



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:07 PM UTC

PDB ID : 6OL1 / pdb_00006ol1
Title : Structure of VcINDY in complex with Succinate
Authors : Sauer, D.B.; Marden, J.J.; Wang, D.N.
Deposited on : 2019-04-15
Resolution : 3.09 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

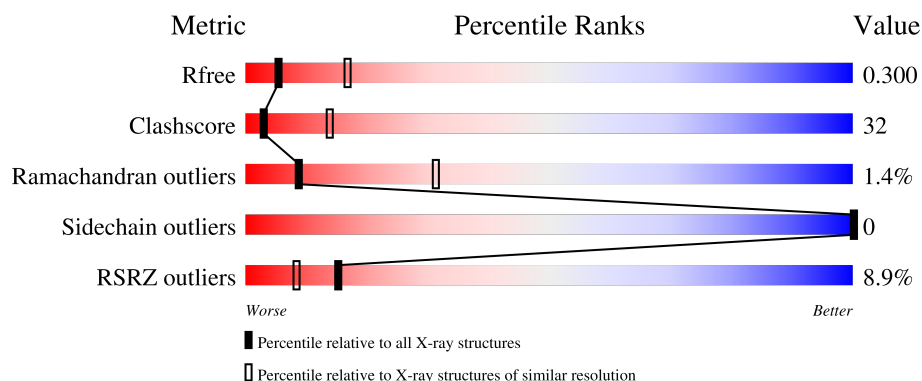
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	449	10% 47% 51% ..
1	B	449	8% 54% 43% ..
1	C	449	11% 55% 43% ..
1	D	449	7% 53% 45% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SIN	A	503	-	-	X	-
3	SIN	D	503	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13381 atoms, of which 16 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.

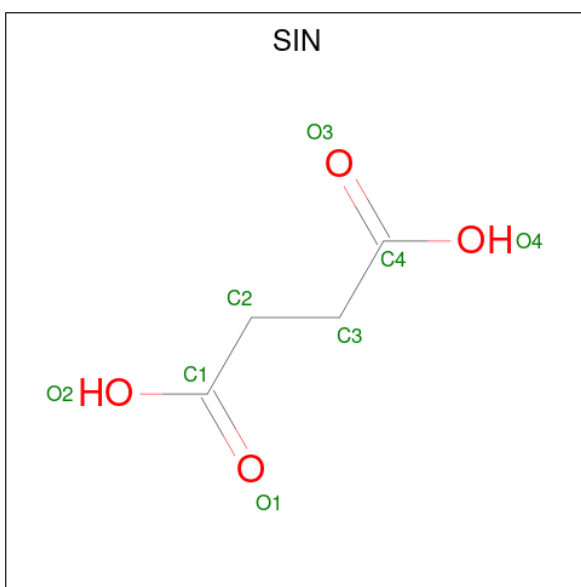
- Molecule 1 is a protein called Transporter, NadC family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	445	Total	C	N	O	S	0	0	0
			3337	2225	522	564	26			
1	D	445	Total	C	N	O	S	0	0	0
			3329	2220	521	562	26			
1	A	445	Total	C	N	O	S	0	0	0
			3331	2220	521	564	26			
1	B	445	Total	C	N	O	S	0	0	0
			3328	2221	519	562	26			

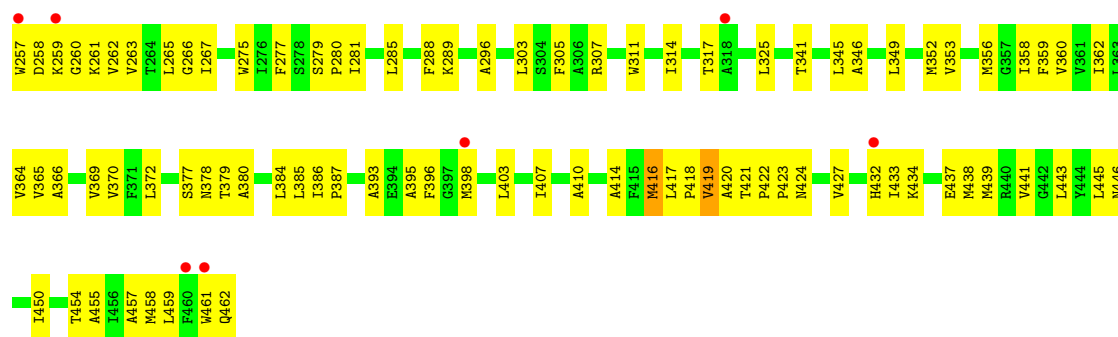
- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total	Na	0	0
			2	2		
2	D	2	Total	Na	0	0
			2	2		
2	A	2	Total	Na	0	0
			2	2		
2	B	2	Total	Na	0	0
			2	2		

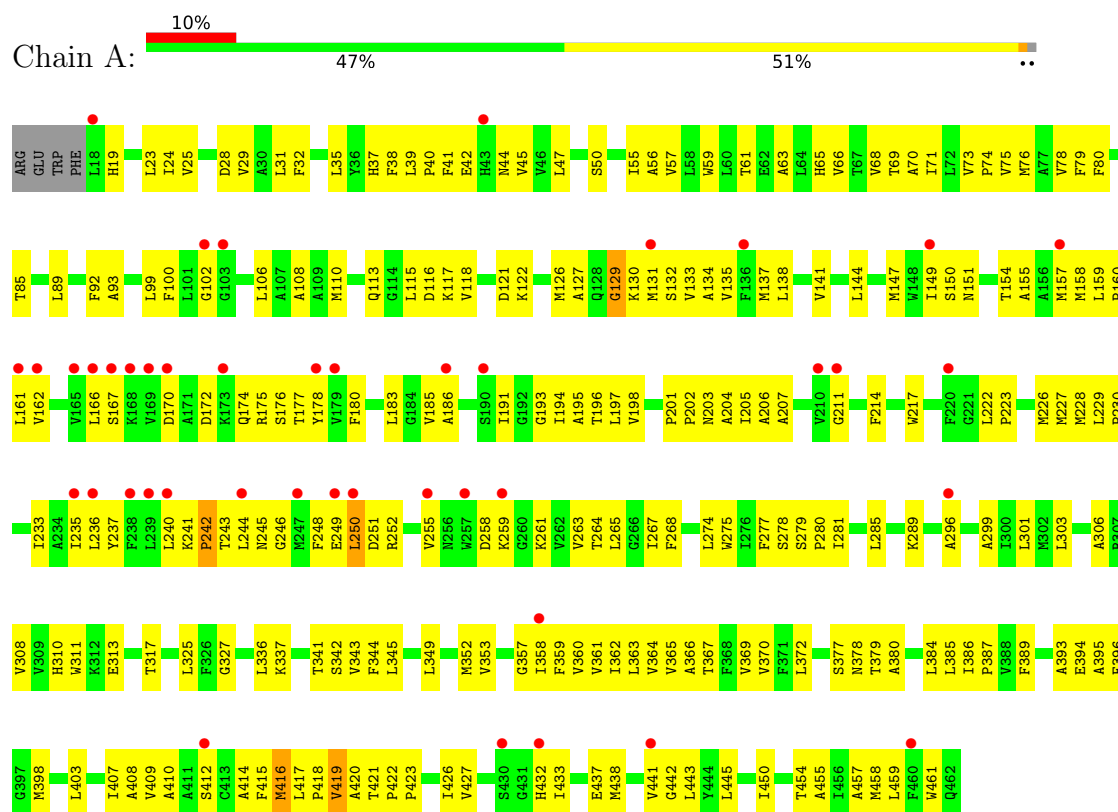
- Molecule 3 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).



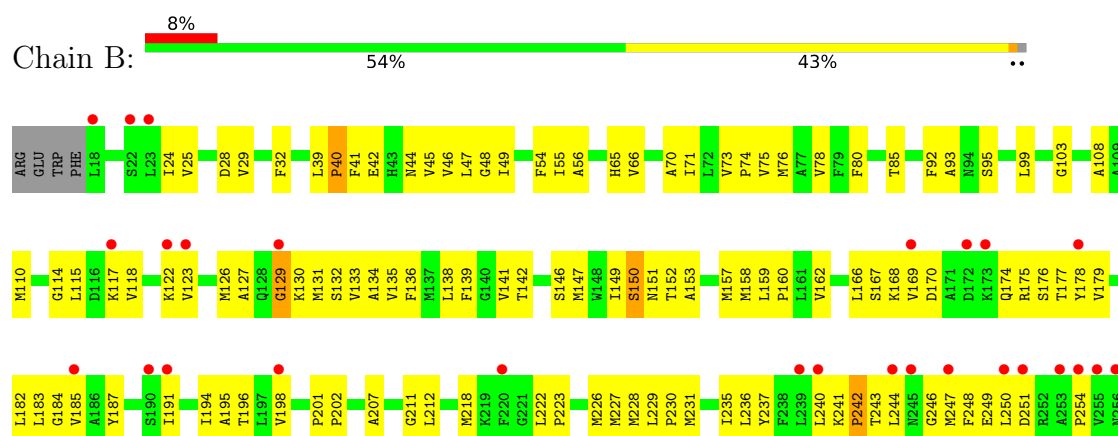
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	0	0
			12	4	4	4		
3	D	1	Total	C	H	O	0	0
			12	4	4	4		
3	A	1	Total	C	H	O	0	0
			12	4	4	4		
3	B	1	Total	C	H	O	0	0
			12	4	4	4		

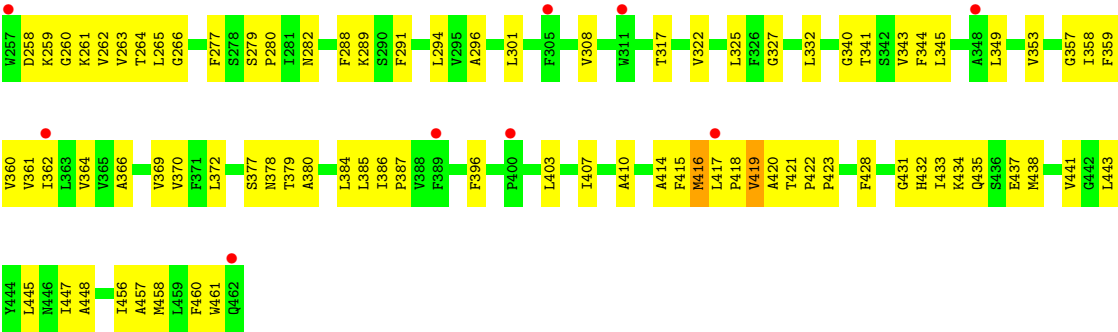


• Molecule 1: Transporter, NadC family



• Molecule 1: Transporter, NadC family





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.53Å 102.54Å 171.12Å 90.00° 98.81° 90.00°	Depositor
Resolution (Å)	46.48 – 3.09 46.48 – 3.09	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.48-3.09) 98.6 (46.48-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.06Å)	Xtriage
Refinement program	PHENIX (1.15.1_3469: ???)	Depositor
R, R_{free}	0.259 , 0.300 0.262 , 0.300	Depositor DCC
R_{free} test set	2000 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13381	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SIN, 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	0.08	0/3410	0.27	0/4652
1	B	0.09	0/3407	0.27	0/4648
1	C	0.09	0/3416	0.29	0/4659
1	D	0.09	0/3408	0.30	0/4648
All	All	0.09	0/13641	0.28	0/18607

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3331	0	3458	253	0
1	B	3328	0	3464	206	0
1	C	3337	0	3477	212	0
1	D	3329	0	3458	230	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	8	4	4	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	4	4	3	0
3	C	8	4	4	3	0
3	D	8	4	4	7	0
All	All	13365	16	13873	869	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 32.

All (869) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:THR:HG22	1:A:423:PRO:HD2	1.33	1.09
1:C:138:LEU:HD13	1:C:162:VAL:HG22	1.33	1.09
1:C:421:THR:HG22	1:C:423:PRO:HD2	1.38	1.05
1:D:421:THR:HG22	1:D:423:PRO:HD2	1.35	1.05
1:A:130:LYS:HB2	1:A:133:VAL:HG12	1.33	1.04
1:C:414:ALA:HB1	1:C:420:ALA:HB1	1.34	1.04
1:B:168:LYS:HG3	1:B:249:GLU:HB3	1.34	1.04
1:B:66:VAL:HG12	1:B:325:LEU:HD13	1.41	1.03
1:D:130:LYS:HB2	1:D:133:VAL:HG12	1.42	1.01
1:D:138:LEU:HD13	1:D:162:VAL:HG22	1.43	1.00
1:B:421:THR:HG22	1:B:423:PRO:HD2	1.45	0.98
1:B:202:PRO:HD3	1:B:379:THR:HG22	1.44	0.98
1:C:167:SER:HB3	1:C:249:GLU:OE2	1.64	0.96
1:A:202:PRO:HD3	1:A:379:THR:HG22	1.46	0.95
1:C:66:VAL:HG12	1:C:325:LEU:HD13	1.47	0.93
1:A:66:VAL:HG12	1:A:325:LEU:HD13	1.49	0.92
1:A:235:ILE:HD12	1:A:445:LEU:HD13	1.50	0.91
1:D:127:ALA:HB1	1:D:133:VAL:HG13	1.50	0.91
1:C:307:ARG:NH2	1:D:63:ALA:O	2.03	0.90
1:A:414:ALA:HB1	1:A:420:ALA:HB1	1.51	0.90
1:C:202:PRO:HD3	1:C:379:THR:HG22	1.53	0.89
1:B:414:ALA:HB1	1:B:420:ALA:HB1	1.55	0.87
1:C:305:PHE:HE1	1:D:64:LEU:HD11	1.39	0.87
1:D:66:VAL:HG12	1:D:325:LEU:HD13	1.57	0.86
1:A:176:SER:HB2	1:A:240:LEU:O	1.76	0.85
1:D:414:ALA:HB1	1:D:420:ALA:HB1	1.57	0.85
1:B:130:LYS:HB2	1:B:133:VAL:HG12	1.57	0.84
1:D:165:VAL:HG22	1:D:248:PHE:CE2	2.12	0.84
1:C:78:VAL:HG11	1:C:85:THR:HG22	1.60	0.83
1:C:168:LYS:HE2	1:C:249:GLU:HB3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ASN:HB2	3:B:503:SIN:O3	1.79	0.82
1:D:362:ILE:HD12	1:D:457:ALA:HB3	1.61	0.82
1:A:118:VAL:HG12	1:A:255:VAL:HG21	1.59	0.82
1:C:129:GLY:HA2	1:C:248:PHE:HB2	1.62	0.82
1:A:362:ILE:HD11	1:A:458:MET:HE2	1.61	0.82
1:D:359:PHE:HA	1:D:458:MET:HE1	1.62	0.81
1:A:113:GLN:NE2	1:A:259:LYS:O	2.11	0.81
1:A:121:ASP:OD2	1:A:252:ARG:NH2	2.13	0.81
1:D:202:PRO:HD3	1:D:379:THR:HG22	1.61	0.80
1:D:182:LEU:HD12	1:D:432:HIS:CE1	2.17	0.80
1:A:78:VAL:HG11	1:A:85:THR:HG22	1.63	0.80
1:A:418:PRO:O	1:A:419:VAL:HG12	1.82	0.79
1:C:337:LYS:NZ	1:C:394:GLU:OE1	2.14	0.79
1:C:437:GLU:O	1:C:441:VAL:HG23	1.83	0.79
1:B:99:LEU:HD12	1:B:296:ALA:HB2	1.64	0.79
1:B:265:LEU:O	1:B:265:LEU:HD13	1.83	0.78
1:C:130:LYS:HB2	1:C:133:VAL:HG12	1.65	0.78
1:D:226:MET:HA	1:D:226:MET:HE2	1.65	0.78
1:C:176:SER:HB2	1:C:240:LEU:O	1.82	0.78
1:A:359:PHE:HA	1:A:458:MET:HE1	1.66	0.78
1:B:127:ALA:HB1	1:B:133:VAL:HG13	1.65	0.77
1:C:250:LEU:HD23	1:C:250:LEU:H	1.48	0.77
1:A:421:THR:HG23	3:A:503:SIN:O1	1.84	0.76
1:B:250:LEU:HD23	1:B:250:LEU:H	1.51	0.76
1:D:78:VAL:HG11	1:D:85:THR:HG22	1.66	0.76
1:D:258:ASP:OD1	1:D:261:LYS:HG3	1.84	0.76
1:A:359:PHE:CD1	1:A:458:MET:HE3	2.20	0.76
1:C:305:PHE:CE1	1:D:64:LEU:HD11	2.21	0.76
1:B:421:THR:HG22	1:B:422:PRO:HD2	1.67	0.75
1:C:39:LEU:HD22	1:C:41:PHE:HE2	1.51	0.75
1:C:129:GLY:C	1:C:248:PHE:HB2	2.11	0.75
1:A:127:ALA:HB2	1:A:137:MET:SD	2.26	0.75
1:C:55:ILE:HD11	1:C:76:MET:HE3	1.69	0.74
1:A:437:GLU:O	1:A:441:VAL:HG23	1.87	0.74
1:A:201:PRO:HG2	1:A:379:THR:HG21	1.67	0.74
1:D:73:VAL:HB	1:D:74:PRO:HD3	1.69	0.74
1:C:129:GLY:CA	1:C:248:PHE:HB2	2.17	0.74
1:B:264:THR:OG1	1:B:308:VAL:HG21	1.88	0.74
1:C:248:PHE:HD2	1:C:249:GLU:H	1.36	0.73
1:A:222:LEU:O	1:A:226:MET:HG2	1.88	0.73
1:D:250:LEU:H	1:D:250:LEU:HD23	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:HD13	1:A:433:ILE:HD13	1.70	0.73
1:A:39:LEU:HD22	1:A:41:PHE:HE2	1.52	0.73
1:B:176:SER:HB2	1:B:240:LEU:O	1.87	0.73
1:B:372:LEU:HD23	1:B:385:LEU:HD11	1.69	0.73
1:D:356:MET:HE3	1:D:360:VAL:HG12	1.69	0.73
1:D:167:SER:HB3	1:D:249:GLU:OE2	1.89	0.73
1:D:421:THR:CG2	1:D:423:PRO:HD2	2.16	0.73
1:D:182:LEU:HD12	1:D:432:HIS:HE1	1.52	0.73
1:A:417:LEU:HD23	1:A:417:LEU:H	1.54	0.73
1:C:183:LEU:HD11	1:C:438:MET:SD	2.29	0.73
1:A:250:LEU:HD23	1:A:250:LEU:H	1.54	0.73
1:B:183:LEU:HD13	1:B:433:ILE:CD1	2.18	0.73
1:A:241:LYS:NZ	1:A:244:LEU:HB2	2.03	0.72
1:C:222:LEU:O	1:C:226:MET:HG2	1.89	0.72
1:A:455:ALA:O	1:A:459:LEU:HG	1.89	0.72
1:C:417:LEU:HD23	1:C:417:LEU:H	1.52	0.72
1:A:421:THR:CG2	1:A:423:PRO:HD2	2.15	0.72
1:B:166:LEU:HD13	1:B:178:TYR:CD1	2.24	0.72
1:C:175:ARG:NH2	1:C:432:HIS:O	2.23	0.72
1:A:175:ARG:HG2	1:A:432:HIS:NE2	2.04	0.72
1:B:258:ASP:OD1	1:B:261:LYS:HG3	1.88	0.72
1:B:437:GLU:O	1:B:441:VAL:HG23	1.90	0.72
1:B:226:MET:HE2	1:B:226:MET:HA	1.70	0.72
1:B:259:LYS:O	1:B:259:LYS:HG3	1.90	0.72
1:C:147:MET:HG2	1:C:195:ALA:HB3	1.71	0.72
1:D:127:ALA:CB	1:D:133:VAL:HG13	2.20	0.72
1:C:182:LEU:HD12	1:C:432:HIS:CE1	2.25	0.72
1:A:248:PHE:HD2	1:A:249:GLU:H	1.38	0.72
1:A:155:ALA:HB3	1:A:426:ILE:HD12	1.72	0.71
1:B:78:VAL:HG11	1:B:85:THR:HG22	1.72	0.71
1:C:259:LYS:O	1:C:259:LYS:HG3	1.91	0.71
1:D:110:MET:HB2	1:D:115:LEU:HB3	1.72	0.71
1:C:108:ALA:HB2	1:C:317:THR:HB	1.73	0.71
1:C:191:ILE:HG12	1:C:228:MET:HE2	1.72	0.71
1:C:226:MET:HE2	1:C:226:MET:HA	1.72	0.71
1:D:353:VAL:HG21	1:D:396:PHE:CE1	2.25	0.71
1:C:429:ALA:HA	1:B:254:PRO:CG	2.19	0.71
1:D:437:GLU:O	1:D:441:VAL:HG23	1.91	0.71
1:C:379:THR:HG23	3:C:503:SIN:O3	1.90	0.70
1:B:129:GLY:HA2	1:B:248:PHE:HB2	1.73	0.70
1:D:421:THR:HG22	1:D:422:PRO:HD2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:TYR:OH	1:B:432:HIS:ND1	2.21	0.70
1:B:132:SER:OG	1:B:244:LEU:HA	1.90	0.70
1:C:35:LEU:HD22	1:C:39:LEU:HD11	1.73	0.70
1:C:359:PHE:CD1	1:C:458:MET:HE3	2.26	0.70
1:B:162:VAL:HG11	1:B:182:LEU:HD23	1.74	0.70
1:D:167:SER:O	1:D:170:ASP:HB2	1.92	0.69
1:B:201:PRO:HG2	1:B:379:THR:HG21	1.74	0.69
1:D:455:ALA:O	1:D:459:LEU:HG	1.93	0.69
1:D:222:LEU:O	1:D:226:MET:HG2	1.92	0.69
1:C:416:MET:O	1:C:438:MET:HG2	1.93	0.69
1:D:259:LYS:O	1:D:259:LYS:HG3	1.91	0.69
1:B:131:MET:HE1	1:B:166:LEU:CD2	2.23	0.69
1:B:134:ALA:HB2	1:B:248:PHE:CE1	2.27	0.69
1:C:129:GLY:HA2	1:C:248:PHE:CB	2.22	0.69
1:D:168:LYS:HG2	1:D:249:GLU:HG2	1.73	0.69
1:D:369:VAL:HG12	1:D:385:LEU:HD12	1.74	0.69
1:B:359:PHE:CD1	1:B:458:MET:HE3	2.27	0.69
1:D:417:LEU:HD23	1:D:417:LEU:H	1.58	0.69
1:A:35:LEU:HD22	1:A:39:LEU:HD11	1.73	0.69
1:D:359:PHE:CD1	1:D:458:MET:HE3	2.29	0.68
1:B:131:MET:HE1	1:B:166:LEU:HD21	1.75	0.68
1:C:421:THR:HG22	1:C:422:PRO:HD2	1.76	0.68
1:B:421:THR:CG2	1:B:423:PRO:HD2	2.21	0.68
1:C:161:LEU:HD21	1:C:252:ARG:NH2	2.08	0.68
1:A:259:LYS:O	1:A:259:LYS:HG3	1.92	0.68
1:C:236:LEU:HD23	1:C:441:VAL:HG11	1.76	0.68
1:D:358:ILE:HD13	1:D:461:TRP:CZ2	2.29	0.68
1:B:241:LYS:HZ1	1:B:244:LEU:HB2	1.58	0.68
1:D:168:LYS:HE2	1:D:249:GLU:HB3	1.76	0.67
1:D:362:ILE:HD11	1:D:458:MET:HE2	1.75	0.67
1:B:138:LEU:HD13	1:B:162:VAL:HG22	1.75	0.67
1:B:235:ILE:HD12	1:B:445:LEU:HD13	1.76	0.67
1:B:369:VAL:HG12	1:B:385:LEU:HD12	1.76	0.67
1:A:110:MET:HB2	1:A:115:LEU:HB3	1.74	0.67
1:B:127:ALA:CB	1:B:133:VAL:HG13	2.25	0.67
1:D:378:ASN:HB2	3:D:503:SIN:C1	2.23	0.67
1:A:226:MET:HE2	1:A:226:MET:HA	1.76	0.67
1:B:55:ILE:HD11	1:B:76:MET:HE3	1.76	0.67
1:B:359:PHE:HA	1:B:458:MET:HE1	1.76	0.67
1:C:237:TYR:CZ	1:C:241:LYS:HD3	2.30	0.67
1:B:73:VAL:HB	1:B:74:PRO:HD3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:LEU:HD11	1:D:75:VAL:HG11	1.77	0.66
1:C:167:SER:HA	1:C:170:ASP:OD2	1.95	0.66
1:C:356:MET:HE3	1:C:360:VAL:HG12	1.76	0.66
1:A:39:LEU:HD22	1:A:41:PHE:CE2	2.31	0.66
1:B:369:VAL:HG12	1:B:385:LEU:CD1	2.26	0.66
1:A:129:GLY:O	1:A:248:PHE:HB2	1.94	0.66
1:A:421:THR:HG22	1:A:422:PRO:HD2	1.76	0.66
1:A:85:THR:OG1	1:B:289:LYS:HB3	1.95	0.66
1:A:337:LYS:NZ	1:A:394:GLU:OE1	2.29	0.66
1:A:369:VAL:HG12	1:A:385:LEU:HD12	1.76	0.66
1:D:379:THR:HG23	3:D:503:SIN:O2	1.96	0.66
1:A:174:GLN:HG3	1:A:177:THR:HB	1.78	0.66
1:C:421:THR:CG2	1:C:423:PRO:HD2	2.20	0.65
1:A:132:SER:OG	1:A:244:LEU:HA	1.96	0.65
1:B:416:MET:O	1:B:438:MET:HG2	1.97	0.65
1:B:417:LEU:HD23	1:B:417:LEU:H	1.60	0.65
1:A:79:PHE:HA	1:B:288:PHE:CE1	2.31	0.65
1:D:99:LEU:HD12	1:D:296:ALA:HB2	1.77	0.65
1:C:168:LYS:HG2	1:C:249:GLU:HG2	1.77	0.65
1:D:414:ALA:HB1	1:D:420:ALA:CB	2.27	0.65
1:A:180:PHE:HD1	1:A:236:LEU:HB3	1.62	0.65
1:A:416:MET:O	1:A:438:MET:HG2	1.96	0.65
1:D:151:ASN:HB2	3:D:503:SIN:C4	2.27	0.65
1:A:393:ALA:HB1	1:A:398:MET:HE3	1.78	0.65
1:D:165:VAL:HG22	1:D:248:PHE:HE2	1.61	0.65
1:A:73:VAL:HB	1:A:74:PRO:HD3	1.79	0.65
1:C:362:ILE:HD11	1:C:454:THR:HG23	1.79	0.65
1:A:129:GLY:HA2	1:A:248:PHE:CD1	2.31	0.65
1:C:79:PHE:HA	1:D:288:PHE:CE1	2.33	0.64
1:C:183:LEU:HD13	1:C:433:ILE:CD1	2.27	0.64
1:A:129:GLY:HA2	1:A:248:PHE:HB2	1.79	0.64
1:B:110:MET:HB2	1:B:115:LEU:HB3	1.78	0.64
1:D:237:TYR:CE2	1:D:241:LYS:HE2	2.33	0.64
1:D:39:LEU:HD22	1:D:41:PHE:HE2	1.63	0.64
1:C:47:LEU:HD11	1:C:80:PHE:CD1	2.33	0.64
1:D:177:THR:OG1	1:D:242:PRO:HG2	1.98	0.64
1:A:241:LYS:HZ1	1:A:244:LEU:HB2	1.61	0.64
1:B:196:THR:OG1	1:B:198:VAL:O	2.13	0.64
1:B:45:VAL:HG11	1:B:344:PHE:CD1	2.32	0.64
1:A:227:MET:O	1:A:230:PRO:HD2	1.98	0.64
1:D:358:ILE:HD13	1:D:461:TRP:CE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ALA:HB2	1:B:93:ALA:HB2	1.80	0.63
1:D:183:LEU:HD13	1:D:433:ILE:CD1	2.29	0.63
1:C:167:SER:HA	1:C:170:ASP:CG	2.23	0.63
1:D:132:SER:OG	1:D:244:LEU:HA	1.99	0.63
1:D:191:ILE:HG12	1:D:228:MET:HE2	1.78	0.63
1:D:176:SER:HB2	1:D:240:LEU:O	1.99	0.63
1:A:118:VAL:HG12	1:A:255:VAL:CG2	2.29	0.63
1:A:129:GLY:HA2	1:A:248:PHE:HD1	1.64	0.63
1:C:73:VAL:HB	1:C:74:PRO:HD3	1.78	0.63
1:B:183:LEU:HD13	1:B:433:ILE:HD13	1.79	0.63
1:A:362:ILE:CD1	1:A:458:MET:HE2	2.28	0.63
1:C:429:ALA:HA	1:B:254:PRO:HG3	1.79	0.62
1:A:222:LEU:HB3	1:A:223:PRO:HD3	1.81	0.62
1:C:359:PHE:HA	1:C:458:MET:HE1	1.81	0.62
1:D:229:LEU:HB3	1:D:230:PRO:HD3	1.81	0.62
1:C:429:ALA:HA	1:B:254:PRO:HG2	1.81	0.62
1:A:193:GLY:O	1:A:203:ASN:ND2	2.30	0.62
1:C:194:ILE:HD13	1:C:409:VAL:HG13	1.81	0.62
1:C:258:ASP:OD1	1:C:261:LYS:HG3	1.99	0.62
1:D:168:LYS:CE	1:D:249:GLU:HB3	2.29	0.62
1:A:183:LEU:HD11	1:A:438:MET:SD	2.39	0.62
1:A:251:ASP:O	1:A:252:ARG:HB3	1.98	0.62
1:C:108:ALA:HB2	1:C:317:THR:CB	2.30	0.62
1:B:174:GLN:NE2	1:B:242:PRO:HB2	2.14	0.62
1:B:222:LEU:O	1:B:226:MET:HG2	2.00	0.62
1:B:349:LEU:O	1:B:353:VAL:HG13	1.98	0.62
1:B:265:LEU:HD13	1:B:265:LEU:C	2.24	0.62
1:A:129:GLY:CA	1:A:248:PHE:HB2	2.29	0.62
1:B:357:GLY:O	1:B:361:VAL:HG23	1.99	0.62
1:C:118:VAL:HA	1:C:255:VAL:HG21	1.82	0.61
1:C:194:ILE:O	1:C:194:ILE:HG22	2.00	0.61
1:D:403:LEU:O	1:D:407:ILE:HG13	1.99	0.61
1:A:194:ILE:O	1:A:194:ILE:HG22	2.00	0.61
1:B:222:LEU:HB3	1:B:223:PRO:HD3	1.81	0.61
1:D:54:PHE:CD2	1:D:76:MET:HE1	2.35	0.61
1:A:417:LEU:HB2	1:A:418:PRO:HD2	1.81	0.61
1:C:139:PHE:CE2	1:C:184:GLY:HA3	2.35	0.61
1:B:194:ILE:HG22	1:B:194:ILE:O	2.00	0.61
1:D:115:LEU:HD21	1:D:265:LEU:HD23	1.83	0.61
1:C:129:GLY:O	1:C:248:PHE:N	2.33	0.61
1:C:161:LEU:HD21	1:C:252:ARG:HH22	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:PRO:C	1:C:420:ALA:H	2.07	0.61
1:C:138:LEU:HD11	1:C:162:VAL:HA	1.82	0.61
1:C:264:THR:OG1	1:C:308:VAL:HG21	2.00	0.61
1:A:117:LYS:HD2	1:A:252:ARG:HH12	1.65	0.61
1:C:118:VAL:HA	1:C:255:VAL:HG11	1.83	0.60
1:D:106:LEU:HD12	1:D:303:LEU:HD11	1.83	0.60
1:D:179:VAL:CG2	1:D:433:ILE:HD12	2.31	0.60
1:A:108:ALA:HB2	1:A:317:THR:CB	2.31	0.60
1:A:183:LEU:HD21	1:A:438:MET:HG3	1.83	0.60
1:B:358:ILE:O	1:B:362:ILE:HG23	2.01	0.60
1:D:418:PRO:O	1:D:419:VAL:HB	2.01	0.60
1:B:414:ALA:HB1	1:B:420:ALA:CB	2.29	0.60
1:D:222:LEU:HB3	1:D:223:PRO:HD3	1.82	0.60
1:A:65:HIS:HB3	1:A:68:VAL:HG23	1.84	0.60
1:B:42:GLU:OE1	1:B:44:ASN:HB2	2.00	0.60
1:B:240:LEU:O	1:B:242:PRO:HD3	2.00	0.60
1:B:179:VAL:HG23	1:B:433:ILE:HB	1.83	0.60
1:A:403:LEU:O	1:A:407:ILE:HG13	2.02	0.60
1:B:362:ILE:HD12	1:B:457:ALA:HB3	1.84	0.60
1:A:135:VAL:HG21	1:A:243:THR:HG21	1.83	0.60
1:C:42:GLU:OE1	1:C:44:ASN:HB2	2.01	0.59
1:C:183:LEU:HD13	1:C:433:ILE:HD13	1.83	0.59
1:A:263:VAL:HG12	1:A:308:VAL:HG21	1.83	0.59
1:A:141:VAL:HG12	1:A:158:MET:CE	2.33	0.59
1:D:194:ILE:HG22	1:D:194:ILE:O	2.02	0.59
1:A:129:GLY:HA2	1:A:248:PHE:CB	2.33	0.59
1:B:167:SER:O	1:B:170:ASP:HB2	2.02	0.59
1:B:279:SER:HB3	1:B:280:PRO:HD3	1.84	0.59
1:B:360:VAL:O	1:B:364:VAL:HG23	2.02	0.59
1:C:305:PHE:HE1	1:D:64:LEU:CD1	2.13	0.59
1:A:349:LEU:O	1:A:353:VAL:HG22	2.02	0.59
1:A:183:LEU:HD13	1:A:433:ILE:CD1	2.31	0.59
1:B:117:LYS:HD3	1:B:157:MET:CE	2.33	0.59
1:D:151:ASN:HB2	3:D:503:SIN:O3	2.02	0.59
1:B:237:TYR:CE1	1:B:241:LYS:HD3	2.37	0.59
1:A:138:LEU:HD13	1:A:162:VAL:HG22	1.84	0.59
1:A:194:ILE:HD11	1:A:412:SER:HB2	1.85	0.59
1:B:241:LYS:HG3	1:B:241:LYS:O	2.01	0.59
1:C:39:LEU:HD22	1:C:41:PHE:CE2	2.37	0.58
1:D:377:SER:HB3	1:D:380:ALA:HB3	1.84	0.58
1:A:79:PHE:HA	1:B:288:PHE:HE1	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:HD3	1:B:157:MET:HE2	1.85	0.58
1:B:151:ASN:HB2	3:B:503:SIN:O2	2.03	0.58
1:A:414:ALA:HB3	1:A:421:THR:OG1	2.02	0.58
1:B:151:ASN:HB2	3:B:503:SIN:C1	2.33	0.58
1:C:84:GLU:OE1	1:D:289:LYS:HE3	2.02	0.58
1:D:66:VAL:HG12	1:D:325:LEU:CD1	2.32	0.58
1:D:418:PRO:HA	1:D:424:ASN:HB3	1.85	0.58
1:A:132:SER:OG	1:A:244:LEU:HD12	2.03	0.58
1:A:418:PRO:C	1:A:420:ALA:H	2.10	0.58
1:C:165:VAL:HG22	1:C:248:PHE:HE2	1.68	0.58
1:D:201:PRO:HG2	1:D:379:THR:HG21	1.84	0.58
1:A:108:ALA:HB2	1:A:317:THR:HB	1.85	0.58
1:B:168:LYS:HG3	1:B:249:GLU:CB	2.22	0.58
1:C:443:LEU:O	1:C:447:ILE:HD12	2.04	0.58
1:A:66:VAL:HG12	1:A:325:LEU:CD1	2.28	0.58
1:A:159:LEU:HB3	1:A:160:PRO:HD3	1.85	0.58
1:B:159:LEU:HB3	1:B:160:PRO:HD3	1.86	0.58
1:C:251:ASP:O	1:C:252:ARG:HB3	2.04	0.58
1:C:378:ASN:HB2	3:C:503:SIN:C4	2.34	0.58
1:C:79:PHE:HA	1:D:288:PHE:HE1	1.68	0.57
1:A:378:ASN:HB2	3:A:503:SIN:C1	2.34	0.57
1:C:117:LYS:HD2	1:C:252:ARG:HH12	1.68	0.57
1:C:222:LEU:HB3	1:C:223:PRO:HD3	1.86	0.57
1:D:253:ALA:HB3	1:B:431:GLY:HA2	1.86	0.57
1:A:117:LYS:HE3	1:A:161:LEU:HD11	1.86	0.57
1:C:165:VAL:HG22	1:C:248:PHE:CE2	2.39	0.57
1:D:108:ALA:HB2	1:D:317:THR:HB	1.87	0.57
1:D:183:LEU:HD13	1:D:433:ILE:HD13	1.86	0.57
1:C:403:LEU:O	1:C:407:ILE:HG13	2.04	0.57
1:D:422:PRO:HB2	1:D:423:PRO:HD3	1.86	0.57
1:B:227:MET:O	1:B:230:PRO:HD2	2.04	0.57
1:A:78:VAL:HG21	1:A:85:THR:HA	1.85	0.57
1:B:135:VAL:HG23	1:B:136:PHE:HD1	1.68	0.57
1:A:191:ILE:HG12	1:A:228:MET:HE2	1.85	0.57
1:C:279:SER:HB3	1:C:280:PRO:HD3	1.85	0.57
1:D:113:GLN:NE2	1:D:259:LYS:O	2.37	0.57
1:C:183:LEU:HD21	1:C:438:MET:HG3	1.85	0.57
1:D:176:SER:HA	1:D:179:VAL:HG12	1.86	0.57
1:A:196:THR:OG1	1:A:198:VAL:O	2.23	0.57
1:D:358:ILE:O	1:D:362:ILE:HG23	2.05	0.56
1:C:237:TYR:CE1	1:C:241:LYS:HD3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:HIS:HB3	1:D:68:VAL:HG23	1.87	0.56
1:D:279:SER:HB3	1:D:280:PRO:HD3	1.87	0.56
1:D:360:VAL:O	1:D:364:VAL:HG23	2.05	0.56
1:C:159:LEU:HB3	1:C:160:PRO:HD3	1.87	0.56
1:D:378:ASN:HB2	3:D:503:SIN:O2	2.05	0.56
1:A:166:LEU:HD12	1:A:178:TYR:HB2	1.87	0.56
1:B:418:PRO:HD3	1:B:438:MET:CE	2.35	0.56
1:A:47:LEU:HD11	1:A:80:PHE:CD1	2.40	0.56
1:A:237:TYR:CE1	1:A:241:LYS:HD3	2.39	0.56
1:D:251:ASP:O	1:B:434:LYS:HG2	2.04	0.56
1:B:191:ILE:HG12	1:B:228:MET:HE2	1.87	0.56
1:C:161:LEU:HD11	1:C:252:ARG:NH1	2.21	0.56
1:A:180:PHE:CD1	1:A:236:LEU:HB3	2.41	0.56
1:B:146:SER:OG	1:B:151:ASN:OD1	2.23	0.56
1:C:127:ALA:HB3	1:C:248:PHE:HE1	1.71	0.56
1:D:115:LEU:HD13	1:D:261:LYS:O	2.06	0.56
1:D:421:THR:HG23	3:D:503:SIN:O1	2.05	0.56
1:A:422:PRO:HB2	1:A:423:PRO:HD3	1.86	0.56
1:C:47:LEU:HD21	1:C:80:PHE:HB3	1.87	0.56
1:B:362:ILE:HD11	1:B:458:MET:HE2	1.86	0.56
1:B:418:PRO:O	1:B:419:VAL:HB	2.06	0.56
1:B:139:PHE:CE2	1:B:184:GLY:HA3	2.40	0.56
1:B:417:LEU:HB2	1:B:418:PRO:HD2	1.88	0.56
1:A:241:LYS:O	1:A:241:LYS:HG3	2.05	0.55
1:B:47:LEU:HD11	1:B:80:PHE:CD1	2.40	0.55
1:C:152:THR:OG1	1:C:422:PRO:HG2	2.06	0.55
1:A:130:LYS:HB2	1:A:133:VAL:CG1	2.22	0.55
1:C:151:ASN:HB2	3:C:503:SIN:C1	2.36	0.55
1:A:47:LEU:HD21	1:A:80:PHE:HB3	1.88	0.55
1:C:422:PRO:HB2	1:C:423:PRO:HD3	1.87	0.55
1:D:58:LEU:CD2	1:D:64:LEU:HD12	2.37	0.55
1:C:194:ILE:HA	1:C:217:TRP:HH2	1.71	0.55
1:C:455:ALA:O	1:C:459:LEU:HG	2.06	0.55
1:D:159:LEU:HB3	1:D:160:PRO:HD3	1.87	0.55
1:D:349:LEU:O	1:D:353:VAL:HG13	2.07	0.55
1:B:129:GLY:C	1:B:248:PHE:HD1	2.13	0.55
1:A:167:SER:O	1:A:170:ASP:HB2	2.07	0.55
1:C:158:MET:O	1:C:162:VAL:HG23	2.06	0.54
1:C:417:LEU:HB2	1:C:418:PRO:HD2	1.89	0.54
1:D:166:LEU:HD13	1:D:178:TYR:HD1	1.72	0.54
1:D:393:ALA:HB2	1:D:403:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:O	1:A:362:ILE:HG23	2.07	0.54
1:D:183:LEU:CD1	1:D:433:ILE:HD13	2.38	0.54
1:A:279:SER:HB3	1:A:280:PRO:HD3	1.88	0.54
1:B:458:MET:O	1:B:461:TRP:HB2	2.07	0.54
1:D:19:HIS:O	1:D:23:LEU:HG	2.07	0.54
1:B:421:THR:CG2	1:B:422:PRO:HD2	2.37	0.54
1:C:42:GLU:CD	1:C:44:ASN:HB2	2.33	0.54
1:A:194:ILE:HA	1:A:217:TRP:HH2	1.73	0.54
1:C:443:LEU:O	1:C:443:LEU:HD12	2.08	0.54
1:B:241:LYS:NZ	1:B:244:LEU:HB2	2.22	0.54
1:C:129:GLY:O	1:C:248:PHE:HB2	2.07	0.54
1:C:340:GLY:O	1:C:343:VAL:HG12	2.08	0.54
1:D:235:ILE:HD12	1:D:445:LEU:HD13	1.90	0.54
1:C:191:ILE:HG12	1:C:228:MET:CE	2.37	0.54
1:A:393:ALA:CB	1:A:398:MET:HE3	2.37	0.54
1:C:365:VAL:HG22	1:C:389:PHE:HE1	1.71	0.54
1:A:122:LYS:O	1:A:126:MET:HG2	2.07	0.54
1:A:360:VAL:O	1:A:364:VAL:HG23	2.07	0.54
1:B:237:TYR:CE2	1:B:241:LYS:HG2	2.43	0.54
1:C:169:VAL:CG2	1:C:246:GLY:HA3	2.38	0.53
1:C:182:LEU:HD12	1:C:432:HIS:HE1	1.70	0.53
1:A:177:THR:HA	1:A:242:PRO:HD2	1.90	0.53
1:A:194:ILE:HD11	1:A:412:SER:CB	2.37	0.53
1:C:67:THR:HG21	1:D:311:TRP:CZ2	2.43	0.53
1:C:132:SER:OG	1:C:244:LEU:HD12	2.08	0.53
1:C:349:LEU:O	1:C:353:VAL:HG13	2.08	0.53
1:D:416:MET:O	1:D:438:MET:HG2	2.08	0.53
1:A:194:ILE:HG21	1:A:409:VAL:HG13	1.91	0.53
1:B:353:VAL:HG21	1:B:396:PHE:CE1	2.43	0.53
1:D:366:ALA:O	1:D:370:VAL:HG23	2.09	0.53
1:D:369:VAL:HG12	1:D:385:LEU:CD1	2.38	0.53
1:D:414:ALA:HB3	1:D:421:THR:OG1	2.08	0.53
1:A:35:LEU:CD2	1:A:39:LEU:HD11	2.38	0.53
1:B:70:ALA:O	1:B:74:PRO:HD3	2.08	0.53
1:A:110:MET:HB2	1:A:115:LEU:HD23	1.90	0.53
1:A:229:LEU:HB3	1:A:230:PRO:HD3	1.90	0.53
1:D:418:PRO:HD3	1:D:438:MET:CE	2.38	0.53
1:A:42:GLU:OE1	1:A:44:ASN:HB2	2.08	0.53
1:A:129:GLY:C	1:A:248:PHE:HB2	2.33	0.53
1:B:422:PRO:HB2	1:B:423:PRO:HD3	1.91	0.53
1:D:393:ALA:HB1	1:D:398:MET:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:PRO:HD2	1:D:41:PHE:CE2	2.43	0.53
1:A:122:LYS:O	1:A:122:LYS:HG3	2.08	0.53
1:B:108:ALA:HB2	1:B:317:THR:CB	2.39	0.53
1:C:201:PRO:HG2	1:C:379:THR:HG21	1.90	0.53
1:A:110:MET:HB3	1:A:264:THR:CG2	2.39	0.53
1:A:113:GLN:O	1:A:261:LYS:HE2	2.09	0.53
1:B:443:LEU:HD12	1:B:443:LEU:O	2.08	0.53
1:D:369:VAL:HA	1:D:372:LEU:HB3	1.91	0.52
1:A:177:THR:CA	1:A:242:PRO:HD2	2.39	0.52
1:C:227:MET:HB3	1:C:452:LEU:HD21	1.91	0.52
1:A:281:ILE:O	1:A:285:LEU:HD12	2.09	0.52
1:B:56:ALA:HB1	1:B:384:LEU:HD21	1.91	0.52
1:C:187:TYR:OH	1:C:415:PHE:O	2.14	0.52
1:A:176:SER:HB3	1:A:240:LEU:HD23	1.91	0.52
1:D:166:LEU:HD11	1:D:181:VAL:CB	2.40	0.52
1:A:367:THR:HG23	1:A:450:ILE:HD13	1.90	0.52
1:A:414:ALA:HB1	1:A:420:ALA:CB	2.32	0.52
1:A:154:THR:O	1:A:158:MET:HB2	2.09	0.52
1:B:147:MET:HG2	1:B:195:ALA:HB3	1.91	0.52
1:D:102:GLY:HA3	1:D:296:ALA:HB1	1.92	0.52
1:D:417:LEU:HB2	1:D:418:PRO:HD2	1.91	0.52
1:A:214:PHE:CD2	1:A:275:TRP:HB3	2.45	0.52
1:A:349:LEU:HB3	1:A:353:VAL:HG13	1.92	0.52
1:A:258:ASP:OD1	1:A:261:LYS:HG3	2.10	0.52
1:A:264:THR:OG1	1:A:308:VAL:HG11	2.10	0.52
1:D:358:ILE:HG13	1:D:359:PHE:N	2.24	0.52
1:B:108:ALA:HB2	1:B:317:THR:HB	1.92	0.52
1:B:229:LEU:HB3	1:B:230:PRO:HD3	1.91	0.52
1:C:115:LEU:HD21	1:C:265:LEU:HD23	1.92	0.51
1:A:141:VAL:HG12	1:A:158:MET:HE1	1.92	0.51
1:A:267:ILE:HG21	1:A:303:LEU:CD2	2.40	0.51
1:B:369:VAL:HG23	1:B:410:ALA:HB1	1.92	0.51
1:D:55:ILE:HD11	1:D:76:MET:HE3	1.93	0.51
1:C:121:ASP:OD2	1:C:252:ARG:NH2	2.43	0.51
1:C:418:PRO:O	1:C:419:VAL:CG1	2.58	0.51
1:B:174:GLN:HE21	1:B:242:PRO:HB2	1.75	0.51
1:C:294:LEU:HD21	1:D:78:VAL:HG11	1.92	0.51
1:A:343:VAL:HG23	1:A:395:ALA:HB1	1.92	0.51
1:D:214:PHE:CD2	1:D:275:TRP:HB3	2.46	0.51
1:A:78:VAL:CG2	1:A:85:THR:HA	2.40	0.51
1:A:147:MET:HG2	1:A:195:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:MET:HG2	1:C:195:ALA:CB	2.41	0.51
1:C:418:PRO:O	1:C:419:VAL:HG12	2.11	0.51
1:A:100:PHE:CE1	1:A:198:VAL:HA	2.46	0.51
1:D:168:LYS:HE2	1:D:249:GLU:CB	2.39	0.51
1:D:251:ASP:OD1	1:B:435:GLN:HB3	2.11	0.51
1:D:461:TRP:O	1:D:462:GLN:HG3	2.11	0.51
1:A:366:ALA:O	1:A:370:VAL:HG23	2.11	0.51
1:D:341:THR:O	1:D:345:LEU:HG	2.11	0.51
1:B:176:SER:CB	1:B:240:LEU:O	2.59	0.51
1:D:29:VAL:HA	1:D:54:PHE:HE1	1.76	0.51
1:D:418:PRO:C	1:D:420:ALA:H	2.18	0.51
1:D:446:ASN:O	1:D:450:ILE:HG13	2.11	0.51
1:B:42:GLU:CD	1:B:44:ASN:HB2	2.35	0.51
1:B:47:LEU:HD21	1:B:80:PHE:HB3	1.92	0.51
1:D:191:ILE:HG12	1:D:228:MET:CE	2.41	0.50
1:A:59:TRP:NE1	1:A:69:THR:HB	2.26	0.50
1:A:177:THR:OG1	1:A:242:PRO:HG2	2.10	0.50
1:C:78:VAL:HG21	1:C:85:THR:HA	1.93	0.50
1:C:414:ALA:HB1	1:C:420:ALA:CB	2.23	0.50
1:D:369:VAL:HG23	1:D:410:ALA:HB1	1.91	0.50
1:C:166:LEU:HD13	1:C:178:TYR:HD1	1.75	0.50
1:B:168:LYS:CG	1:B:249:GLU:HB3	2.25	0.50
1:C:42:GLU:OE2	1:C:44:ASN:HB2	2.12	0.50
1:A:311:TRP:HB3	1:B:65:HIS:CD2	2.46	0.50
1:C:229:LEU:HB3	1:C:230:PRO:HD3	1.94	0.50
1:C:362:ILE:CD1	1:C:454:THR:HG23	2.41	0.50
1:C:214:PHE:CD2	1:C:275:TRP:HB3	2.47	0.50
1:A:131:MET:HA	1:A:134:ALA:HB3	1.93	0.50
1:A:362:ILE:HD12	1:A:457:ALA:HB3	1.94	0.50
1:A:367:THR:HA	1:A:450:ILE:CD1	2.42	0.50
1:C:207:ALA:O	1:C:211:GLY:N	2.45	0.49
1:C:418:PRO:O	1:C:420:ALA:N	2.45	0.49
1:D:418:PRO:HA	1:D:424:ASN:CB	2.42	0.49
1:A:25:VAL:O	1:A:29:VAL:HG23	2.12	0.49
1:B:169:VAL:HG21	1:B:246:GLY:CA	2.42	0.49
1:D:54:PHE:HE2	1:D:72:LEU:HD21	1.77	0.49
1:D:132:SER:HG	1:D:244:LEU:HA	1.77	0.49
1:D:248:PHE:HD2	1:D:249:GLU:H	1.58	0.49
1:C:168:LYS:HG2	1:C:249:GLU:HB3	1.94	0.49
1:B:277:PHE:O	1:B:280:PRO:HD2	2.12	0.49
1:B:421:THR:HG22	1:B:422:PRO:CD	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:LEU:HD21	1:D:438:MET:HG3	1.95	0.49
1:A:99:LEU:HD21	1:A:197:LEU:HD13	1.94	0.49
1:A:362:ILE:HG13	1:A:454:THR:HG23	1.94	0.49
1:D:370:VAL:HG23	1:D:410:ALA:HB1	1.94	0.49
1:D:227:MET:O	1:D:230:PRO:HD2	2.12	0.49
1:D:251:ASP:O	1:D:252:ARG:HB3	2.13	0.49
1:D:267:ILE:HG21	1:D:303:LEU:CD2	2.43	0.49
1:D:108:ALA:HB2	1:D:317:THR:CB	2.43	0.49
1:B:54:PHE:CD2	1:B:76:MET:HE1	2.48	0.49
1:B:231:MET:SD	1:B:448:ALA:HB1	2.53	0.49
1:C:360:VAL:O	1:C:364:VAL:HG23	2.13	0.49
1:D:260:GLY:CA	1:D:263:VAL:HB	2.43	0.49
1:A:150:SER:OG	1:A:151:ASN:N	2.44	0.49
1:A:237:TYR:O	1:A:241:LYS:HB3	2.12	0.49
1:A:349:LEU:O	1:A:353:VAL:HG13	2.13	0.49
1:B:92:PHE:CD2	1:B:327:GLY:HA3	2.48	0.49
1:B:241:LYS:O	1:B:241:LYS:CG	2.60	0.49
1:C:294:LEU:HD21	1:D:85:THR:HG22	1.95	0.49
1:C:419:VAL:O	1:C:419:VAL:HG22	2.13	0.49
1:D:42:GLU:OE2	1:D:44:ASN:HB2	2.13	0.49
1:D:369:VAL:HG21	1:D:410:ALA:HB3	1.95	0.49
1:D:421:THR:CG2	1:D:422:PRO:HD2	2.41	0.49
1:A:336:LEU:HB3	1:A:342:SER:OG	2.13	0.49
1:C:71:ILE:O	1:C:74:PRO:HD2	2.13	0.49
1:D:47:LEU:HD11	1:D:80:PHE:CD1	2.48	0.49
1:B:237:TYR:CZ	1:B:241:LYS:HD3	2.48	0.49
1:B:418:PRO:C	1:B:420:ALA:H	2.20	0.49
1:D:28:ASP:OD2	1:D:57:VAL:HB	2.12	0.48
1:D:370:VAL:CG2	1:D:410:ALA:HB1	2.43	0.48
1:D:386:ILE:HB	1:D:387:PRO:HD3	1.94	0.48
1:B:237:TYR:CD2	1:B:241:LYS:HG2	2.48	0.48
1:C:141:VAL:HG12	1:C:158:MET:HE2	1.95	0.48
1:C:341:THR:O	1:C:345:LEU:HG	2.13	0.48
1:C:366:ALA:O	1:C:370:VAL:HG23	2.12	0.48
1:B:49:ILE:HD11	1:B:345:LEU:HD21	1.94	0.48
1:B:236:LEU:HD23	1:B:441:VAL:HG11	1.95	0.48
1:C:168:LYS:HG2	1:C:249:GLU:CG	2.44	0.48
1:B:56:ALA:HA	1:B:384:LEU:HD22	1.94	0.48
1:C:369:VAL:HG23	1:C:410:ALA:HB1	1.94	0.48
1:D:362:ILE:HG13	1:D:454:THR:HG23	1.94	0.48
1:D:443:LEU:HD12	1:D:443:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:VAL:CG1	1:A:158:MET:HE1	2.44	0.48
1:B:366:ALA:O	1:B:370:VAL:HG23	2.13	0.48
1:C:418:PRO:C	1:C:420:ALA:N	2.71	0.48
1:C:421:THR:CG2	1:C:422:PRO:HD2	2.43	0.48
1:C:161:LEU:HD11	1:C:252:ARG:HH12	1.79	0.48
1:C:262:VAL:O	1:C:266:GLY:N	2.43	0.48
1:D:58:LEU:HD21	1:D:64:LEU:HD12	1.95	0.48
1:D:139:PHE:CE2	1:D:184:GLY:HA3	2.48	0.48
1:D:256:ASN:OD1	1:D:256:ASN:N	2.47	0.48
1:A:263:VAL:CG1	1:A:308:VAL:HG21	2.43	0.48
1:A:267:ILE:HG21	1:A:303:LEU:HD23	1.94	0.48
1:A:151:ASN:HB2	3:A:503:SIN:C4	2.44	0.48
1:A:421:THR:CG2	1:A:422:PRO:HD2	2.44	0.48
1:B:434:LYS:HB2	1:B:437:GLU:CD	2.39	0.48
1:D:39:LEU:HD22	1:D:41:PHE:CE2	2.47	0.48
1:C:93:ALA:HB2	1:D:93:ALA:HB2	1.96	0.48
1:A:363:LEU:HD13	1:A:454:THR:OG1	2.13	0.48
1:B:66:VAL:HG12	1:B:325:LEU:CD1	2.29	0.48
1:C:149:ILE:HG22	1:C:150:SER:N	2.28	0.48
1:A:183:LEU:HD22	1:A:433:ILE:HD11	1.95	0.48
1:D:122:LYS:HE2	1:D:257:TRP:HH2	1.79	0.47
1:B:207:ALA:O	1:B:211:GLY:N	2.47	0.47
1:D:72:LEU:HA	1:D:75:VAL:HG12	1.96	0.47
1:A:191:ILE:HG12	1:A:228:MET:CE	2.44	0.47
1:B:40:PRO:HD2	1:B:41:PHE:CE2	2.50	0.47
1:B:178:TYR:HH	1:B:432:HIS:CE1	2.25	0.47
1:C:256:ASN:N	1:C:256:ASN:OD1	2.46	0.47
1:A:174:GLN:NE2	1:A:177:THR:OG1	2.47	0.47
1:A:386:ILE:HB	1:A:387:PRO:HD3	1.97	0.47
1:C:131:MET:HE2	1:C:169:VAL:CG2	2.44	0.47
1:C:418:PRO:C	1:C:419:VAL:HG12	2.38	0.47
1:A:116:ASP:OD2	1:A:157:MET:HE3	2.14	0.47
1:A:201:PRO:O	1:A:205:ILE:HG13	2.14	0.47
1:A:367:THR:HG23	1:A:450:ILE:CD1	2.44	0.47
1:A:418:PRO:O	1:A:419:VAL:CG1	2.59	0.47
1:B:169:VAL:O	1:B:169:VAL:HG12	2.14	0.47
1:D:42:GLU:OE1	1:D:44:ASN:HB2	2.15	0.47
1:C:228:MET:HG3	1:C:452:LEU:HD23	1.96	0.47
1:D:253:ALA:HB2	1:B:428:PHE:O	2.14	0.47
1:A:131:MET:HG3	1:A:246:GLY:HA3	1.97	0.47
1:A:186:ALA:HB2	1:A:427:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:VAL:HG11	1:B:344:PHE:CG	2.49	0.47
1:C:99:LEU:HD12	1:C:296:ALA:HB2	1.95	0.47
1:D:42:GLU:CD	1:D:44:ASN:HB2	2.40	0.47
1:D:265:LEU:HD13	1:D:265:LEU:O	2.15	0.47
1:A:56:ALA:HB1	1:A:384:LEU:HD21	1.97	0.47
1:A:110:MET:HB3	1:A:264:THR:HG21	1.97	0.47
1:A:186:ALA:HB2	1:A:427:VAL:CG1	2.45	0.47
1:B:168:LYS:HD2	1:B:248:PHE:O	2.13	0.47
1:B:237:TYR:O	1:B:241:LYS:HB3	2.15	0.47
1:D:346:ALA:HB2	1:D:395:ALA:HB3	1.96	0.47
1:A:42:GLU:CD	1:A:44:ASN:HB2	2.40	0.47
1:A:75:VAL:HG11	1:B:301:LEU:HD11	1.96	0.47
1:A:353:VAL:HG21	1:A:396:PHE:CE1	2.49	0.47
1:B:262:VAL:O	1:B:266:GLY:N	2.39	0.47
1:C:367:THR:HA	1:C:450:ILE:HD13	1.97	0.47
1:A:135:VAL:CG2	1:A:243:THR:HG21	2.45	0.47
1:B:66:VAL:CG1	1:B:325:LEU:HD13	2.29	0.47
1:D:149:ILE:HG22	1:D:150:SER:N	2.29	0.47
1:A:149:ILE:HG22	1:A:150:SER:N	2.29	0.47
1:A:357:GLY:O	1:A:361:VAL:HG23	2.14	0.47
1:B:135:VAL:HG21	1:B:243:THR:HG21	1.97	0.47
1:C:92:PHE:CD2	1:C:327:GLY:HA3	2.51	0.46
1:D:137:MET:O	1:D:141:VAL:HG23	2.15	0.46
1:B:103:GLY:HA3	1:B:198:VAL:HG11	1.96	0.46
1:D:416:MET:HG2	1:D:439:MET:O	2.16	0.46
1:A:201:PRO:HB2	1:A:379:THR:HB	1.96	0.46
1:A:265:LEU:HD13	1:A:265:LEU:O	2.15	0.46
1:A:310:HIS:HB2	1:A:313:GLU:HG2	1.98	0.46
1:B:114:GLY:O	1:B:118:VAL:HG13	2.15	0.46
1:C:120:ALA:O	1:C:124:LEU:HB2	2.15	0.46
1:D:196:THR:OG1	1:D:198:VAL:O	2.32	0.46
1:D:369:VAL:HG23	1:D:410:ALA:CB	2.45	0.46
1:A:85:THR:O	1:A:89:LEU:HD13	2.15	0.46
1:A:176:SER:OG	1:A:242:PRO:HG3	2.16	0.46
1:B:142:THR:OG1	1:B:158:MET:HG3	2.16	0.46
1:B:176:SER:HB2	1:B:240:LEU:HB3	1.97	0.46
1:B:177:THR:OG1	1:B:242:PRO:HG2	2.15	0.46
1:A:367:THR:HA	1:A:450:ILE:HD13	1.97	0.46
1:B:265:LEU:C	1:B:265:LEU:CD1	2.88	0.46
1:C:70:ALA:O	1:C:74:PRO:HD3	2.16	0.46
1:C:196:THR:OG1	1:C:198:VAL:O	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:VAL:O	1:C:369:VAL:HG22	2.15	0.46
1:A:141:VAL:HG12	1:A:158:MET:HE2	1.98	0.46
1:A:418:PRO:C	1:A:420:ALA:N	2.74	0.46
1:B:279:SER:HB3	1:B:280:PRO:CD	2.46	0.46
1:C:416:MET:HG3	1:C:442:GLY:C	2.41	0.46
1:A:258:ASP:CG	1:A:261:LYS:HE3	2.41	0.46
1:D:175:ARG:HH12	1:D:434:LYS:HG3	1.80	0.46
1:D:251:ASP:OD1	1:B:435:GLN:N	2.49	0.46
1:D:175:ARG:HH12	1:D:434:LYS:CD	2.29	0.46
1:A:418:PRO:HD3	1:A:438:MET:CE	2.45	0.46
1:B:177:THR:OG1	1:B:242:PRO:HD2	2.16	0.46
1:D:152:THR:N	3:D:503:SIN:O3	2.39	0.46
1:A:249:GLU:O	1:A:251:ASP:N	2.49	0.46
1:C:227:MET:O	1:C:230:PRO:HD2	2.16	0.46
1:D:362:ILE:CD1	1:D:458:MET:HE2	2.44	0.46
1:A:106:LEU:HG	1:A:268:PHE:HD1	1.81	0.46
1:C:182:LEU:O	1:C:185:VAL:HG22	2.16	0.45
1:D:197:LEU:HD12	1:D:214:PHE:HA	1.97	0.45
1:A:202:PRO:HG3	1:A:379:THR:HA	1.99	0.45
1:A:207:ALA:O	1:A:211:GLY:N	2.49	0.45
1:A:365:VAL:HG22	1:A:389:PHE:HE1	1.82	0.45
1:B:246:GLY:O	1:B:247:MET:HG3	2.16	0.45
1:C:279:SER:HB3	1:C:280:PRO:CD	2.45	0.45
1:D:262:VAL:O	1:D:266:GLY:N	2.44	0.45
1:A:183:LEU:HD22	1:A:433:ILE:CD1	2.45	0.45
1:B:122:LYS:HG3	1:B:122:LYS:O	2.15	0.45
1:A:241:LYS:O	1:A:241:LYS:CG	2.64	0.45
1:A:358:ILE:HG13	1:A:359:PHE:N	2.31	0.45
1:B:456:ILE:HG22	1:B:460:PHE:HD2	1.81	0.45
1:D:277:PHE:O	1:D:280:PRO:HD2	2.16	0.45
1:A:71:ILE:O	1:A:74:PRO:HD2	2.16	0.45
1:A:78:VAL:HG11	1:A:85:THR:CG2	2.42	0.45
1:A:235:ILE:CD1	1:A:445:LEU:HD13	2.35	0.45
1:B:175:ARG:O	1:B:178:TYR:N	2.36	0.45
1:C:45:VAL:O	1:C:49:ILE:HG12	2.16	0.45
1:D:259:LYS:HE3	1:D:259:LYS:HB2	1.83	0.45
1:D:362:ILE:HD12	1:D:457:ALA:CB	2.41	0.45
1:A:110:MET:HA	1:A:264:THR:HG21	1.97	0.45
1:B:201:PRO:HB2	1:B:379:THR:CG2	2.46	0.45
1:C:277:PHE:O	1:C:280:PRO:HD2	2.16	0.45
1:C:369:VAL:HG12	1:C:385:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:LEU:HA	1:D:75:VAL:CG1	2.46	0.45
1:A:274:LEU:O	1:A:278:SER:N	2.50	0.45
1:C:367:THR:HA	1:C:450:ILE:CD1	2.47	0.45
1:C:418:PRO:HD3	1:C:438:MET:CE	2.46	0.45
1:C:421:THR:HG22	1:C:422:PRO:CD	2.45	0.45
1:D:241:LYS:O	1:D:241:LYS:HG3	2.17	0.45
1:D:267:ILE:CD1	1:D:303:LEU:HD23	2.47	0.45
1:A:201:PRO:HB2	1:A:202:PRO:HD3	1.99	0.45
1:A:369:VAL:HG12	1:A:385:LEU:CD1	2.44	0.45
1:D:56:ALA:HB1	1:D:384:LEU:HD21	1.99	0.45
1:C:369:VAL:HG21	1:C:410:ALA:HB3	1.98	0.45
1:D:123:VAL:O	1:D:126:MET:HB2	2.17	0.45
1:D:233:ILE:HD13	1:D:236:LEU:HD12	2.00	0.45
1:B:349:LEU:O	1:B:353:VAL:HG22	2.17	0.45
1:C:59:TRP:NE1	1:C:69:THR:HB	2.32	0.44
1:B:25:VAL:O	1:B:29:VAL:HG23	2.17	0.44
1:B:39:LEU:HB2	1:B:46:VAL:HG13	1.99	0.44
1:C:45:VAL:HG11	1:C:344:PHE:CD1	2.52	0.44
1:C:78:VAL:CG2	1:C:85:THR:HA	2.47	0.44
1:C:241:LYS:O	1:C:241:LYS:HG3	2.17	0.44
1:D:421:THR:HG22	1:D:422:PRO:CD	2.44	0.44
1:A:78:VAL:HG11	1:B:294:LEU:HD11	1.99	0.44
1:A:89:LEU:HD23	1:B:95:SER:HA	2.00	0.44
1:A:263:VAL:HG11	1:A:306:ALA:HB1	1.99	0.44
1:A:301:LEU:HD11	1:B:75:VAL:HG11	1.98	0.44
1:B:250:LEU:H	1:B:250:LEU:CD2	2.26	0.44
1:B:418:PRO:HD3	1:B:438:MET:HE3	1.99	0.44
1:C:197:LEU:HD23	1:C:197:LEU:O	2.17	0.44
1:D:183:LEU:HD12	1:D:427:VAL:HG21	2.00	0.44
1:D:352:MET:HE3	1:D:352:MET:HB2	1.82	0.44
1:B:176:SER:CB	1:B:240:LEU:HB3	2.48	0.44
1:B:258:ASP:CG	1:B:261:LYS:HE3	2.42	0.44
1:D:356:MET:CE	1:D:360:VAL:HG12	2.43	0.44
1:B:201:PRO:HB2	1:B:202:PRO:HD3	1.99	0.44
1:A:42:GLU:OE2	1:A:44:ASN:HB2	2.18	0.44
1:A:378:ASN:HB2	3:A:503:SIN:O1	2.17	0.44
1:A:110:MET:CB	1:A:264:THR:HG21	2.48	0.44
1:B:218:MET:HG2	1:B:222:LEU:HB2	1.98	0.44
1:C:386:ILE:HB	1:C:387:PRO:HD3	2.00	0.44
1:C:449:CYS:O	1:C:453:LEU:HG	2.18	0.44
1:A:32:PHE:CD1	1:A:50:SER:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:MET:CA	1:A:264:THR:HG21	2.47	0.44
1:A:175:ARG:HG2	1:A:432:HIS:CD2	2.53	0.44
1:A:289:LYS:HA	1:A:289:LYS:HD2	1.74	0.44
1:C:194:ILE:O	1:C:194:ILE:CG2	2.66	0.44
1:A:162:VAL:HG21	1:A:185:VAL:HG11	1.99	0.44
1:C:114:GLY:O	1:C:118:VAL:HG13	2.18	0.44
1:D:133:VAL:O	1:D:133:VAL:HG22	2.17	0.44
1:A:92:PHE:CD2	1:A:327:GLY:HA3	2.53	0.44
1:A:194:ILE:O	1:A:194:ILE:CG2	2.66	0.44
1:B:169:VAL:HG21	1:B:246:GLY:HA3	2.00	0.44
1:C:201:PRO:HB2	1:C:379:THR:CG2	2.48	0.43
1:D:207:ALA:O	1:D:211:GLY:N	2.51	0.43
1:D:240:LEU:O	1:D:242:PRO:HD3	2.18	0.43
1:D:369:VAL:CG2	1:D:410:ALA:HB3	2.48	0.43
1:A:417:LEU:H	1:A:417:LEU:CD2	2.28	0.43
1:C:117:LYS:HD2	1:C:252:ARG:NH1	2.32	0.43
1:C:133:VAL:HG22	1:C:133:VAL:O	2.18	0.43
1:C:169:VAL:HG21	1:C:246:GLY:HA3	2.00	0.43
1:D:20:ARG:HD3	1:D:21:ASN:OD1	2.18	0.43
1:A:19:HIS:O	1:A:23:LEU:HG	2.19	0.43
1:A:31:LEU:HD11	1:A:35:LEU:HD11	2.00	0.43
1:A:45:VAL:HG11	1:A:344:PHE:CD1	2.53	0.43
1:A:352:MET:HE3	1:A:352:MET:HB2	1.88	0.43
1:B:194:ILE:O	1:B:194:ILE:CG2	2.66	0.43
1:D:147:MET:HG2	1:D:195:ALA:HB3	1.99	0.43
1:A:228:MET:HE3	1:A:415:PHE:HZ	1.82	0.43
1:C:358:ILE:HG13	1:C:359:PHE:N	2.32	0.43
1:D:279:SER:HB3	1:D:280:PRO:CD	2.47	0.43
1:D:365:VAL:O	1:D:369:VAL:HG22	2.19	0.43
1:C:78:VAL:CG1	1:C:85:THR:HG22	2.41	0.43
1:C:131:MET:HE2	1:C:169:VAL:HB	2.01	0.43
1:A:70:ALA:O	1:A:74:PRO:HD3	2.19	0.43
1:A:279:SER:HB3	1:A:280:PRO:CD	2.48	0.43
1:A:308:VAL:O	1:A:308:VAL:CG1	2.66	0.43
1:A:367:THR:OG1	1:A:450:ILE:HG21	2.18	0.43
1:D:150:SER:OG	1:D:151:ASN:N	2.50	0.43
1:D:369:VAL:CG1	1:D:385:LEU:HD12	2.47	0.43
1:A:176:SER:CB	1:A:240:LEU:HG	2.49	0.43
1:A:369:VAL:HG21	1:A:410:ALA:HB3	2.00	0.43
1:A:416:MET:HG3	1:A:442:GLY:C	2.43	0.43
1:B:166:LEU:HD13	1:B:178:TYR:HD1	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:LEU:O	1:B:407:ILE:HG13	2.19	0.43
1:C:178:TYR:O	1:C:178:TYR:CG	2.71	0.43
1:C:304:SER:CB	1:D:68:VAL:HG11	2.48	0.43
1:D:144:LEU:HD23	1:D:144:LEU:HA	1.89	0.43
1:A:172:ASP:O	1:A:175:ARG:HG3	2.19	0.43
1:A:443:LEU:HD12	1:A:443:LEU:O	2.18	0.43
1:B:207:ALA:HA	1:B:212:LEU:HB2	2.00	0.43
1:B:282:ASN:HB2	1:B:291:PHE:CD2	2.54	0.43
1:C:39:LEU:HB2	1:C:46:VAL:HG13	2.01	0.43
1:D:182:LEU:HD23	1:D:182:LEU:HA	1.75	0.43
1:A:155:ALA:HB3	1:A:426:ILE:CD1	2.47	0.43
1:C:417:LEU:H	1:C:417:LEU:CD2	2.26	0.43
1:D:169:VAL:HG12	1:D:169:VAL:O	2.18	0.43
1:B:71:ILE:O	1:B:74:PRO:HD2	2.19	0.43
1:D:183:LEU:CD1	1:D:433:ILE:CD1	2.95	0.43
1:D:253:ALA:CB	1:B:428:PHE:O	2.67	0.43
1:B:332:LEU:HD23	1:B:387:PRO:HG2	2.01	0.43
1:B:340:GLY:O	1:B:343:VAL:HG12	2.19	0.43
1:C:70:ALA:HB2	1:C:325:LEU:HD12	2.01	0.42
1:C:197:LEU:HD12	1:C:214:PHE:HA	2.01	0.42
1:C:201:PRO:HB2	1:C:202:PRO:HD3	2.01	0.42
1:C:243:THR:HG22	1:C:243:THR:O	2.19	0.42
1:D:260:GLY:HA3	1:D:263:VAL:HB	2.00	0.42
1:A:59:TRP:HE1	1:A:69:THR:HB	1.83	0.42
1:A:110:MET:HB2	1:A:115:LEU:CD2	2.48	0.42
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.87	0.42
1:C:109:ALA:HB2	1:C:309:VAL:HG11	2.01	0.42
1:D:233:ILE:HD13	1:D:233:ILE:HA	1.88	0.42
1:A:421:THR:HG22	1:A:422:PRO:CD	2.46	0.42
1:B:259:LYS:HE3	1:B:259:LYS:HB2	1.87	0.42
1:B:414:ALA:HB3	1:B:421:THR:OG1	2.18	0.42
1:B:443:LEU:O	1:B:447:ILE:HD12	2.18	0.42
1:C:142:THR:OG1	1:C:158:MET:HG3	2.18	0.42
1:D:135:VAL:HG23	1:D:136:PHE:HD1	1.85	0.42
1:D:281:ILE:O	1:D:285:LEU:HD12	2.19	0.42
1:B:240:LEU:HA	1:B:240:LEU:HD12	1.82	0.42
1:C:201:PRO:O	1:C:205:ILE:HG13	2.19	0.42
1:C:250:LEU:H	1:C:250:LEU:CD2	2.23	0.42
1:D:115:LEU:HD21	1:D:265:LEU:CD2	2.47	0.42
1:D:193:GLY:O	1:D:203:ASN:ND2	2.46	0.42
1:D:372:LEU:CD2	1:D:385:LEU:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ALA:HB2	1:A:408:ALA:HB2	2.02	0.42
1:A:237:TYR:CZ	1:A:241:LYS:HD3	2.54	0.42
1:A:277:PHE:O	1:A:280:PRO:HD2	2.20	0.42
1:B:129:GLY:CA	1:B:248:PHE:HB2	2.45	0.42
1:C:141:VAL:HG12	1:C:158:MET:CE	2.49	0.42
1:C:377:SER:HB3	1:C:380:ALA:HB3	2.02	0.42
1:A:100:PHE:CE1	1:A:204:ALA:HB2	2.55	0.42
1:B:42:GLU:OE2	1:B:44:ASN:HB2	2.19	0.42
1:B:55:ILE:HD11	1:B:76:MET:CE	2.47	0.42
1:D:105:ALA:HA	1:D:314:ILE:HG12	2.02	0.42
1:D:194:ILE:O	1:D:194:ILE:CG2	2.67	0.42
1:A:459:LEU:C	1:A:461:TRP:H	2.28	0.42
1:C:265:LEU:HD13	1:C:265:LEU:O	2.19	0.42
1:C:358:ILE:O	1:C:362:ILE:HG23	2.19	0.42
1:D:175:ARG:HH12	1:D:434:LYS:CG	2.33	0.42
1:D:201:PRO:N	1:D:202:PRO:CD	2.83	0.42
1:D:237:TYR:CD2	1:D:241:LYS:HG2	2.55	0.42
1:D:358:ILE:CD1	1:D:461:TRP:CE2	3.01	0.42
1:A:201:PRO:CG	1:A:379:THR:HG21	2.44	0.42
1:C:150:SER:OG	1:C:151:ASN:N	2.51	0.42
1:D:142:THR:OG1	1:D:158:MET:HG3	2.19	0.42
1:D:267:ILE:HD13	1:D:303:LEU:HD23	2.01	0.42
1:A:133:VAL:O	1:A:133:VAL:HG22	2.19	0.42
1:C:362:ILE:HD11	1:C:454:THR:CG2	2.49	0.42
1:B:249:GLU:O	1:B:251:ASP:N	2.52	0.42
1:B:133:VAL:HG22	1:B:133:VAL:O	2.20	0.41
1:B:182:LEU:O	1:B:185:VAL:HG22	2.20	0.41
1:B:377:SER:HB3	1:B:380:ALA:HB3	2.01	0.41
1:D:345:LEU:O	1:D:349:LEU:HG	2.20	0.41
1:D:377:SER:HB3	1:D:380:ALA:CB	2.49	0.41
1:A:28:ASP:OD2	1:A:57:VAL:HB	2.21	0.41
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.96	0.41
1:A:250:LEU:H	1:A:250:LEU:CD2	2.29	0.41
1:B:32:PHE:HB2	1:B:54:PHE:HD1	1.85	0.41
1:B:149:ILE:HG22	1:B:150:SER:N	2.34	0.41
1:C:177:THR:O	1:C:177:THR:HG22	2.20	0.41
1:C:201:PRO:N	1:C:202:PRO:CD	2.84	0.41
1:D:130:LYS:O	1:D:134:ALA:HB2	2.21	0.41
1:D:131:MET:HE2	1:D:169:VAL:HG21	2.02	0.41
1:A:55:ILE:HD11	1:A:76:MET:HE3	2.03	0.41
1:A:233:ILE:HD13	1:A:233:ILE:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:THR:HG23	3:A:503:SIN:O2	2.21	0.41
1:C:311:TRP:HB3	1:D:65:HIS:CD2	2.55	0.41
1:D:110:MET:HE2	1:D:149:ILE:HG13	2.02	0.41
1:B:152:THR:OG1	1:B:422:PRO:HG2	2.20	0.41
1:B:386:ILE:HB	1:B:387:PRO:HD3	2.00	0.41
1:C:258:ASP:CG	1:C:261:LYS:HE3	2.45	0.41
1:D:305:PHE:O	1:D:307:ARG:HD2	2.21	0.41
1:A:25:VAL:HG23	1:A:63:ALA:HB1	2.03	0.41
1:B:260:GLY:CA	1:B:263:VAL:HB	2.51	0.41
1:C:99:LEU:HD21	1:C:197:LEU:HD13	2.02	0.41
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.76	0.41
1:C:425:ALA:HA	1:C:428:PHE:HB3	2.03	0.41
1:B:250:LEU:HG	1:B:250:LEU:O	2.21	0.41
1:B:282:ASN:HB2	1:B:291:PHE:CG	2.55	0.41
1:B:358:ILE:HG13	1:B:359:PHE:N	2.34	0.41
1:C:120:ALA:O	1:C:124:LEU:N	2.33	0.41
1:D:122:LYS:O	1:D:122:LYS:HG3	2.20	0.41
1:D:165:VAL:HG22	1:D:248:PHE:CZ	2.54	0.41
1:D:201:PRO:HB2	1:D:202:PRO:HD3	2.03	0.41
1:D:241:LYS:O	1:D:241:LYS:CG	2.68	0.41
1:B:169:VAL:HG21	1:B:246:GLY:HA2	2.02	0.41
1:B:187:TYR:OH	1:B:415:PHE:O	2.33	0.41
1:C:303:LEU:HB3	1:C:309:VAL:HG12	2.01	0.41
1:C:402:LEU:HD23	1:C:403:LEU:N	2.36	0.41
1:D:166:LEU:HD23	1:D:166:LEU:HA	1.93	0.41
1:A:102:GLY:HA3	1:A:296:ALA:HB1	2.03	0.41
1:A:341:THR:O	1:A:345:LEU:HG	2.21	0.41
1:A:377:SER:HB3	1:A:380:ALA:HB3	2.03	0.41
1:B:150:SER:OG	1:B:151:ASN:N	2.53	0.41
1:B:322:VAL:O	1:B:325:LEU:HB3	2.20	0.41
1:A:37:HIS:C	1:A:38:PHE:HD1	2.29	0.41
1:B:24:ILE:O	1:B:28:ASP:HB2	2.20	0.41
1:B:141:VAL:HG12	1:B:158:MET:CE	2.51	0.41
1:C:175:ARG:O	1:C:178:TYR:N	2.42	0.41
1:C:231:MET:SD	1:C:448:ALA:HB1	2.61	0.41
1:A:24:ILE:HD13	1:A:61:THR:HB	2.03	0.41
1:B:150:SER:HB3	1:B:153:ALA:HB3	2.03	0.41
1:D:175:ARG:HH22	1:D:434:LYS:HE3	1.87	0.40
1:D:240:LEU:HD12	1:D:240:LEU:HA	1.93	0.40
1:D:356:MET:HB3	1:D:360:VAL:HB	2.02	0.40
1:D:418:PRO:HD3	1:D:438:MET:HE1	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:PRO:HD3	1:A:438:MET:HE3	2.04	0.40
1:B:289:LYS:HD2	1:B:289:LYS:HA	1.86	0.40
1:D:25:VAL:O	1:D:29:VAL:HG23	2.22	0.40
1:D:116:ASP:OD2	1:D:157:MET:HE3	2.22	0.40
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.92	0.40
1:A:201:PRO:N	1:A:202:PRO:CD	2.84	0.40
1:A:243:THR:C	1:A:245:ASN:H	2.29	0.40
1:B:48:GLY:HA3	1:B:341:THR:OG1	2.21	0.40
1:D:122:LYS:HE2	1:D:257:TRP:CH2	2.56	0.40
1:D:168:LYS:HA	1:D:168:LYS:HD3	1.91	0.40
1:D:212:LEU:HD22	1:D:216:ASP:HB3	2.03	0.40
1:A:250:LEU:O	1:A:250:LEU:HG	2.22	0.40
1:A:299:ALA:O	1:A:303:LEU:HG	2.22	0.40
1:B:201:PRO:N	1:B:202:PRO:CD	2.84	0.40
1:C:289:LYS:HA	1:C:289:LYS:HD2	1.76	0.40
1:C:356:MET:HB3	1:C:360:VAL:HB	2.03	0.40
1:C:370:VAL:HG23	1:C:410:ALA:HB1	2.04	0.40
1:A:372:LEU:HD23	1:A:385:LEU:HD11	2.03	0.40
1:B:123:VAL:O	1:B:126:MET:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/449 (99%)	395 (89%)	42 (10%)	6 (1%)	9	31
1	B	443/449 (99%)	398 (90%)	39 (9%)	6 (1%)	9	31
1	C	443/449 (99%)	393 (89%)	43 (10%)	7 (2%)	7	28
1	D	443/449 (99%)	400 (90%)	38 (9%)	5 (1%)	11	36
All	All	1772/1796 (99%)	1586 (90%)	162 (9%)	24 (1%)	9	31

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	242	PRO
1	C	416	MET
1	C	419	VAL
1	D	242	PRO
1	D	419	VAL
1	A	242	PRO
1	A	416	MET
1	A	419	VAL
1	B	242	PRO
1	B	416	MET
1	B	419	VAL
1	D	416	MET
1	C	129	GLY
1	D	129	GLY
1	A	40	PRO
1	A	129	GLY
1	B	40	PRO
1	B	129	GLY
1	C	150	SER
1	D	40	PRO
1	A	250	LEU
1	B	150	SER
1	C	40	PRO
1	C	418	PRO

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	349/357 (98%)	349 (100%)	0	100	100
1	B	349/357 (98%)	349 (100%)	0	100	100
1	C	351/357 (98%)	351 (100%)	0	100	100
1	D	348/357 (98%)	348 (100%)	0	100	100
All	All	1397/1428 (98%)	1397 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	435	GLN
1	D	37	HIS
1	D	432	HIS
1	A	174	GLN
1	A	256	ASN
1	B	112	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
3	SIN	C	503	-	7,7,7	1.24	0	8,8,8	0.69	0
3	SIN	D	503	-	7,7,7	1.29	0	8,8,8	1.07	0
3	SIN	B	503	-	7,7,7	1.24	0	8,8,8	0.99	0
3	SIN	A	503	-	7,7,7	1.30	0	8,8,8	1.40	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SIN	C	503	-	-	0/5/5/5	-
3	SIN	D	503	-	-	4/5/5/5	-
3	SIN	B	503	-	-	2/5/5/5	-
3	SIN	A	503	-	-	5/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	SIN	O4-C4-C3	2.05	120.47	114.00
3	A	503	SIN	O2-C1-C2	2.00	120.32	114.00

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	SIN	C1-C2-C3-C4
3	A	503	SIN	C2-C3-C4-O3
3	A	503	SIN	C2-C3-C4-O4
3	B	503	SIN	O2-C1-C2-C3
3	D	503	SIN	O2-C1-C2-C3
3	B	503	SIN	O1-C1-C2-C3
3	D	503	SIN	O1-C1-C2-C3
3	D	503	SIN	C2-C3-C4-O3
3	D	503	SIN	C2-C3-C4-O4
3	A	503	SIN	O2-C1-C2-C3
3	A	503	SIN	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	SIN	3	0
3	D	503	SIN	7	0
3	B	503	SIN	3	0
3	A	503	SIN	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	445/449 (99%)	0.70	43 (9%) 13 7	49, 84, 157, 189	0
1	B	445/449 (99%)	0.49	36 (8%) 18 10	44, 76, 132, 173	0
1	C	445/449 (99%)	0.68	50 (11%) 10 5	39, 74, 145, 179	0
1	D	445/449 (99%)	0.45	30 (6%) 24 12	40, 70, 122, 156	0
All	All	1780/1796 (99%)	0.58	159 (8%) 15 8	39, 76, 142, 189	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	LYS	6.0
1	A	169	VAL	5.8
1	D	18	LEU	5.4
1	C	169	VAL	5.4
1	A	170	ASP	5.3
1	C	136	PHE	5.2
1	C	173	LYS	4.8
1	B	169	VAL	4.7
1	C	137	MET	4.7
1	A	190	SER	4.6
1	C	178	TYR	4.6
1	B	257	TRP	4.5
1	C	358	ILE	4.4
1	D	250	LEU	4.4
1	A	210	VAL	4.4
1	C	133	VAL	4.3
1	C	244	LEU	4.2
1	C	268	PHE	4.2
1	C	42	GLU	4.2
1	D	248	PHE	4.1
1	D	162	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	256	ASN	4.1
1	D	157	MET	4.0
1	C	243	THR	4.0
1	D	239	LEU	4.0
1	A	165	VAL	3.9
1	B	172	ASP	3.9
1	C	461	TRP	3.8
1	C	402	LEU	3.8
1	C	250	LEU	3.8
1	D	243	THR	3.7
1	A	167	SER	3.7
1	D	155	ALA	3.6
1	D	212	LEU	3.6
1	C	401	VAL	3.6
1	D	160	PRO	3.6
1	A	161	LEU	3.5
1	C	240	LEU	3.5
1	A	162	VAL	3.3
1	D	318	ALA	3.3
1	B	250	LEU	3.3
1	B	23	LEU	3.3
1	D	259	LYS	3.2
1	A	244	LEU	3.2
1	B	239	LEU	3.2
1	D	240	LEU	3.2
1	A	250	LEU	3.2
1	B	117	LYS	3.2
1	D	159	LEU	3.2
1	C	237	TYR	3.1
1	C	431	GLY	3.1
1	C	157	MET	3.1
1	A	186	ALA	3.1
1	B	22	SER	3.1
1	D	247	MET	3.0
1	A	149	ILE	3.0
1	C	132	SER	3.0
1	C	174	GLN	3.0
1	A	173	LYS	3.0
1	D	398	MET	3.0
1	A	259	LYS	2.9
1	B	244	LEU	2.9
1	A	220	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	110	MET	2.9
1	C	44	ASN	2.9
1	B	123	VAL	2.9
1	C	460	PHE	2.9
1	D	178	TYR	2.9
1	C	432	HIS	2.9
1	A	430	SER	2.9
1	C	172	ASP	2.9
1	D	244	LEU	2.9
1	D	213	SER	2.8
1	B	240	LEU	2.8
1	A	257	TRP	2.8
1	A	358	ILE	2.8
1	A	102	GLY	2.7
1	B	18	LEU	2.7
1	C	257	TRP	2.7
1	D	169	VAL	2.7
1	B	305	PHE	2.7
1	C	239	LEU	2.7
1	A	247	MET	2.7
1	C	176	SER	2.7
1	B	190	SER	2.7
1	D	432	HIS	2.7
1	B	389	PHE	2.6
1	A	249	GLU	2.6
1	D	161	LEU	2.6
1	A	43	HIS	2.6
1	B	178	TYR	2.6
1	A	166	LEU	2.6
1	C	375	PHE	2.6
1	A	136	PHE	2.6
1	A	240	LEU	2.6
1	B	173	LYS	2.5
1	A	296	ALA	2.5
1	C	20	ARG	2.5
1	A	179	VAL	2.5
1	C	43	HIS	2.5
1	B	129	GLY	2.5
1	A	157	MET	2.4
1	C	117	LYS	2.4
1	C	177	THR	2.4
1	A	236	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	247	MET	2.4
1	D	460	PHE	2.4
1	D	211	GLY	2.4
1	B	417	LEU	2.4
1	A	412	SER	2.4
1	C	194	ILE	2.3
1	B	253	ALA	2.3
1	A	178	TYR	2.3
1	B	254	PRO	2.3
1	A	211	GLY	2.3
1	C	217	TRP	2.3
1	B	122	LYS	2.3
1	B	198	VAL	2.3
1	B	362	ILE	2.2
1	D	257	TRP	2.2
1	B	311	TRP	2.2
1	D	37	HIS	2.2
1	A	238	PHE	2.2
1	A	460	PHE	2.2
1	B	220	PHE	2.2
1	C	255	VAL	2.2
1	C	18	LEU	2.2
1	A	131	MET	2.2
1	B	247	MET	2.2
1	A	235	ILE	2.2
1	D	461	TRP	2.2
1	C	245	ASN	2.2
1	B	245	ASN	2.2
1	B	348	ALA	2.2
1	C	171	ALA	2.2
1	B	251	ASP	2.2
1	A	18	LEU	2.1
1	C	170	ASP	2.1
1	A	255	VAL	2.1
1	C	149	ILE	2.1
1	C	362	ILE	2.1
1	C	193	GLY	2.1
1	A	103	GLY	2.1
1	B	255	VAL	2.1
1	D	158	MET	2.1
1	D	19	HIS	2.1
1	B	191	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	175	ARG	2.1
1	C	124	LEU	2.1
1	D	149	ILE	2.1
1	C	310	HIS	2.1
1	C	444	TYR	2.1
1	C	429	ALA	2.0
1	A	441	VAL	2.0
1	B	185	VAL	2.0
1	A	432	HIS	2.0
1	B	400	PRO	2.0
1	B	462	GLN	2.0
1	A	239	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	A	502	1/1	0.80	0.10	101,101,101,101	0
3	SIN	B	503	8/8	0.85	0.20	67,83,118,121	0
2	NA	D	502	1/1	0.86	0.14	78,78,78,78	0
2	NA	C	502	1/1	0.87	0.17	81,81,81,81	0
3	SIN	D	503	8/8	0.88	0.18	77,90,111,111	0
3	SIN	C	503	8/8	0.89	0.14	60,78,101,101	0
3	SIN	A	503	8/8	0.93	0.10	53,79,107,107	0
2	NA	B	502	1/1	0.93	0.09	85,85,85,85	0
2	NA	C	501	1/1	0.94	0.07	76,76,76,76	0
2	NA	B	501	1/1	0.97	0.09	57,57,57,57	0
2	NA	D	501	1/1	0.97	0.05	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	A	501	1/1	0.98	0.03	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.