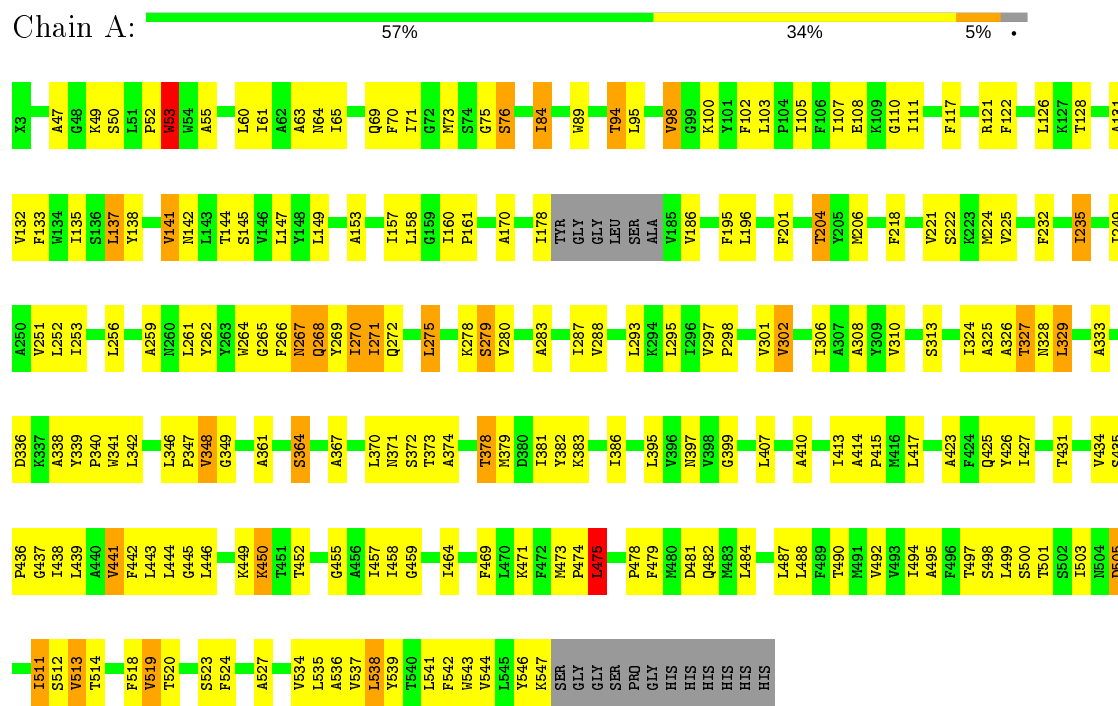
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

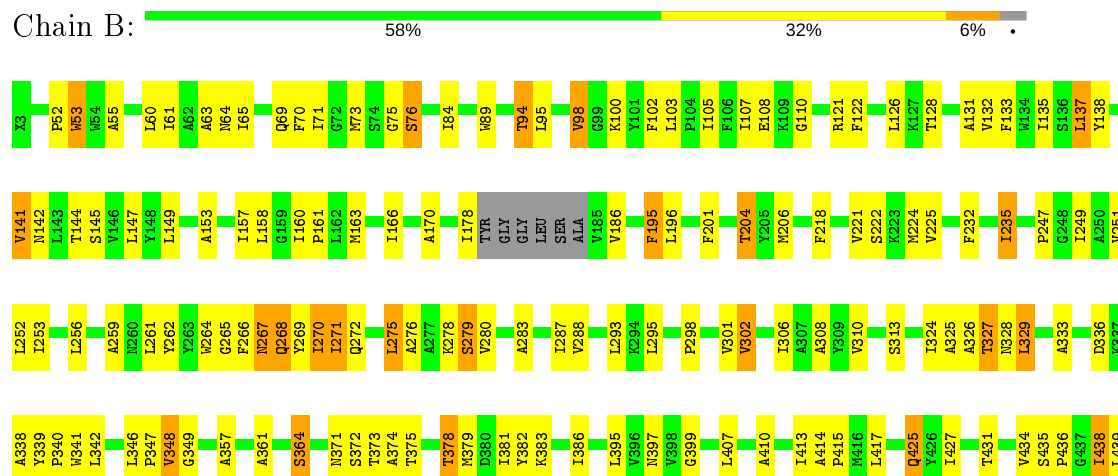
3 Residue-property plots

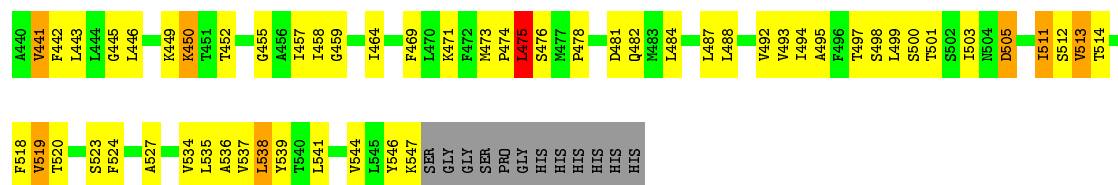
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Sodium/glucose cotransporter



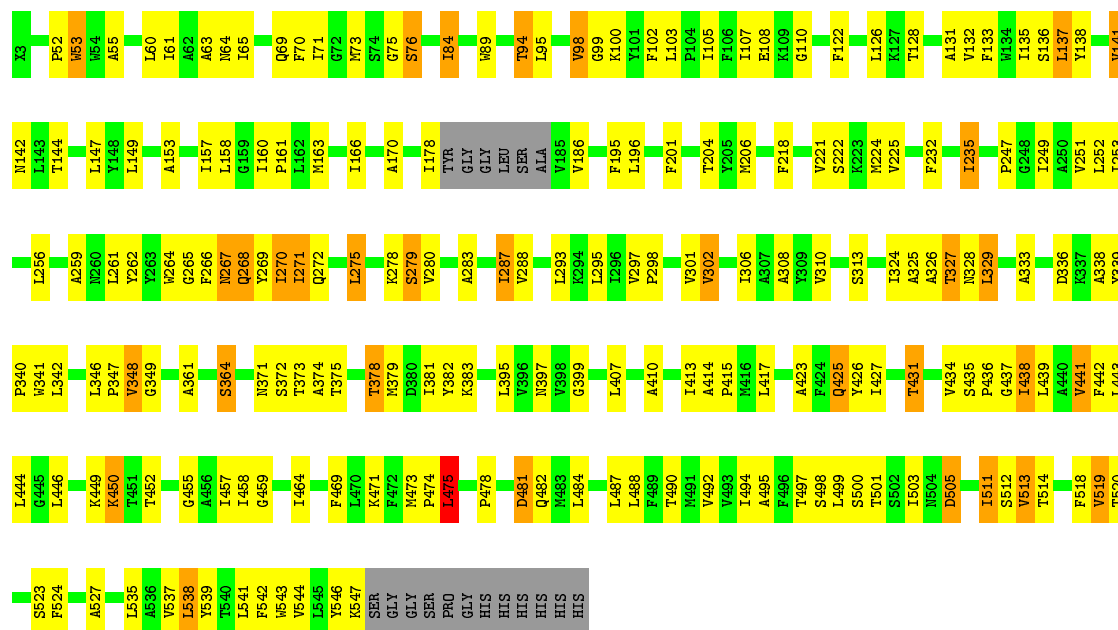
- Molecule 1: Sodium/glucose cotransporter





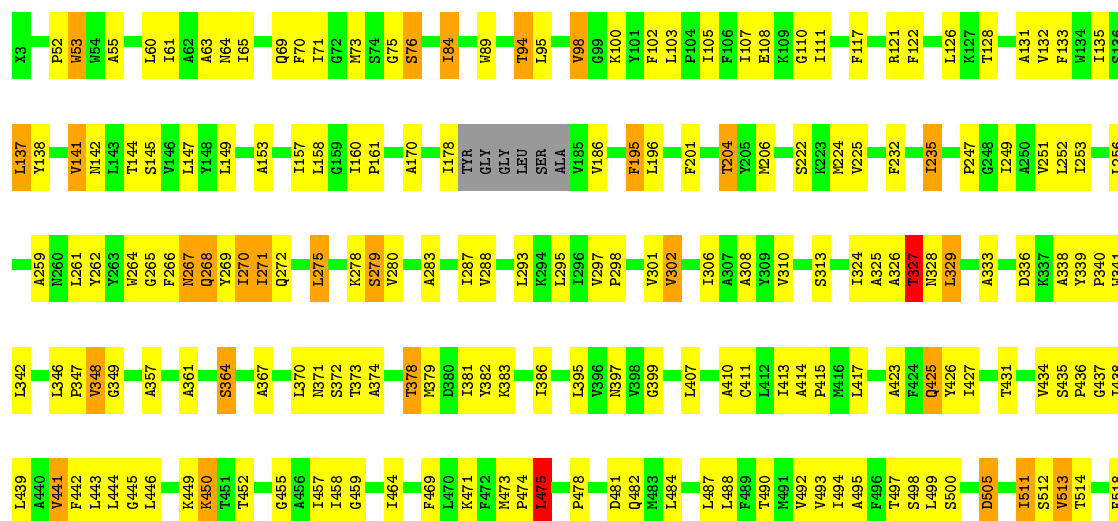
- Molecule 1: Sodium/glucose cotransporter

Chain C: 58% 32% 6% .



- Molecule 1: Sodium/glucose cotransporter

Chain D: 58% 33% 5% .



V519	T520	S523	F524	N525	V534	L535	A536	V537	L538	Y539	T540	L541	F542	W543	V544	L545	Y546	K547	SER	GLY	GLY	SER	SER	PRO	GLY	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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 29.50 – 2.70	Depositor EDS
% Data completeness (in resolution range)	53.3 (30.00-2.70) 91.3 (29.50-2.70)	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 (5.02%)	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)	0.17 , 32.5	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: NA, GAL, ER3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/3867	0.57	0/5279
1	B	0.48	0/3867	0.57	0/5279
1	C	0.48	1/3867 (0.0%)	0.57	0/5279
1	D	0.47	0/3867	0.57	0/5279
All	All	0.48	1/15468 (0.0%)	0.57	0/21116

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	481	ASP	CB-CG	5.38	1.63	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	B	122	PHE	Peptide
1	C	122	PHE	Peptide
1	D	122	PHE	Peptide

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	3854	0	3887	180	0
1	B	3854	0	3887	164	0
1	C	3854	0	3887	164	0
1	D	3854	0	3887	188	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	668	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 22.

All (668) 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:O	1:D:475:LEU:HD23	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:D:271:ILE:HG22	1:D:272:GLN:N	2.04	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: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: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: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: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: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
1:D:271:ILE:CG2	1:D:272:GLN:N	2.58	0.67
1:C:224:MET:HB2	1:C:310:VAL:HG21	1.77	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:511:ILE:C	1:A:511:ILE:HD13	2.14	0.66
1:A:63:ALA:CB	1:A:270:ILE:HG21	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:511:ILE:HD13	1:D:511:ILE:C	2.16	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:C:511:ILE:HD13	1:C:511:ILE:C	2.16	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: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:B:511:ILE:HD13	1:B:511:ILE:C	2.18	0.64
1:C:141:VAL:HG22	1:C:142:ASN:N	2.13	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
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:B:144:THR:HG23	1:B:414:ALA:HA	1.81	0.62
1:B:63:ALA:HB1	1:B:270:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:538:LEU:HD12	1:A:538:LEU:C	2.20	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:308:ALA:HB2	1:C:342:LEU:HD11	1.81	0.60
1:C:95:LEU:HA	1:C:98:VAL:HG13	1.83	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: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:100:LYS:NZ	1:C:520:THR:HG22	2.17	0.60
1:C:98:VAL:HB	1:C:265:GLY:HA2	1.83	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:D:538:LEU:C	1:D:538:LEU:HD12	2.22	0.60
1:A:458:ILE:HD12	1:A:497:THR:HG21	1.84	0.59
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: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:484:LEU:HD23	1:B:484:LEU:C	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:484:LEU:C	1:C:484:LEU:HD23	2.23	0.58
1:D:107:ILE:HD12	1:D:108:GLU:N	2.19	0.58
1:D:95:LEU:HA	1:D:98:VAL:HG13	1.84	0.58
1:C:107:ILE:HD12	1:C:108:GLU:N	2.19	0.58
1:D:249:ILE:HD12	1:D:253:ILE:HD11	1.86	0.58
1:D:206:MET:CE	1:D:346:LEU:HD12	2.33	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:249:ILE:HD12	1:A:253:ILE:HD11	1.84	0.57
1:A:50:SER:N	1:D:513:VAL:HG22	2.18	0.57
1:C:327:THR:O	1:C:329:LEU:HD13	2.05	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
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: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: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:D:324:ILE:O	1:D:324:ILE:HG22	2.06	0.56
1:B:71:ILE:HG22	1:B:149:LEU:HD22	1.88	0.56
1:B:538:LEU:HD12	1:B:538:LEU:C	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:SER:N	1:D:513:VAL:HG21	2.21	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: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: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:B:206:MET:CE	1:B:346:LEU:HD12	2.37	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: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:HA	1:C:425:GLN:HE21	1.73	0.54
1:D:478:PRO:O	1:D:482:GLN:HB2	2.07	0.54
1:A:100:LYS:HZ3	1:A:520:THR:HG22	1.72	0.54
1:B:417:LEU:HD23	1:B:417:LEU:N	2.22	0.54
1:D:329:LEU:HD12	1:D:341:TRP:NE1	2.23	0.54
1:D:262:TYR:HB2	1:D:439:LEU:HD22	1.89	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:N	1:A:417:LEU:HD23	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:474:PRO:O	1:B:475:LEU:C	2.45	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:HG22	1:C:324:ILE:O	2.08	0.53
1:D:133:PHE:HB3	1:D:434:VAL:HG21	1.90	0.53
1:D:98:VAL:HA	1:D:102:PHE:CD1	2.43	0.53
1:A:324:ILE:HG22	1:A:324:ILE:O	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:538:LEU:C	1:C:538:LEU:HD12	2.28	0.53
1:A:327:THR:C	1:A:329:LEU:HD13	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:469:PHE:O	1:C:473:MET:HB2	2.08	0.52
1:D:71:ILE:HG22	1:D:149:LEU:HD22	1.91	0.52
1:D:235:ILE:HD12	1:D:235:ILE:H	1.74	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:458:ILE:HD12	1:A:497:THR:CG2	2.40	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:C:371:ASN:OD1	1:C:372:SER:N	2.43	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:D:484:LEU:HD23	1:D:484:LEU:C	2.30	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:N	1:C:417:LEU:HD23	2.24	0.52
1:C:295:LEU:HD22	1:C:535:LEU:HD21	1.92	0.51
1:C:71:ILE:HG22	1:C:149:LEU:HD22	1.91	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:C:327:THR:C	1:C:329:LEU:HD13	2.30	0.51
1:D:196:LEU:HD11	1:D:361:ALA:CB	2.40	0.51
1:D:100:LYS:HZ3	1:D:520:THR:HG22	1.76	0.51
1:A:484:LEU:HD23	1:A:484:LEU:C	2.31	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:D:301:VAL:HG23	1:D:302:VAL:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:LEU:HD22	1:D:535:LEU:HD21	1.92	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
1:B:275:LEU:HD23	1:B:283:ALA:CB	2.34	0.51
1:B:196:LEU:HD11	1:B:361:ALA:CB	2.41	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:196:LEU:HD11	1:D:361:ALA:HB2	1.93	0.50
1:D:69:GLN:O	1:D:73:MET:HB3	2.11	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: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:A:474:PRO:O	1:A:475:LEU:C	2.50	0.50
1:B:288:VAL:CG2	1:B:524:PHE:CD1	2.95	0.50
1:B:425:GLN:HA	1:B:425:GLN:HE21	1.77	0.50
1:B:327:THR:C	1:B:329:LEU:HD13	2.32	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:A:288:VAL:CG2	1:A:524:PHE:CD1	2.95	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:327:THR:C	1:D:329:LEU:HD13	2.32	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: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:D:474:PRO:O	1:D:475:LEU:C	2.49	0.49
1:B:395:LEU:HD23	1:B:395:LEU:C	2.33	0.49
1:D:224:MET:HE3	1:D:306:ILE:HG22	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:LEU:O	1:B:544:VAL:HG12	2.12	0.49
1:B:407:LEU:HD23	1:B:407:LEU:C	2.33	0.49
1:B:266:PHE:CZ	1:B:446:LEU:HD12	2.48	0.49
1:C:512:SER:O	1:C:514:THR:N	2.46	0.49
1:C:69:GLN:O	1:C:73:MET:HB3	2.13	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:C:61:ILE:HG13	1:C:293:LEU:HD12	1.94	0.49
1:D:178:ILE:HD12	1:D:178:ILE:N	2.28	0.49
1:D:100:LYS:HZ2	1:D:520:THR:HG22	1.77	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: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: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:D:61:ILE:HG13	1:D:293:LEU:HD12	1.95	0.48
1:B:178:ILE:HD12	1:B:178:ILE:N	2.28	0.48
1:B:61:ILE:HG13	1:B:293:LEU:HD12	1.95	0.48
1:C:348:VAL:HG23	1:C:349:GLY:H	1.78	0.48
1:C:100:LYS:HZ2	1:C:520:THR:HG22	1.77	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: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:474:PRO:O	1:C:475:LEU:C	2.51	0.48
1:C:178:ILE:HD12	1:C:178:ILE:N	2.28	0.48
1:C:107:ILE:CD1	1:C:280:VAL:HG21	2.35	0.48
1:C:339:TYR:N	1:C:340:PRO:HD2	2.29	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:49:LYS:HG2	1:D:512:SER:OG	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:VAL:HG13	1:B:538:LEU:N	2.29	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:D:518:PHE:O	1:D:519:VAL:C	2.53	0.48
1:A:267:ASN:O	1:A:269:TYR:N	2.47	0.47
1:D:225:VAL:HG23	1:D:232:PHE:CD1	2.49	0.47
1:A:407:LEU:HD23	1:A:407:LEU:C	2.35	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:C:511:ILE:CD1	1:C:511:ILE:C	2.82	0.47
1:C:450:LYS:NZ	1:C:505:ASP:OD1	2.41	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:C:407:LEU:C	1:C:407:LEU:HD23	2.35	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:288:VAL:CG2	1:D:524:PHE:CD1	2.97	0.47
1:A:379:MET:O	1:A:383:LYS:HB3	2.15	0.47
1:B:201:PHE:HA	1:B:204:THR:HG22	1.95	0.47
1:C:224:MET:HE3	1:C:306:ILE:HG22	1.95	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:128:THR:O	1:A:131:ALA:HB3	2.14	0.47
1:A:75:GLY:HA3	1:A:336:ASP:HA	1.96	0.47
1:C:262:TYR:HB2	1:C:439:LEU:HD22	1.97	0.47
1:A:201:PHE:HA	1:A:204:THR:HG22	1.97	0.47
1:D:137:LEU:O	1:D:141:VAL:HG13	2.15	0.47
1:D:126:LEU:HD12	1:D:457:ILE:HD13	1.97	0.47
1:A:71:ILE:CG2	1:A:149:LEU:HD22	2.44	0.47
1:B:271:ILE:HG23	1:B:275:LEU:HD12	1.96	0.47
1:D:206:MET:HE2	1:D:346:LEU:HD12	1.96	0.47
1:D:511:ILE:C	1:D:511:ILE:CD1	2.83	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:D:201:PHE:HA	1:D:204:THR:HG22	1.96	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:LEU:HD12	1:D:410:ALA:HB1	1.97	0.46
1:A:518:PHE:O	1:A:519:VAL:C	2.53	0.46
1:B:71:ILE:CG2	1:B:149:LEU:HD22	2.44	0.46
1:C:484:LEU:C	1:C:484:LEU:CD2	2.83	0.46
1:B:325:ALA:O	1:B:329:LEU:HD11	2.15	0.46
1:B:75:GLY:HA3	1:B:336:ASP:HA	1.97	0.46
1:C:201:PHE:HA	1:C:204:THR:HG22	1.97	0.46
1:B:256:LEU:O	1:B:259:ALA:HB3	2.14	0.46
1:B:518:PHE:O	1:B:519:VAL:C	2.53	0.46
1:A:50:SER:HB3	1:D:513:VAL:CG2	2.46	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:439:LEU:HG	1:D:443:LEU:CD2	2.45	0.46
1:D:94:THR:HG22	1:D:95:LEU:N	2.31	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:D:407:LEU:HD23	1:D:407:LEU:C	2.35	0.46
1:A:50:SER:CA	1:D:513:VAL:CG2	2.90	0.46
1:B:534:VAL:O	1:B:537:VAL:HG12	2.16	0.46
1:B:71:ILE:HD11	1:B:153:ALA:HB2	1.98	0.46
1:C:435:SER:N	1:C:436:PRO:CD	2.79	0.46
1:B:206:MET:HE2	1:B:346:LEU:HD12	1.97	0.46
1:B:94:THR:HG22	1:B:95:LEU:N	2.31	0.46
1:D:379:MET:O	1:D:383:LYS:HB3	2.15	0.46
1:A:224:MET:HE3	1:A:306:ILE:HG22	1.98	0.46
1:A:61:ILE:HG13	1:A:293:LEU:HD12	1.98	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:B:484:LEU:C	1:B:484:LEU:CD2	2.84	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:A:511:ILE:C	1:A:511:ILE:CD1	2.81	0.45
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: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
1:B:225:VAL:HG23	1:B:232:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:LEU:C	1:C:395:LEU:HD23	2.37	0.45
1:A:235:ILE:H	1:A:235:ILE:HD12	1.82	0.45
1:A:266:PHE:CZ	1:A:442:PHE:HB3	2.51	0.45
1:A:495:ALA:O	1:A:499:LEU:HB2	2.17	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:B:235:ILE:H	1:B:235:ILE:HD12	1.82	0.45
1:B:371:ASN:O	1:B:375:THR:HG23	2.17	0.45
1:D:395:LEU:C	1:D:395:LEU:HD23	2.37	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:C:324:ILE:C	1:C:326:ALA:N	2.70	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:A:324:ILE:C	1:A:326:ALA:N	2.70	0.45
1:D:89:TRP:NE1	1:D:298:PRO:HG2	2.32	0.45
1:D:378:THR:HG21	1:D:399:GLY:HA2	1.97	0.45
1:D:374:ALA:HB1	1:D:399:GLY:O	2.17	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:B:324:ILE:C	1:B:326:ALA:N	2.70	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: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: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:224:MET:CE	1:A:306:ILE:HG22	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:324:ILE:C	1:D:326:ALA:N	2.71	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:145:SER:HB2	1:D:427:ILE:HD11	1.99	0.44
1:D:71:ILE:CG2	1:D:149:LEU:HD22	2.48	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:141:VAL:CG2	1:D:142:ASN:N	2.79	0.43
1:D:435:SER:N	1:D:436:PRO:CD	2.81	0.43
1:B:271:ILE:C	1:B:275:LEU:HD12	2.38	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:382:TYR:HA	1:A:386:ILE:HD12	2.00	0.43
1:A:374:ALA:HB1	1:A:399:GLY:O	2.17	0.43
1:D:450:LYS:NZ	1:D:505:ASP:OD1	2.41	0.43
1:A:395:LEU:C	1:A:395:LEU:HD23	2.38	0.43
1:B:121:ARG:NH1	1:B:445:GLY:O	2.51	0.43
1:C:135:ILE:HA	1:C:373:THR:HG23	2.00	0.43
1:C:63:ALA:HB1	1:C:270:ILE:CD1	2.48	0.43
1:D:65:ILE:HA	1:D:69:GLN:HG3	2.00	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:301:VAL:HG23	1:D:302:VAL:N	2.33	0.43
1:D:295:LEU:CD2	1:D:535:LEU:HD21	2.48	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: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:B:145:SER:HB2	1:B:427:ILE:HD11	2.00	0.43
1:C:103:LEU:HD13	1:C:272:GLN:HE22	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:121:ARG:NH1	1:A:445:GLY:O	2.52	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:C:518:PHE:O	1:C:519:VAL:C	2.55	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:A:271:ILE:C	1:A:275:LEU:HD12	2.39	0.43
1:B:495:ALA:O	1:B:499:LEU:HB2	2.19	0.43
1:C:141:VAL:CG2	1:C:142:ASN:N	2.80	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:126:LEU:HD12	1:A:457:ILE:HD13	2.00	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:414:ALA:HB3	1:D:415:PRO:HD3	2.00	0.42
1:D:121:ARG:NH1	1:D:445:GLY:O	2.52	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: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: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: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:C:65:ILE:HA	1:C:69:GLN:HG3	2.01	0.42
1:D:278:LYS:O	1:D:279:SER:C	2.57	0.42
1:D:475:LEU:O	1:D:475:LEU:CD2	2.57	0.42
1:A:288:VAL:HG23	1:A:524:PHE:CE1	2.54	0.42
1:A:535:LEU:O	1:A:536:ALA:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:535:LEU:O	1:B:536:ALA:C	2.58	0.42
1:C:346:LEU:HG	1:C:347:PRO:CD	2.49	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:C:247:PRO:HG3	1:C:478:PRO:HB3	2.00	0.42
1:C:99:GLY:HA2	1:C:287:ILE:HD13	2.01	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:266:PHE:O	1:A:267:ASN:C	2.58	0.42
1:A:278:LYS:O	1:A:279:SER:C	2.58	0.42
1:C:278:LYS:O	1:C:279:SER:C	2.58	0.42
1:A:111:ILE:HG21	1:A:117:PHE:HB2	2.01	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:439:LEU:HG	1:C:443:LEU:HD21	2.02	0.42
1:C:288:VAL:HG11	1:C:527:ALA:CB	2.50	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:295:LEU:CD2	1:A:535:LEU:HD21	2.50	0.41
1:A:63:ALA:HB1	1:A:270:ILE:CD1	2.47	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: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:C:271:ILE:C	1:C:275:LEU:HD12	2.40	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:A:542:PHE:O	1:A:543:TRP:C	2.58	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
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:346:LEU:HG	1:D:347:PRO:CD	2.50	0.41
1:D:63:ALA:HB1	1:D:270:ILE:CD1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:271:ILE:C	1:D:275:LEU:HD12	2.39	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:266:PHE:O	1:D:267:ASN:C	2.59	0.41
1:D:495:ALA:O	1:D:499:LEU:HB2	2.20	0.41
1:A:52:PRO:O	1:A:53:TRP:C	2.59	0.41
1:B:218:PHE:O	1:B:221:VAL:HB	2.20	0.41
1:B:278:LYS:O	1:B:279:SER:C	2.59	0.41
1:B:346:LEU:HG	1:B:347:PRO:CD	2.50	0.41
1:B:224:MET:HE3	1:B:306:ILE:HG22	2.02	0.41
1:B:267:ASN:O	1:B:269:TYR:N	2.54	0.41
1:C:542:PHE:O	1:C:543:TRP:C	2.59	0.41
1:D:542:PHE:O	1:D:543:TRP:C	2.59	0.41
1:A:288:VAL:HG11	1:A:527:ALA:CB	2.51	0.41
1:A:488:LEU:HA	1:A:488:LEU:HD23	1.96	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:B:271:ILE:O	1:B:275:LEU:N	2.51	0.41
1:B:511:ILE:CD1	1:B:511:ILE:C	2.85	0.41
1:B:474:PRO:O	1:B:476:SER:N	2.54	0.41
1:B:76:SER:HB3	1:B:84:ILE:HD13	2.01	0.41
1:D:247:PRO:HG3	1:D:478:PRO:HB3	2.02	0.41
1:A:206:MET:HE1	1:A:346:LEU:HD12	2.02	0.40
1:B:158:LEU:HB2	1:B:160:ILE:HD12	2.04	0.40
1:D:297:VAL:HB	1:D:298:PRO:HD3	2.03	0.40
1:D:262:TYR:HA	1:D:439:LEU:HD13	2.03	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:475:LEU:CD2	1:B:475:LEU:O	2.55	0.40
1:D:298:PRO:HA	1:D:302:VAL:HG13	2.03	0.40
1:D:379:MET:HE3	1:D:395:LEU:HD21	2.04	0.40
1:D:525:ASN:HA	1:D:525:ASN:HD22	1.68	0.40
1:B:163:MET:SD	1:B:166:ILE:HD11	2.62	0.40
1:C:378:THR:O	1:C:382:TYR:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:ALA:O	1:C:426:TYR:HB3	2.22	0.40
1:D:535:LEU:O	1:D:536:ALA:C	2.60	0.40
1:A:218:PHE:O	1:A:221:VAL:HB	2.21	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%)	4	10
1	B	491/530 (93%)	417 (85%)	59 (12%)	15 (3%)	4	9
1	C	491/530 (93%)	418 (85%)	59 (12%)	14 (3%)	4	10
1	D	491/530 (93%)	421 (86%)	54 (11%)	16 (3%)	4	8
All	All	1964/2120 (93%)	1680 (86%)	225 (12%)	59 (3%)	4	10

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
1	A	513	VAL
1	A	519	VAL
1	B	53	TRP
1	B	110	GLY
1	B	268	GLN

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Mol	Chain	Res	Type
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
1	B	333	ALA
1	B	338	ALA
1	C	333	ALA
1	C	338	ALA
1	C	364	SER

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Mol	Chain	Res	Type
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%)	357 (90%)	39 (10%)	8	18
1	B	396/413 (96%)	357 (90%)	39 (10%)	8	18
1	C	396/413 (96%)	356 (90%)	40 (10%)	7	17
1	D	396/413 (96%)	356 (90%)	40 (10%)	7	17
All	All	1584/1652 (96%)	1426 (90%)	158 (10%)	7	18

All (158) 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
1	A	137	LEU
1	A	141	VAL
1	A	186	VAL
1	A	195	PHE
1	A	204	THR

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Mol	Chain	Res	Type
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	364	SER
1	A	378	THR
1	A	397	ASN
1	A	413	ILE
1	A	438	ILE
1	A	441	VAL
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	538	LEU
1	B	53	TRP
1	B	60	LEU
1	B	64	ASN
1	B	70	PHE
1	B	76	SER
1	B	94	THR
1	B	98	VAL
1	B	137	LEU
1	B	141	VAL
1	B	186	VAL
1	B	195	PHE
1	B	204	THR
1	B	235	ILE
1	B	261	LEU
1	B	270	ILE
1	B	271	ILE

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Mol	Chain	Res	Type
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	364	SER
1	B	378	THR
1	B	397	ASN
1	B	413	ILE
1	B	425	GLN
1	B	438	ILE
1	B	441	VAL
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	500	SER
1	B	511	ILE
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	195	PHE
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

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Mol	Chain	Res	Type
1	C	313	SER
1	C	327	THR
1	C	329	LEU
1	C	364	SER
1	C	378	THR
1	C	397	ASN
1	C	413	ILE
1	C	425	GLN
1	C	431	THR
1	C	438	ILE
1	C	441	VAL
1	C	449	LYS
1	C	450	LYS
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	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	195	PHE
1	D	204	THR
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

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Mol	Chain	Res	Type
1	D	327	THR
1	D	329	LEU
1	D	364	SER
1	D	378	THR
1	D	397	ASN
1	D	413	ILE
1	D	425	GLN
1	D	438	ILE
1	D	441	VAL
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	500	SER
1	D	511	ILE
1	D	538	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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	397	ASN
1	B	425	GLN
1	B	525	ASN
1	C	142	ASN
1	C	245	ASN
1	C	260	ASN

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Mol	Chain	Res	Type
1	C	272	GLN
1	C	397	ASN
1	C	425	GLN
1	C	525	ASN
1	D	123	ASN
1	D	142	ASN
1	D	245	ASN
1	D	260	ASN
1	D	272	GLN
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 monosaccharides 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	D	701	-	12,12,12	0.55	0	17,17,17	0.61	0
2	GAL	C	701	-	12,12,12	0.55	0	17,17,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	B	701	-	12,12,12	0.55	0	17,17,17	0.58	0
2	GAL	A	701	-	12,12,12	0.55	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	D	701	-	-	0/2/22/22	0/1/1/1
2	GAL	C	701	-	-	0/2/22/22	0/1/1/1
2	GAL	B	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	A	1
1	D	1
1	C	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.