



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:14 PM UTC

PDB ID : 6OKZ / pdb_00006okz
Title : Structure of VcINDY bound to Fumarate
Authors : Sauer, D.B.; Marden, J.; Wang, D.N.
Deposited on : 2019-04-15
Resolution : 3.29 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

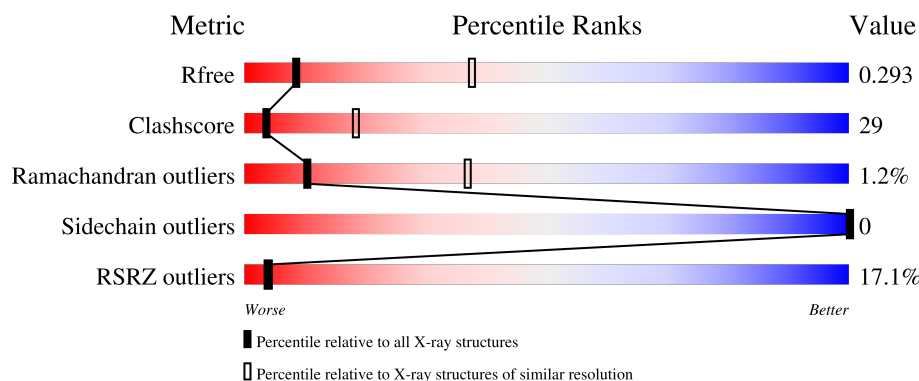
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	17% 54% 42% .
1	B	449	19% 52% 47% ..
1	C	449	16% 54% 41% ..
1	D	449	15% 52% 46% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13124 atoms, of which 4 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.

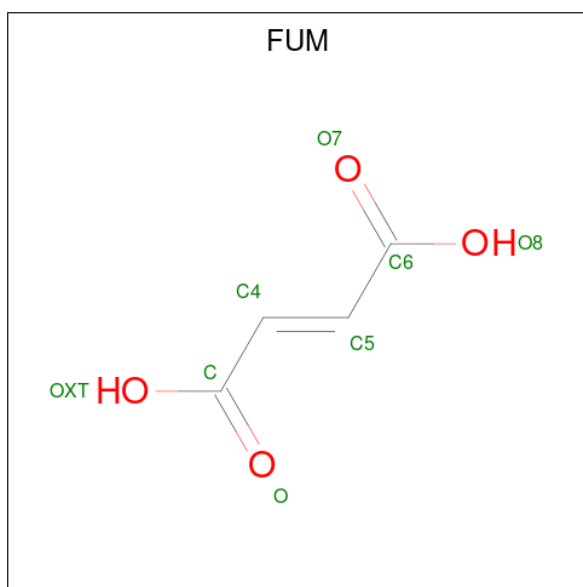
- Molecule 1 is a protein called Transporter, NadC family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	432	Total	C	N	O	S	0	0	0
			3229	2153	505	546	25			
1	D	444	Total	C	N	O	S	0	0	0
			3319	2213	519	561	26			
1	A	432	Total	C	N	O	S	0	0	0
			3231	2156	504	546	25			
1	B	444	Total	C	N	O	S	0	0	0
			3318	2213	518	561	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	1	Total	Na	0	0
			1	1		

- Molecule 3 is FUMARIC ACID (CCD ID: FUM) (formula: C₄H₄O₄).

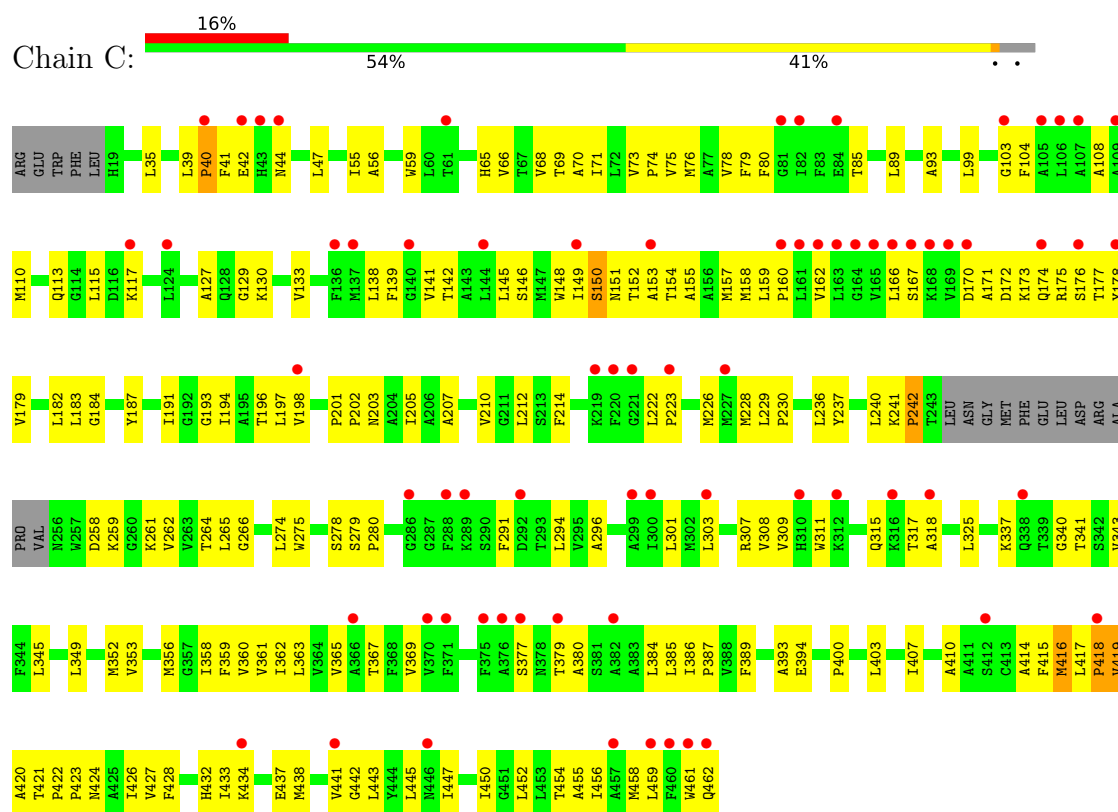


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	0	0
			10	4	2	4		
3	B	1	Total	C	H	O	0	0
			10	4	2	4		

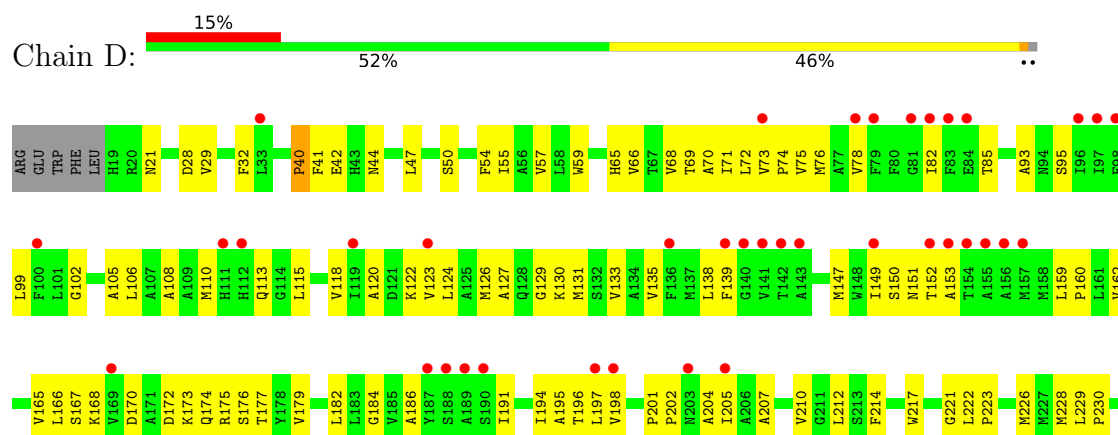
3 Residue-property plots

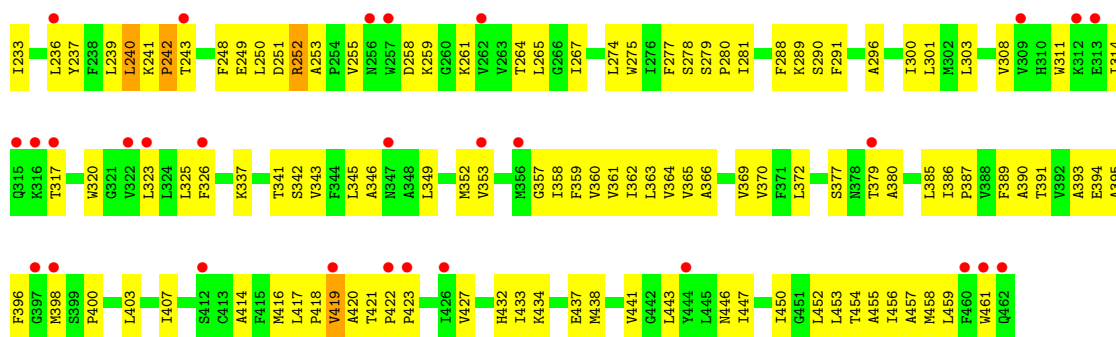
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Transporter, NadC family

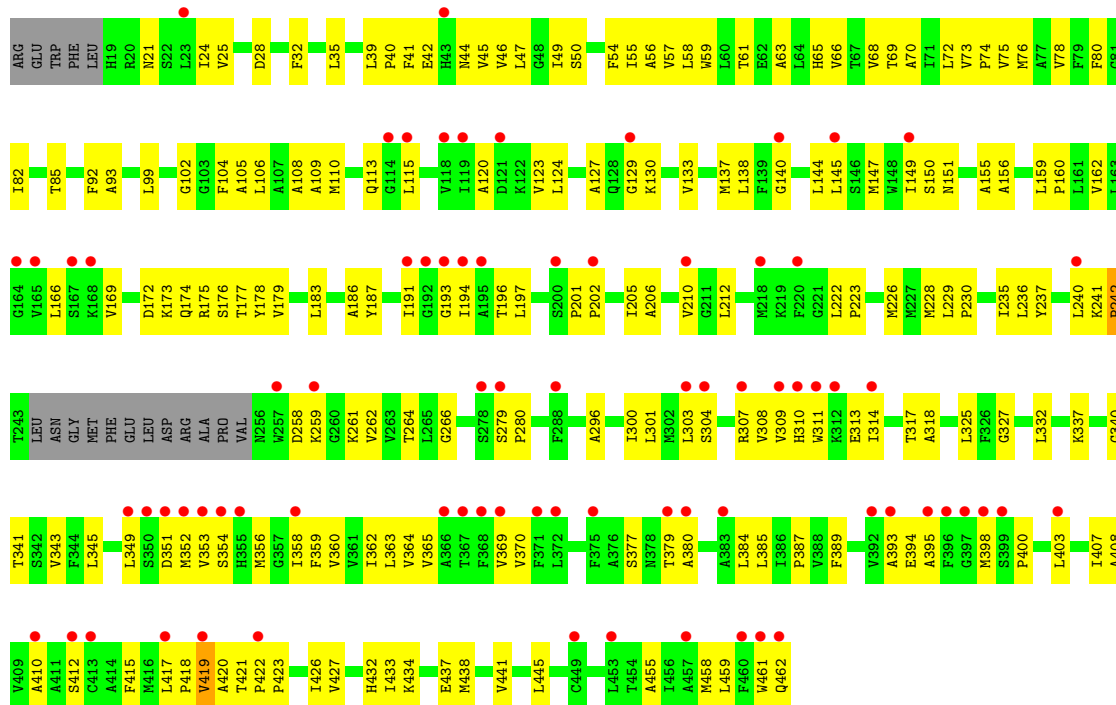


- Molecule 1: Transporter, NadC family

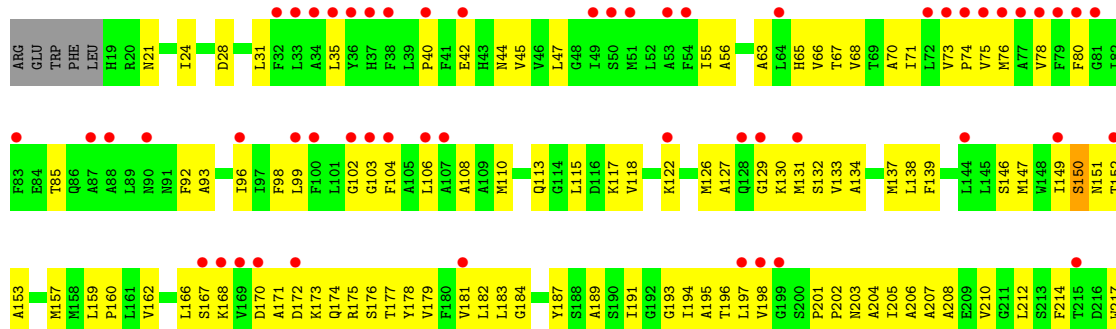


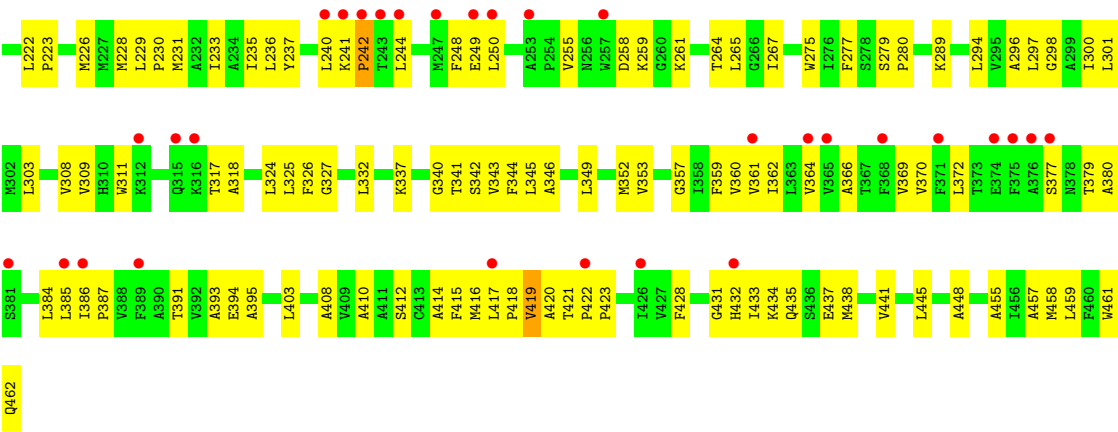


• Molecule 1: Transporter, NadC family



• 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	105.80Å 102.06Å 171.17Å 90.00° 98.94° 90.00°	Depositor
Resolution (Å)	47.90 – 3.29 47.90 – 3.29	Depositor EDS
% Data completeness (in resolution range)	93.5 (47.90-3.29) 93.5 (47.90-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.15.1_3469: ???)	Depositor
R, R_{free}	0.247 , 0.286 0.250 , 0.293	Depositor DCC
R_{free} test set	2000 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å ²)	110.6	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 24.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13124	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: FUM, 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	0.09	0/3307	0.27	0/4511
1	B	0.08	0/3397	0.26	0/4634
1	C	0.08	0/3304	0.27	0/4506
1	D	0.11	0/3398	0.27	0/4635
All	All	0.09	0/13406	0.27	0/18286

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	3231	0	3360	213	0
1	B	3318	0	3445	212	0
1	C	3229	0	3364	184	0
1	D	3319	0	3446	205	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	B	8	2	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	2	1	0	0
All	All	13120	4	13617	783	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 29.

All (783) 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:D:177:THR:HG23	1:D:243:THR:HG22	1.24	1.19
1:A:421:THR:HG22	1:A:423:PRO:HD2	1.21	1.16
1:B:421:THR:HG22	1:B:423:PRO:HD2	1.16	1.16
1:C:421:THR:HG22	1:C:423:PRO:HD2	1.22	1.13
1:D:421:THR:HG22	1:D:423:PRO:HD2	1.17	1.09
1:B:130:LYS:HB2	1:B:133:VAL:HG12	1.36	1.05
1:A:166:LEU:HD11	1:A:178:TYR:HA	1.36	1.04
1:B:202:PRO:HD3	1:B:379:THR:HG22	1.40	1.02
1:C:414:ALA:HB1	1:C:420:ALA:HB1	1.40	1.00
1:D:202:PRO:HD3	1:D:379:THR:HG22	1.40	0.98
1:A:127:ALA:HB1	1:A:133:VAL:HG11	1.46	0.98
1:C:78:VAL:HG11	1:C:85:THR:HG22	1.47	0.96
1:A:113:GLN:NE2	1:A:259:LYS:O	2.00	0.94
1:D:78:VAL:HG11	1:D:85:THR:HG22	1.49	0.94
1:A:138:LEU:HD13	1:A:162:VAL:HG22	1.51	0.93
1:D:253:ALA:HB3	1:B:431:GLY:HA2	1.51	0.93
1:C:301:LEU:HD11	1:D:75:VAL:HG11	1.51	0.93
1:A:202:PRO:HD3	1:A:379:THR:HG22	1.50	0.91
1:C:359:PHE:HA	1:C:458:MET:HE1	1.50	0.91
1:D:66:VAL:HG12	1:D:325:LEU:HD13	1.51	0.91
1:A:175:ARG:HH12	1:A:434:LYS:HG3	1.33	0.91
1:A:66:VAL:HG12	1:A:325:LEU:HD13	1.51	0.90
1:C:202:PRO:HD3	1:C:379:THR:HG22	1.54	0.90
1:D:418:PRO:O	1:D:419:VAL:HG12	1.71	0.90
1:B:78:VAL:HG11	1:B:85:THR:HG22	1.55	0.89
1:A:166:LEU:HD21	1:A:178:TYR:HB2	1.57	0.87
1:D:138:LEU:HD13	1:D:162:VAL:HG22	1.54	0.86
1:A:166:LEU:HD13	1:A:178:TYR:HD1	1.41	0.85
1:D:414:ALA:HB1	1:D:420:ALA:HB1	1.58	0.85
1:A:78:VAL:HG11	1:A:85:THR:HG22	1.57	0.85
1:D:127:ALA:HB1	1:D:133:VAL:HG13	1.60	0.83
1:C:337:LYS:NZ	1:C:394:GLU:OE1	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:SER:OG	1:B:151:ASN:ND2	2.12	0.82
1:C:66:VAL:HG12	1:C:325:LEU:HD13	1.59	0.82
1:B:103:GLY:HA3	1:B:198:VAL:HG11	1.63	0.81
1:A:236:LEU:HD23	1:A:441:VAL:HG11	1.63	0.81
1:A:337:LYS:NZ	1:A:394:GLU:OE1	2.14	0.81
1:B:236:LEU:HD23	1:B:441:VAL:HG11	1.63	0.81
1:C:117:LYS:HD3	1:C:157:MET:HE2	1.61	0.81
1:D:130:LYS:HB2	1:D:133:VAL:HG12	1.63	0.81
1:C:176:SER:HA	1:C:179:VAL:HG12	1.62	0.80
1:A:75:VAL:HG11	1:B:301:LEU:HD11	1.63	0.80
1:A:175:ARG:O	1:A:178:TYR:N	2.14	0.80
1:C:130:LYS:HB2	1:C:133:VAL:HG12	1.64	0.79
1:A:235:ILE:HD12	1:A:445:LEU:HD13	1.63	0.79
1:B:377:SER:HB3	1:B:380:ALA:HB3	1.65	0.79
1:D:168:LYS:HE2	1:D:249:GLU:HB3	1.63	0.79
1:D:118:VAL:HA	1:D:255:VAL:HG21	1.63	0.79
1:B:66:VAL:HG12	1:B:325:LEU:HD13	1.63	0.79
1:B:191:ILE:HG12	1:B:228:MET:HE2	1.65	0.78
1:C:461:TRP:HE3	1:C:462:GLN:HG3	1.48	0.78
1:C:359:PHE:CD1	1:C:458:MET:HE3	2.19	0.78
1:A:359:PHE:CD1	1:A:458:MET:HE3	2.19	0.78
1:D:167:SER:HB3	1:D:249:GLU:OE2	1.84	0.78
1:B:461:TRP:HE3	1:B:462:GLN:HG3	1.48	0.77
1:A:311:TRP:HB3	1:B:65:HIS:CD2	2.20	0.77
1:A:127:ALA:H	1:A:137:MET:HE1	1.48	0.77
1:D:165:VAL:HG22	1:D:248:PHE:HE2	1.50	0.77
1:B:240:LEU:O	1:B:242:PRO:HD3	1.86	0.76
1:D:349:LEU:HB3	1:D:353:VAL:HG13	1.68	0.76
1:C:236:LEU:HD23	1:C:441:VAL:HG11	1.67	0.75
1:D:175:ARG:HH12	1:D:434:LYS:HG3	1.50	0.75
1:D:455:ALA:O	1:D:459:LEU:HG	1.87	0.75
1:D:201:PRO:HG2	1:D:379:THR:HG21	1.68	0.74
1:D:337:LYS:NZ	1:D:394:GLU:OE1	2.19	0.74
1:D:106:LEU:HD12	1:D:303:LEU:HD11	1.67	0.74
1:C:35:LEU:HD22	1:C:39:LEU:HD11	1.70	0.74
1:A:65:HIS:HB3	1:A:68:VAL:HG23	1.68	0.74
1:D:418:PRO:HD3	1:D:438:MET:HE3	1.69	0.74
1:A:359:PHE:HE2	1:A:363:LEU:HD22	1.53	0.74
1:A:418:PRO:O	1:A:419:VAL:HG12	1.87	0.74
1:A:264:THR:OG1	1:A:308:VAL:HG21	1.88	0.74
1:B:201:PRO:HG2	1:B:379:THR:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:PHE:CD1	1:B:458:MET:HE3	2.23	0.73
1:A:155:ALA:HB3	1:A:426:ILE:HD12	1.70	0.73
1:C:258:ASP:OD1	1:C:261:LYS:HG3	1.89	0.73
1:D:258:ASP:OD1	1:D:261:LYS:HG3	1.88	0.73
1:B:235:ILE:HD12	1:B:445:LEU:HD13	1.71	0.73
1:A:109:ALA:HA	1:A:309:VAL:HB	1.69	0.72
1:A:437:GLU:O	1:A:441:VAL:HG23	1.89	0.72
1:B:196:THR:OG1	1:B:198:VAL:O	2.05	0.72
1:C:177:THR:OG1	1:C:242:PRO:HG2	1.89	0.72
1:A:73:VAL:HB	1:A:74:PRO:HD3	1.70	0.72
1:D:177:THR:CG2	1:D:243:THR:HG22	2.14	0.72
1:B:258:ASP:OD1	1:B:261:LYS:HG3	1.89	0.72
1:D:250:LEU:H	1:D:250:LEU:HD23	1.55	0.72
1:B:182:LEU:HD12	1:B:432:HIS:CE1	2.23	0.72
1:C:191:ILE:HG12	1:C:228:MET:HE2	1.71	0.71
1:A:176:SER:OG	1:A:242:PRO:HG3	1.90	0.71
1:A:176:SER:HB2	1:A:240:LEU:O	1.89	0.71
1:A:201:PRO:HG2	1:A:379:THR:HG21	1.72	0.71
1:C:210:VAL:HG23	1:C:212:LEU:HG	1.72	0.71
1:C:264:THR:OG1	1:C:308:VAL:HG21	1.91	0.71
1:A:35:LEU:HD22	1:A:39:LEU:HD11	1.73	0.71
1:A:362:ILE:HD11	1:A:458:MET:HE2	1.71	0.71
1:B:166:LEU:HB3	1:B:178:TYR:HD1	1.54	0.71
1:C:240:LEU:O	1:C:242:PRO:HD3	1.91	0.70
1:C:362:ILE:HD11	1:C:458:MET:HE2	1.73	0.70
1:B:226:MET:HE2	1:B:226:MET:HA	1.73	0.70
1:D:343:VAL:HA	1:D:395:ALA:HB1	1.74	0.70
1:C:187:TYR:OH	1:C:415:PHE:O	2.05	0.70
1:C:356:MET:HB3	1:C:360:VAL:HB	1.73	0.70
1:D:226:MET:HA	1:D:226:MET:HE2	1.73	0.70
1:A:226:MET:HE2	1:A:226:MET:HA	1.74	0.70
1:D:228:MET:HG3	1:D:452:LEU:HD23	1.73	0.70
1:D:240:LEU:O	1:D:242:PRO:HD3	1.91	0.70
1:A:124:LEU:HA	1:A:137:MET:SD	2.31	0.70
1:A:183:LEU:HD13	1:A:433:ILE:HD13	1.72	0.70
1:B:337:LYS:NZ	1:B:394:GLU:OE1	2.24	0.69
1:D:182:LEU:HD12	1:D:432:HIS:CE1	2.27	0.69
1:C:461:TRP:CE3	1:C:462:GLN:HG3	2.27	0.69
1:D:349:LEU:O	1:D:353:VAL:HG22	1.93	0.69
1:B:168:LYS:HE2	1:B:249:GLU:HB3	1.74	0.69
1:D:414:ALA:HB1	1:D:420:ALA:CB	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD22	1:A:41:PHE:HE2	1.56	0.69
1:B:78:VAL:CG1	1:B:85:THR:HG22	2.22	0.69
1:D:165:VAL:HG22	1:D:248:PHE:CE2	2.27	0.69
1:B:250:LEU:HD23	1:B:250:LEU:H	1.56	0.69
1:C:416:MET:O	1:C:438:MET:HG2	1.92	0.69
1:B:177:THR:OG1	1:B:242:PRO:HG2	1.92	0.69
1:C:307:ARG:HH22	1:D:21:ASN:HD22	1.41	0.69
1:C:196:THR:OG1	1:C:198:VAL:O	2.12	0.68
1:A:99:LEU:HD12	1:A:296:ALA:HB2	1.74	0.68
1:A:176:SER:HA	1:A:179:VAL:HG12	1.75	0.68
1:A:365:VAL:HG22	1:A:389:PHE:HE1	1.57	0.68
1:C:222:LEU:O	1:C:226:MET:HG2	1.95	0.67
1:D:176:SER:HA	1:D:179:VAL:HG12	1.76	0.67
1:B:166:LEU:HD11	1:B:181:VAL:CB	2.25	0.67
1:B:461:TRP:CE3	1:B:462:GLN:HG3	2.29	0.67
1:C:113:GLN:HG3	1:C:261:LYS:HG2	1.77	0.67
1:C:367:THR:HG23	1:C:450:ILE:HD13	1.77	0.67
1:C:171:ALA:HB3	1:C:174:GLN:HB2	1.77	0.67
1:B:176:SER:HA	1:B:179:VAL:HG12	1.76	0.67
1:D:78:VAL:CG1	1:D:85:THR:HG22	2.23	0.67
1:A:127:ALA:HB2	1:A:137:MET:HE3	1.77	0.67
1:D:233:ILE:HD13	1:D:236:LEU:HD12	1.77	0.66
1:D:65:HIS:HB3	1:D:68:VAL:HG23	1.77	0.66
1:A:349:LEU:O	1:A:353:VAL:HG22	1.95	0.66
1:C:194:ILE:O	1:C:194:ILE:HG22	1.96	0.66
1:A:166:LEU:HD11	1:A:178:TYR:CA	2.19	0.66
1:C:55:ILE:HD11	1:C:76:MET:HE3	1.77	0.66
1:B:66:VAL:CG1	1:B:325:LEU:HD13	2.26	0.66
1:B:176:SER:OG	1:B:242:PRO:HG3	1.95	0.66
1:C:191:ILE:HG12	1:C:228:MET:CE	2.26	0.65
1:B:108:ALA:HB2	1:B:317:THR:CB	2.26	0.65
1:D:437:GLU:O	1:D:441:VAL:HG23	1.96	0.65
1:D:66:VAL:CG1	1:D:325:LEU:HD13	2.25	0.65
1:B:167:SER:O	1:B:170:ASP:HB2	1.97	0.65
1:D:167:SER:O	1:D:170:ASP:HB2	1.97	0.65
1:B:102:GLY:HA3	1:B:296:ALA:HB1	1.79	0.65
1:A:194:ILE:HD11	1:A:412:SER:HB2	1.79	0.65
1:C:437:GLU:O	1:C:441:VAL:HG23	1.97	0.65
1:B:237:TYR:O	1:B:241:LYS:HB3	1.96	0.64
1:C:73:VAL:HB	1:C:74:PRO:HD3	1.78	0.64
1:A:194:ILE:O	1:A:194:ILE:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:HD12	1:A:445:LEU:CD1	2.27	0.64
1:B:231:MET:SD	1:B:448:ALA:HB1	2.38	0.64
1:B:73:VAL:HB	1:B:74:PRO:HD3	1.80	0.64
1:B:264:THR:OG1	1:B:308:VAL:HG21	1.96	0.64
1:C:99:LEU:HD12	1:C:296:ALA:HB2	1.80	0.64
1:D:377:SER:HB3	1:D:380:ALA:HB3	1.78	0.64
1:A:455:ALA:O	1:A:459:LEU:HG	1.97	0.64
1:A:110:MET:HB2	1:A:115:LEU:HB3	1.78	0.64
1:B:117:LYS:HD3	1:B:157:MET:HE2	1.80	0.63
1:A:393:ALA:HB2	1:A:403:LEU:HD12	1.80	0.63
1:C:78:VAL:CG1	1:C:85:THR:HG22	2.26	0.63
1:C:259:LYS:O	1:C:259:LYS:HG3	1.98	0.63
1:A:183:LEU:HD13	1:A:433:ILE:CD1	2.28	0.63
1:B:194:ILE:HG22	1:B:194:ILE:O	1.98	0.63
1:C:183:LEU:HD13	1:C:433:ILE:CD1	2.27	0.63
1:A:301:LEU:HD11	1:B:75:VAL:HG11	1.80	0.63
1:A:362:ILE:HD11	1:A:458:MET:CE	2.28	0.63
1:B:183:LEU:HD13	1:B:433:ILE:CD1	2.28	0.63
1:D:73:VAL:HB	1:D:74:PRO:HD3	1.80	0.63
1:A:78:VAL:CG1	1:A:85:THR:HG22	2.28	0.63
1:B:437:GLU:O	1:B:441:VAL:HG23	1.99	0.63
1:B:150:SER:HB3	1:B:153:ALA:HB3	1.81	0.63
1:B:259:LYS:O	1:B:259:LYS:HG3	1.98	0.63
1:C:356:MET:HE3	1:C:360:VAL:HG12	1.81	0.62
1:C:377:SER:HB3	1:C:380:ALA:HB3	1.81	0.62
1:D:194:ILE:HG22	1:D:194:ILE:O	1.98	0.62
1:B:129:GLY:HA2	1:B:248:PHE:HB2	1.81	0.62
1:D:253:ALA:HB2	1:B:428:PHE:O	1.99	0.62
1:A:175:ARG:NH1	1:A:434:LYS:HG3	2.12	0.62
1:B:132:SER:OG	1:B:244:LEU:HA	1.99	0.62
1:C:182:LEU:HD12	1:C:432:HIS:CE1	2.34	0.62
1:A:177:THR:OG1	1:A:242:PRO:HG2	1.99	0.62
1:C:99:LEU:HD21	1:C:197:LEU:HD13	1.81	0.62
1:D:207:ALA:HA	1:D:212:LEU:HB2	1.80	0.62
1:D:222:LEU:O	1:D:226:MET:HG2	1.99	0.62
1:D:418:PRO:HD3	1:D:438:MET:CE	2.30	0.62
1:B:134:ALA:HB2	1:B:248:PHE:CE1	2.35	0.62
1:C:159:LEU:HB3	1:C:160:PRO:HD3	1.82	0.62
1:C:237:TYR:O	1:C:241:LYS:HB3	2.00	0.61
1:D:259:LYS:O	1:D:259:LYS:HG3	1.99	0.61
1:D:341:THR:O	1:D:345:LEU:HG	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ASP:OD1	1:A:261:LYS:HG3	1.99	0.61
1:B:222:LEU:O	1:B:226:MET:HG2	1.98	0.61
1:C:171:ALA:HB3	1:C:174:GLN:CB	2.30	0.61
1:A:127:ALA:CB	1:A:133:VAL:HG11	2.25	0.61
1:A:159:LEU:HB3	1:A:160:PRO:HD3	1.83	0.61
1:D:127:ALA:CB	1:D:133:VAL:HG13	2.28	0.61
1:C:201:PRO:HG2	1:C:379:THR:HG21	1.83	0.61
1:D:196:THR:OG1	1:D:198:VAL:O	2.18	0.61
1:A:422:PRO:HB2	1:A:423:PRO:HD3	1.81	0.61
1:C:365:VAL:HG22	1:C:389:PHE:HE1	1.65	0.61
1:C:175:ARG:O	1:C:178:TYR:N	2.27	0.61
1:B:421:THR:CG2	1:B:423:PRO:HD2	2.10	0.61
1:C:141:VAL:HG12	1:C:158:MET:HE2	1.83	0.61
1:C:210:VAL:CG2	1:C:212:LEU:HG	2.31	0.61
1:D:131:MET:O	1:D:135:VAL:HG22	2.01	0.61
1:D:159:LEU:HB3	1:D:160:PRO:HD3	1.83	0.61
1:C:171:ALA:CB	1:C:174:GLN:HB2	2.31	0.60
1:C:418:PRO:O	1:C:419:VAL:HG12	2.00	0.60
1:D:239:LEU:O	1:D:240:LEU:HB2	2.01	0.60
1:C:79:PHE:HA	1:D:288:PHE:CE1	2.36	0.60
1:A:259:LYS:O	1:A:259:LYS:HG3	1.99	0.60
1:A:179:VAL:HB	1:A:432:HIS:CE1	2.36	0.60
1:D:222:LEU:HB3	1:D:223:PRO:HD3	1.83	0.60
1:D:453:LEU:O	1:D:457:ALA:N	2.21	0.60
1:B:108:ALA:HB2	1:B:317:THR:HB	1.83	0.60
1:B:359:PHE:HA	1:B:458:MET:HE1	1.83	0.60
1:A:138:LEU:CD1	1:A:162:VAL:HG22	2.30	0.60
1:A:377:SER:HB3	1:A:380:ALA:HB3	1.83	0.60
1:B:377:SER:HB3	1:B:380:ALA:CB	2.32	0.60
1:C:214:PHE:CD2	1:C:275:TRP:HB3	2.37	0.60
1:D:229:LEU:HB3	1:D:230:PRO:HD3	1.84	0.60
1:D:359:PHE:HE2	1:D:363:LEU:HD22	1.67	0.60
1:A:262:VAL:O	1:A:266:GLY:N	2.32	0.59
1:B:241:LYS:HZ1	1:B:244:LEU:HB2	1.67	0.59
1:C:113:GLN:O	1:C:261:LYS:HE2	2.03	0.59
1:A:201:PRO:O	1:A:205:ILE:HG13	2.02	0.59
1:A:418:PRO:C	1:A:420:ALA:H	2.10	0.59
1:B:159:LEU:HB3	1:B:160:PRO:HD3	1.84	0.59
1:A:106:LEU:HA	1:A:303:LEU:HD11	1.83	0.59
1:B:207:ALA:HA	1:B:212:LEU:HB2	1.83	0.59
1:D:452:LEU:HD11	1:D:456:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:CD1	1:A:178:TYR:HD1	2.14	0.59
1:D:362:ILE:HD11	1:D:454:THR:HG23	1.84	0.59
1:C:150:SER:HB3	1:C:153:ALA:HB3	1.85	0.59
1:C:226:MET:HE2	1:C:226:MET:HA	1.85	0.59
1:A:104:PHE:CD1	1:A:318:ALA:HA	2.38	0.59
1:A:113:GLN:O	1:A:261:LYS:HE2	2.03	0.59
1:C:422:PRO:HB2	1:C:423:PRO:HD3	1.85	0.59
1:A:124:LEU:HD12	1:A:137:MET:SD	2.42	0.59
1:B:349:LEU:O	1:B:353:VAL:HG22	2.02	0.59
1:C:65:HIS:CD2	1:D:311:TRP:HB3	2.37	0.59
1:C:201:PRO:O	1:C:205:ILE:HG13	2.02	0.59
1:D:251:ASP:O	1:D:252:ARG:HB3	2.03	0.58
1:B:222:LEU:HB3	1:B:223:PRO:HD3	1.85	0.58
1:B:162:VAL:HG11	1:B:182:LEU:HD23	1.84	0.58
1:B:241:LYS:NZ	1:B:244:LEU:HB2	2.17	0.58
1:A:172:ASP:O	1:A:175:ARG:HG3	2.03	0.58
1:C:104:PHE:CD1	1:C:318:ALA:HA	2.39	0.58
1:A:222:LEU:HB3	1:A:223:PRO:HD3	1.86	0.58
1:B:241:LYS:HG3	1:B:241:LYS:O	2.03	0.57
1:C:75:VAL:HG11	1:D:301:LEU:HD11	1.85	0.57
1:C:127:ALA:HB1	1:C:133:VAL:HG13	1.85	0.57
1:B:214:PHE:CD2	1:B:275:TRP:HB3	2.40	0.57
1:B:340:GLY:O	1:B:343:VAL:HG12	2.04	0.57
1:C:85:THR:O	1:C:89:LEU:HD13	2.04	0.57
1:C:152:THR:OG1	1:C:422:PRO:HG2	2.04	0.57
1:B:177:THR:HA	1:B:242:PRO:HD2	1.86	0.57
1:A:42:GLU:OE1	1:A:44:ASN:HB2	2.05	0.57
1:A:359:PHE:CE2	1:A:363:LEU:HD22	2.36	0.57
1:C:358:ILE:O	1:C:362:ILE:HG23	2.04	0.57
1:D:32:PHE:CD1	1:D:50:SER:HB3	2.40	0.57
1:D:422:PRO:HB2	1:D:423:PRO:HD3	1.86	0.57
1:C:108:ALA:HB2	1:C:317:THR:HB	1.86	0.57
1:C:359:PHE:HA	1:C:458:MET:CE	2.29	0.57
1:A:109:ALA:HB2	1:A:303:LEU:HD13	1.86	0.57
1:D:99:LEU:HD12	1:D:296:ALA:HB2	1.86	0.56
1:A:175:ARG:HG2	1:A:432:HIS:NE2	2.20	0.56
1:D:365:VAL:O	1:D:369:VAL:HG22	2.05	0.56
1:A:108:ALA:HB2	1:A:317:THR:HB	1.86	0.56
1:B:174:GLN:NE2	1:B:177:THR:OG1	2.38	0.56
1:C:42:GLU:OE1	1:C:44:ASN:HB2	2.05	0.56
1:D:210:VAL:HG23	1:D:212:LEU:HG	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:LEU:CD1	1:D:75:VAL:HG11	2.31	0.56
1:A:183:LEU:HD11	1:A:438:MET:SD	2.46	0.56
1:B:70:ALA:O	1:B:74:PRO:HD3	2.06	0.56
1:D:110:MET:HB2	1:D:115:LEU:HB3	1.88	0.56
1:B:418:PRO:HD3	1:B:438:MET:CE	2.35	0.56
1:C:222:LEU:HB3	1:C:223:PRO:HD3	1.88	0.56
1:C:311:TRP:HB3	1:D:65:HIS:CD2	2.40	0.56
1:D:201:PRO:O	1:D:205:ILE:HG13	2.05	0.56
1:A:417:LEU:HD23	1:A:417:LEU:H	1.71	0.56
1:B:210:VAL:HG23	1:B:212:LEU:HG	1.88	0.56
1:B:191:ILE:HG12	1:B:228:MET:CE	2.33	0.56
1:B:194:ILE:HD11	1:B:412:SER:HB2	1.87	0.56
1:B:417:LEU:HD23	1:B:417:LEU:H	1.70	0.56
1:D:360:VAL:O	1:D:364:VAL:HG23	2.06	0.56
1:C:307:ARG:NH2	1:D:21:ASN:HD22	2.04	0.55
1:C:108:ALA:HB2	1:C:317:THR:CB	2.37	0.55
1:C:417:LEU:HD23	1:C:417:LEU:H	1.71	0.55
1:D:362:ILE:HD11	1:D:458:MET:HE2	1.88	0.55
1:B:175:ARG:O	1:B:178:TYR:N	2.27	0.55
1:C:39:LEU:HD22	1:C:41:PHE:HE2	1.71	0.55
1:D:191:ILE:HG12	1:D:228:MET:HE2	1.88	0.55
1:D:362:ILE:CD1	1:D:454:THR:HG23	2.37	0.55
1:D:113:GLN:NE2	1:D:259:LYS:O	2.40	0.55
1:D:251:ASP:OD1	1:B:435:GLN:N	2.40	0.55
1:A:55:ILE:HD11	1:A:76:MET:HE3	1.89	0.55
1:B:56:ALA:HA	1:B:384:LEU:HD22	1.88	0.55
1:C:158:MET:O	1:C:162:VAL:HG23	2.07	0.55
1:A:47:LEU:HD21	1:A:82:ILE:HD11	1.87	0.55
1:C:113:GLN:NE2	1:C:259:LYS:O	2.39	0.55
1:C:193:GLY:O	1:C:203:ASN:ND2	2.38	0.55
1:D:152:THR:HG23	1:D:422:PRO:HB2	1.89	0.54
1:B:341:THR:O	1:B:345:LEU:HG	2.07	0.54
1:C:377:SER:HB3	1:C:380:ALA:CB	2.37	0.54
1:A:187:TYR:OH	1:A:415:PHE:O	2.18	0.54
1:B:303:LEU:HB3	1:B:309:VAL:CG1	2.36	0.54
1:B:422:PRO:HB2	1:B:423:PRO:HD3	1.90	0.54
1:D:102:GLY:HA3	1:D:296:ALA:HB1	1.88	0.54
1:A:183:LEU:HD22	1:A:433:ILE:HD11	1.88	0.54
1:D:59:TRP:NE1	1:D:69:THR:HB	2.23	0.54
1:A:130:LYS:O	1:A:133:VAL:HG12	2.07	0.54
1:D:102:GLY:HA2	1:D:300:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:LEU:O	1:D:407:ILE:HG13	2.08	0.54
1:A:417:LEU:HB2	1:A:418:PRO:HD2	1.89	0.54
1:D:29:VAL:HA	1:D:54:PHE:HE1	1.73	0.54
1:D:417:LEU:HD23	1:D:417:LEU:H	1.71	0.54
1:C:241:LYS:O	1:C:241:LYS:HG3	2.06	0.54
1:A:39:LEU:HB2	1:A:46:VAL:HG13	1.88	0.54
1:B:175:ARG:HH22	1:B:434:LYS:HE3	1.73	0.54
1:C:66:VAL:CG1	1:C:325:LEU:HD13	2.36	0.53
1:C:394:GLU:OE2	1:C:400:PRO:HG3	2.08	0.53
1:D:150:SER:HB3	1:D:153:ALA:HB3	1.90	0.53
1:B:99:LEU:HD21	1:B:197:LEU:HD13	1.91	0.53
1:D:147:MET:O	1:D:196:THR:OG1	2.26	0.53
1:B:176:SER:HB2	1:B:240:LEU:O	2.07	0.53
1:B:418:PRO:C	1:B:420:ALA:H	2.16	0.53
1:A:140:GLY:O	1:A:144:LEU:HB2	2.08	0.53
1:C:369:VAL:HG12	1:C:385:LEU:HD12	1.89	0.53
1:D:414:ALA:CB	1:D:420:ALA:HB1	2.37	0.53
1:A:32:PHE:HB2	1:A:54:PHE:HD1	1.72	0.53
1:A:229:LEU:HB3	1:A:230:PRO:HD3	1.90	0.53
1:D:129:GLY:HA2	1:D:248:PHE:HB2	1.90	0.53
1:D:346:ALA:HA	1:D:396:PHE:CZ	2.44	0.53
1:A:92:PHE:CD2	1:A:327:GLY:HA3	2.44	0.53
1:C:415:PHE:CG	1:C:445:LEU:HD23	2.44	0.53
1:D:197:LEU:HD23	1:D:197:LEU:O	2.09	0.53
1:A:28:ASP:OD2	1:A:57:VAL:HB	2.09	0.53
1:C:99:LEU:CD2	1:C:197:LEU:HD13	2.39	0.53
1:A:461:TRP:HE3	1:A:462:GLN:HG3	1.74	0.53
1:B:152:THR:HG23	1:B:422:PRO:HB2	1.90	0.53
1:C:103:GLY:HA3	1:C:198:VAL:HG11	1.91	0.53
1:A:175:ARG:HG2	1:A:432:HIS:CD2	2.44	0.53
1:A:237:TYR:CE2	1:A:241:LYS:HE2	2.44	0.53
1:C:65:HIS:HB3	1:C:68:VAL:HG23	1.89	0.53
1:B:99:LEU:CD2	1:B:197:LEU:HD13	2.39	0.53
1:B:294:LEU:O	1:B:298:GLY:N	2.29	0.53
1:C:174:GLN:HG3	1:C:177:THR:HB	1.90	0.52
1:C:294:LEU:HD21	1:D:78:VAL:HG11	1.91	0.52
1:C:393:ALA:HB2	1:C:403:LEU:HD12	1.90	0.52
1:C:418:PRO:C	1:C:420:ALA:H	2.17	0.52
1:D:179:VAL:CG2	1:D:433:ILE:HD12	2.38	0.52
1:C:403:LEU:O	1:C:407:ILE:HG13	2.09	0.52
1:D:251:ASP:O	1:B:434:LYS:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ALA:HA	1:A:314:ILE:HG12	1.91	0.52
1:A:108:ALA:HB2	1:A:317:THR:CB	2.40	0.52
1:B:207:ALA:HA	1:B:212:LEU:HD12	1.91	0.52
1:D:369:VAL:HA	1:D:372:LEU:HB3	1.90	0.52
1:A:113:GLN:HG3	1:A:261:LYS:HG2	1.92	0.52
1:A:403:LEU:O	1:A:407:ILE:HG13	2.08	0.52
1:B:104:PHE:CD1	1:B:318:ALA:HA	2.45	0.52
1:D:369:VAL:HG12	1:D:385:LEU:HD12	1.92	0.52
1:B:117:LYS:HD3	1:B:157:MET:CE	2.39	0.52
1:C:422:PRO:O	1:C:426:ILE:N	2.42	0.52
1:B:204:ALA:HB3	1:B:326:PHE:CZ	2.45	0.52
1:B:362:ILE:HD11	1:B:458:MET:HE2	1.92	0.52
1:A:65:HIS:CD2	1:B:311:TRP:HB3	2.44	0.52
1:C:340:GLY:O	1:C:343:VAL:HG12	2.10	0.52
1:A:105:ALA:HB3	1:A:300:ILE:HG12	1.91	0.52
1:B:118:VAL:HA	1:B:255:VAL:HG11	1.91	0.52
1:C:138:LEU:HD13	1:C:162:VAL:HG22	1.91	0.52
1:A:59:TRP:NE1	1:A:69:THR:HB	2.25	0.52
1:D:108:ALA:HB2	1:D:317:THR:CB	2.40	0.51
1:D:179:VAL:HG23	1:D:433:ILE:HB	1.92	0.51
1:B:303:LEU:HB3	1:B:309:VAL:HG12	1.92	0.51
1:D:59:TRP:HE1	1:D:69:THR:HB	1.75	0.51
1:A:47:LEU:HD11	1:A:80:PHE:CD1	2.45	0.51
1:B:130:LYS:HB2	1:B:133:VAL:CG1	2.26	0.51
1:C:229:LEU:HB3	1:C:230:PRO:HD3	1.93	0.51
1:D:418:PRO:C	1:D:420:ALA:H	2.19	0.51
1:D:343:VAL:HA	1:D:395:ALA:CB	2.40	0.51
1:D:416:MET:O	1:D:438:MET:HG2	2.11	0.51
1:A:369:VAL:HG12	1:A:385:LEU:HD12	1.92	0.51
1:B:357:GLY:O	1:B:361:VAL:HG23	2.09	0.51
1:C:417:LEU:HB2	1:C:418:PRO:HD2	1.92	0.51
1:A:210:VAL:HG23	1:A:212:LEU:HG	1.91	0.51
1:B:207:ALA:CB	1:B:212:LEU:HB2	2.41	0.51
1:B:206:ALA:HB2	1:B:408:ALA:HB2	1.93	0.51
1:B:229:LEU:HB3	1:B:230:PRO:HD3	1.91	0.51
1:C:152:THR:HG23	1:C:422:PRO:HB2	1.93	0.51
1:C:278:SER:HB2	1:C:291:PHE:HD2	1.76	0.51
1:D:366:ALA:O	1:D:370:VAL:HG23	2.11	0.51
1:A:201:PRO:HB2	1:A:379:THR:CG2	2.41	0.51
1:C:142:THR:OG1	1:C:158:MET:HG3	2.10	0.51
1:D:320:TRP:CE3	1:D:323:LEU:HD12	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:SER:HB3	1:D:380:ALA:CB	2.41	0.51
1:C:167:SER:HA	1:C:170:ASP:CG	2.36	0.51
1:D:47:LEU:HD21	1:D:82:ILE:HD11	1.93	0.51
1:B:45:VAL:HG11	1:B:344:PHE:CD1	2.46	0.51
1:D:54:PHE:CD2	1:D:76:MET:HE1	2.46	0.50
1:B:55:ILE:HD11	1:B:76:MET:HE3	1.93	0.50
1:C:369:VAL:HG21	1:C:410:ALA:HB3	1.93	0.50
1:D:417:LEU:HB2	1:D:418:PRO:HD2	1.91	0.50
1:A:120:ALA:O	1:A:124:LEU:HB2	2.10	0.50
1:A:237:TYR:CZ	1:A:241:LYS:HE2	2.46	0.50
1:A:191:ILE:HG12	1:A:228:MET:HE2	1.92	0.50
1:A:240:LEU:O	1:A:242:PRO:HD3	2.12	0.50
1:A:304:SER:CB	1:B:68:VAL:HG11	2.41	0.50
1:A:370:VAL:CG2	1:A:410:ALA:HB1	2.42	0.50
1:B:267:ILE:CD1	1:B:303:LEU:HD23	2.41	0.50
1:C:56:ALA:HA	1:C:384:LEU:HD22	1.93	0.50
1:A:28:ASP:OD1	1:A:58:LEU:HD13	2.11	0.50
1:A:65:HIS:HD2	1:B:311:TRP:HB3	1.77	0.50
1:D:115:LEU:HD21	1:D:265:LEU:HD23	1.94	0.50
1:A:174:GLN:HA	1:A:174:GLN:OE1	2.10	0.50
1:B:366:ALA:O	1:B:370:VAL:HG23	2.12	0.50
1:A:123:VAL:O	1:A:137:MET:HE2	2.12	0.50
1:A:206:ALA:HB2	1:A:408:ALA:HB2	1.93	0.50
1:A:222:LEU:O	1:A:226:MET:HG2	2.12	0.50
1:B:174:GLN:HG3	1:B:177:THR:HB	1.94	0.50
1:B:414:ALA:HB1	1:B:420:ALA:HB1	1.94	0.50
1:B:416:MET:O	1:B:438:MET:HG2	2.12	0.50
1:A:102:GLY:HA2	1:A:300:ILE:HD11	1.94	0.50
1:C:146:SER:HA	1:C:150:SER:O	2.11	0.50
1:D:342:SER:OG	1:D:391:THR:HB	2.11	0.49
1:D:359:PHE:CD1	1:D:458:MET:HE3	2.47	0.49
1:D:446:ASN:O	1:D:450:ILE:HG13	2.12	0.49
1:D:72:LEU:HA	1:D:75:VAL:HG12	1.93	0.49
1:D:204:ALA:HB3	1:D:326:PHE:CZ	2.47	0.49
1:A:127:ALA:CB	1:A:137:MET:CE	2.91	0.49
1:A:358:ILE:O	1:A:362:ILE:HG23	2.12	0.49
1:B:127:ALA:HB1	1:B:133:VAL:HG13	1.95	0.49
1:C:207:ALA:HA	1:C:212:LEU:HB2	1.94	0.49
1:A:133:VAL:O	1:A:133:VAL:HG22	2.12	0.49
1:A:303:LEU:HB3	1:A:309:VAL:HG12	1.95	0.49
1:A:21:ASN:HB3	1:A:63:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LEU:HB3	1:B:178:TYR:CD1	2.43	0.49
1:B:187:TYR:OH	1:B:415:PHE:O	2.25	0.49
1:A:356:MET:CE	1:A:360:VAL:HG12	2.43	0.49
1:A:359:PHE:HA	1:A:458:MET:HE1	1.93	0.49
1:B:182:LEU:HD12	1:B:432:HIS:HE1	1.75	0.49
1:B:279:SER:HB3	1:B:280:PRO:HD3	1.95	0.49
1:C:172:ASP:C	1:C:174:GLN:H	2.21	0.49
1:C:311:TRP:NE1	1:C:315:GLN:OE1	2.46	0.49
1:D:194:ILE:O	1:D:221:GLY:HA3	2.12	0.49
1:D:349:LEU:HB3	1:D:353:VAL:CG1	2.39	0.49
1:A:25:VAL:HG23	1:A:63:ALA:HB1	1.94	0.49
1:B:346:ALA:HB2	1:B:395:ALA:HB3	1.94	0.49
1:B:362:ILE:HD12	1:B:457:ALA:HB3	1.93	0.49
1:C:262:VAL:O	1:C:266:GLY:N	2.40	0.49
1:D:113:GLN:O	1:D:261:LYS:HE2	2.13	0.49
1:D:443:LEU:O	1:D:447:ILE:HD12	2.13	0.49
1:A:356:MET:HB3	1:A:360:VAL:HB	1.94	0.49
1:B:99:LEU:HD12	1:B:296:ALA:HB2	1.94	0.49
1:B:421:THR:HG22	1:B:423:PRO:CD	2.11	0.49
1:D:168:LYS:HG2	1:D:249:GLU:HG2	1.94	0.49
1:B:92:PHE:CD2	1:B:327:GLY:HA3	2.48	0.49
1:D:72:LEU:HD12	1:D:75:VAL:CG1	2.43	0.49
1:D:131:MET:HE1	1:D:166:LEU:CD2	2.43	0.49
1:B:113:GLN:NE2	1:B:259:LYS:O	2.46	0.49
1:D:147:MET:HG2	1:D:195:ALA:HB3	1.95	0.49
1:D:267:ILE:CD1	1:D:303:LEU:HD23	2.43	0.49
1:B:201:PRO:O	1:B:205:ILE:HG13	2.13	0.49
1:C:359:PHE:HE2	1:C:363:LEU:HD22	1.77	0.48
1:B:342:SER:OG	1:B:391:THR:HB	2.14	0.48
1:C:115:LEU:HD21	1:C:265:LEU:HD23	1.94	0.48
1:B:231:MET:HE3	1:B:445:LEU:HD12	1.94	0.48
1:C:182:LEU:HD12	1:C:432:HIS:HE1	1.78	0.48
1:C:311:TRP:HB3	1:D:65:HIS:HD2	1.75	0.48
1:D:168:LYS:CE	1:D:249:GLU:HB3	2.39	0.48
1:B:129:GLY:C	1:B:248:PHE:HD1	2.21	0.48
1:B:201:PRO:CG	1:B:379:THR:HG21	2.41	0.48
1:C:152:THR:HG23	1:C:422:PRO:CB	2.43	0.48
1:A:74:PRO:HG2	1:A:92:PHE:CE1	2.49	0.48
1:A:241:LYS:O	1:A:241:LYS:HG3	2.13	0.48
1:C:352:MET:HE3	1:C:352:MET:HB2	1.76	0.48
1:C:356:MET:CE	1:C:360:VAL:HG12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:ALA:O	1:D:300:ILE:HG13	2.14	0.48
1:A:340:GLY:O	1:A:343:VAL:HG12	2.14	0.48
1:C:341:THR:O	1:C:345:LEU:HG	2.14	0.48
1:C:365:VAL:HG22	1:C:389:PHE:CE1	2.46	0.48
1:D:182:LEU:HD12	1:D:432:HIS:HE1	1.73	0.48
1:A:183:LEU:HD21	1:A:438:MET:HG3	1.96	0.48
1:A:418:PRO:O	1:A:419:VAL:CG1	2.59	0.48
1:D:359:PHE:CE2	1:D:363:LEU:HD22	2.47	0.48
1:B:24:ILE:O	1:B:28:ASP:HB2	2.13	0.48
1:B:172:ASP:OD1	1:B:173:LYS:N	2.47	0.48
1:C:428:PHE:HA	1:C:433:ILE:CG2	2.44	0.47
1:A:102:GLY:HA3	1:A:296:ALA:HB1	1.95	0.47
1:C:155:ALA:HB3	1:C:426:ILE:HD12	1.96	0.47
1:C:99:LEU:HA	1:C:296:ALA:CB	2.45	0.47
1:A:155:ALA:HB3	1:A:426:ILE:CD1	2.43	0.47
1:C:89:LEU:HD23	1:D:95:SER:HA	1.97	0.47
1:A:360:VAL:O	1:A:364:VAL:HG23	2.14	0.47
1:C:418:PRO:O	1:C:419:VAL:CG1	2.62	0.47
1:B:110:MET:HB2	1:B:115:LEU:HB3	1.97	0.47
1:B:204:ALA:HB3	1:B:326:PHE:CE1	2.49	0.47
1:D:174:GLN:OE1	1:D:174:GLN:HA	2.13	0.47
1:D:278:SER:HB2	1:D:291:PHE:HD2	1.80	0.47
1:A:394:GLU:OE2	1:A:400:PRO:HG3	2.14	0.47
1:B:139:PHE:CE2	1:B:184:GLY:HA3	2.49	0.47
1:C:139:PHE:CE2	1:C:184:GLY:HA3	2.50	0.47
1:A:191:ILE:HG12	1:A:228:MET:CE	2.43	0.47
1:C:35:LEU:CD2	1:C:39:LEU:HD11	2.42	0.47
1:C:175:ARG:O	1:C:179:VAL:N	2.48	0.47
1:D:201:PRO:CG	1:D:379:THR:HG21	2.41	0.47
1:D:390:ALA:HB1	1:D:400:PRO:HB2	1.97	0.47
1:A:150:SER:OG	1:A:151:ASN:N	2.47	0.47
1:A:393:ALA:HB1	1:A:398:MET:HE3	1.96	0.47
1:B:417:LEU:HB2	1:B:418:PRO:HD2	1.97	0.47
1:C:349:LEU:O	1:C:353:VAL:HG22	2.15	0.47
1:B:237:TYR:CD2	1:B:241:LYS:HG2	2.49	0.47
1:C:236:LEU:CD2	1:C:441:VAL:HG11	2.40	0.46
1:A:133:VAL:O	1:A:137:MET:HB2	2.15	0.46
1:A:310:HIS:O	1:A:313:GLU:HB2	2.15	0.46
1:C:59:TRP:NE1	1:C:69:THR:HB	2.30	0.46
1:D:40:PRO:HD2	1:D:41:PHE:CE2	2.50	0.46
1:A:147:MET:O	1:A:196:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:LYS:O	1:D:126:MET:HG2	2.15	0.46
1:D:177:THR:OG1	1:D:242:PRO:HG2	2.14	0.46
1:A:24:ILE:HG21	1:A:61:THR:CB	2.45	0.46
1:A:179:VAL:CA	1:A:432:HIS:HE1	2.27	0.46
1:A:127:ALA:HB2	1:A:137:MET:CE	2.44	0.46
1:B:98:PHE:HB3	1:B:297:LEU:HD21	1.97	0.46
1:D:150:SER:OG	1:D:151:ASN:N	2.49	0.46
1:A:74:PRO:HG2	1:A:92:PHE:CZ	2.50	0.46
1:A:461:TRP:CE3	1:A:462:GLN:HG3	2.51	0.46
1:B:418:PRO:O	1:B:419:VAL:HB	2.16	0.46
1:C:70:ALA:O	1:C:74:PRO:HD3	2.16	0.46
1:C:93:ALA:HB2	1:D:93:ALA:HB2	1.98	0.46
1:C:419:VAL:O	1:C:419:VAL:HG22	2.15	0.46
1:D:386:ILE:HB	1:D:387:PRO:HD3	1.97	0.46
1:A:303:LEU:HB3	1:A:309:VAL:CG1	2.46	0.46
1:B:267:ILE:HD12	1:B:303:LEU:HD23	1.96	0.46
1:C:303:LEU:HB3	1:C:309:VAL:CG1	2.46	0.46
1:D:32:PHE:CE1	1:D:50:SER:HB3	2.51	0.46
1:D:241:LYS:O	1:D:241:LYS:HG3	2.16	0.46
1:A:377:SER:HB3	1:A:380:ALA:CB	2.44	0.46
1:B:138:LEU:HD13	1:B:162:VAL:HG22	1.98	0.46
1:D:365:VAL:HG22	1:D:389:PHE:HE1	1.81	0.46
1:A:172:ASP:OD1	1:A:173:LYS:N	2.48	0.46
1:A:418:PRO:HD3	1:A:438:MET:CE	2.46	0.46
1:C:369:VAL:HG23	1:C:410:ALA:HB1	1.97	0.45
1:A:72:LEU:HA	1:A:75:VAL:HG12	1.98	0.45
1:C:183:LEU:HD11	1:C:438:MET:SD	2.56	0.45
1:B:122:LYS:O	1:B:126:MET:HG2	2.16	0.45
1:D:55:ILE:HD11	1:D:76:MET:HE3	1.97	0.45
1:D:139:PHE:CE2	1:D:184:GLY:HA3	2.51	0.45
1:A:70:ALA:O	1:A:74:PRO:HD3	2.16	0.45
1:D:194:ILE:O	1:D:194:ILE:CG2	2.64	0.45
1:D:393:ALA:CB	1:D:398:MET:HE3	2.47	0.45
1:A:56:ALA:HA	1:A:384:LEU:HD22	1.98	0.45
1:A:109:ALA:HB2	1:A:309:VAL:HG11	1.98	0.45
1:A:341:THR:O	1:A:345:LEU:HG	2.16	0.45
1:D:418:PRO:O	1:D:419:VAL:CG1	2.56	0.45
1:D:461:TRP:C	1:D:461:TRP:CE3	2.95	0.45
1:A:418:PRO:C	1:A:420:ALA:N	2.74	0.45
1:A:418:PRO:HD3	1:A:438:MET:HE3	1.97	0.45
1:B:115:LEU:HD21	1:B:265:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:SER:OG	1:B:151:ASN:N	2.50	0.45
1:C:47:LEU:HD11	1:C:80:PHE:CD1	2.52	0.45
1:C:182:LEU:O	1:C:427:VAL:HG11	2.17	0.45
1:C:432:HIS:CG	1:C:433:ILE:N	2.84	0.45
1:D:207:ALA:CB	1:D:212:LEU:HB2	2.46	0.45
1:B:259:LYS:HE3	1:B:259:LYS:HB2	1.86	0.45
1:C:150:SER:OG	1:C:151:ASN:N	2.50	0.45
1:D:194:ILE:HA	1:D:217:TRP:HH2	1.81	0.45
1:D:152:THR:OG1	1:D:422:PRO:HG2	2.16	0.45
1:C:421:THR:CG2	1:C:422:PRO:HD2	2.46	0.45
1:A:309:VAL:CG2	1:A:313:GLU:HB2	2.46	0.45
1:B:171:ALA:HB3	1:B:174:GLN:CB	2.46	0.45
1:D:70:ALA:O	1:D:74:PRO:HD3	2.17	0.45
1:D:175:ARG:NH1	1:D:434:LYS:HG3	2.26	0.45
1:D:393:ALA:HB2	1:D:403:LEU:HD12	1.98	0.45
1:A:24:ILE:HD13	1:A:61:THR:HB	1.98	0.45
1:A:106:LEU:O	1:A:110:MET:HG2	2.17	0.45
1:B:171:ALA:HB3	1:B:174:GLN:HB2	1.98	0.45
1:C:133:VAL:HG22	1:C:133:VAL:O	2.17	0.44
1:A:186:ALA:HB2	1:A:427:VAL:CG2	2.47	0.44
1:B:172:ASP:O	1:B:175:ARG:HG3	2.16	0.44
1:A:109:ALA:HB1	1:A:303:LEU:HD22	1.98	0.44
1:A:151:ASN:HD21	1:A:193:GLY:HA3	1.82	0.44
1:A:311:TRP:CZ2	1:B:67:THR:HG21	2.52	0.44
1:A:370:VAL:HG23	1:A:410:ALA:HB1	1.99	0.44
1:B:21:ASN:HB3	1:B:63:ALA:HB1	1.99	0.44
1:C:65:HIS:HD2	1:D:311:TRP:HB3	1.82	0.44
1:C:110:MET:HB2	1:C:115:LEU:HB3	1.98	0.44
1:B:212:LEU:HD13	1:B:217:TRP:HD1	1.82	0.44
1:C:279:SER:HB3	1:C:280:PRO:HD3	1.99	0.44
1:D:108:ALA:HB2	1:D:317:THR:HB	1.99	0.44
1:D:253:ALA:HB3	1:B:431:GLY:CA	2.35	0.44
1:A:32:PHE:CD1	1:A:50:SER:HB3	2.53	0.44
1:B:183:LEU:HD13	1:B:433:ILE:HD13	1.99	0.44
1:C:194:ILE:O	1:C:194:ILE:CG2	2.64	0.44
1:C:201:PRO:HB2	1:C:379:THR:CG2	2.48	0.44
1:C:356:MET:HE2	1:C:361:VAL:HA	2.00	0.44
1:A:309:VAL:HG22	1:A:313:GLU:HB2	1.98	0.44
1:B:210:VAL:CG2	1:B:212:LEU:HG	2.48	0.44
1:C:138:LEU:HD23	1:C:138:LEU:HA	1.90	0.44
1:D:274:LEU:HD23	1:D:281:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:SER:HB3	1:A:280:PRO:HD3	1.99	0.44
1:A:369:VAL:HG11	1:A:407:ILE:HG23	1.98	0.44
1:B:201:PRO:HB2	1:B:379:THR:CG2	2.47	0.44
1:A:144:LEU:HD23	1:A:144:LEU:O	2.18	0.44
1:A:349:LEU:HB3	1:A:353:VAL:HG13	2.00	0.44
1:A:352:MET:HE3	1:A:352:MET:HB2	1.78	0.44
1:B:31:LEU:HD11	1:B:35:LEU:HD11	1.99	0.44
1:B:207:ALA:CA	1:B:212:LEU:HB2	2.46	0.44
1:D:72:LEU:HA	1:D:75:VAL:CG1	2.48	0.44
1:A:85:THR:OG1	1:B:289:LYS:HB3	2.18	0.43
1:A:369:VAL:HG21	1:A:410:ALA:HB3	1.99	0.43
1:C:166:LEU:HD13	1:C:178:TYR:HA	2.01	0.43
1:A:307:ARG:NH1	1:B:63:ALA:O	2.36	0.43
1:A:461:TRP:HZ3	1:A:462:GLN:HE21	1.66	0.43
1:B:174:GLN:OE1	1:B:174:GLN:HA	2.17	0.43
1:C:443:LEU:O	1:C:447:ILE:HD12	2.18	0.43
1:D:346:ALA:HA	1:D:396:PHE:CE2	2.53	0.43
1:A:25:VAL:HG23	1:A:63:ALA:CB	2.48	0.43
1:B:129:GLY:HA2	1:B:248:PHE:CD1	2.53	0.43
1:B:133:VAL:HG22	1:B:133:VAL:O	2.18	0.43
1:B:151:ASN:ND2	1:B:189:ALA:O	2.51	0.43
1:B:193:GLY:O	1:B:203:ASN:ND2	2.38	0.43
1:C:418:PRO:C	1:C:420:ALA:N	2.77	0.43
1:A:99:LEU:HA	1:A:296:ALA:CB	2.48	0.43
1:A:310:HIS:H	1:A:313:GLU:HG3	1.84	0.43
1:B:147:MET:O	1:B:196:THR:OG1	2.37	0.43
1:C:142:THR:O	1:C:154:THR:HG21	2.19	0.43
1:A:343:VAL:HG23	1:A:395:ALA:HB1	2.01	0.43
1:B:167:SER:HB3	1:B:249:GLU:OE2	2.18	0.43
1:D:71:ILE:O	1:D:74:PRO:HD2	2.18	0.43
1:D:279:SER:HB3	1:D:280:PRO:HD3	2.01	0.43
1:A:66:VAL:CG1	1:A:325:LEU:HD13	2.35	0.43
1:A:332:LEU:HD23	1:A:387:PRO:HG2	2.01	0.43
1:B:168:LYS:HD3	1:B:168:LYS:HA	1.90	0.43
1:B:172:ASP:C	1:B:174:GLN:N	2.77	0.43
1:B:194:ILE:O	1:B:194:ILE:CG2	2.65	0.43
1:C:85:THR:OG1	1:D:289:LYS:HB3	2.17	0.43
1:C:148:TRP:CH2	1:C:196:THR:HG21	2.54	0.43
1:B:237:TYR:CE2	1:B:241:LYS:HG2	2.54	0.43
1:C:71:ILE:O	1:C:74:PRO:HD2	2.19	0.43
1:C:362:ILE:CD1	1:C:454:THR:HG23	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ALA:HB1	1:C:420:ALA:CB	2.28	0.43
1:A:149:ILE:HG22	1:A:150:SER:N	2.34	0.43
1:A:179:VAL:HG23	1:A:433:ILE:HB	2.01	0.43
1:D:110:MET:CE	1:D:149:ILE:HG13	2.49	0.43
1:D:120:ALA:O	1:D:124:LEU:HB2	2.18	0.43
1:A:197:LEU:HD23	1:A:197:LEU:O	2.19	0.43
1:C:117:LYS:CD	1:C:157:MET:HE2	2.39	0.43
1:C:386:ILE:HB	1:C:387:PRO:HD3	2.01	0.43
1:C:416:MET:HG3	1:C:442:GLY:C	2.44	0.43
1:D:42:GLU:OE1	1:D:44:ASN:HB2	2.18	0.43
1:D:172:ASP:OD1	1:D:173:LYS:N	2.52	0.43
1:D:201:PRO:N	1:D:202:PRO:CD	2.82	0.43
1:A:194:ILE:O	1:A:194:ILE:CG2	2.65	0.43
1:B:237:TYR:CZ	1:B:241:LYS:HE2	2.54	0.43
1:B:296:ALA:O	1:B:300:ILE:HG13	2.18	0.43
1:D:210:VAL:CG2	1:D:212:LEU:HG	2.49	0.42
1:A:236:LEU:CD2	1:A:441:VAL:HG11	2.39	0.42
1:B:421:THR:CG2	1:B:422:PRO:HD2	2.48	0.42
1:C:85:THR:HG21	1:D:290:SER:H	1.84	0.42
1:D:237:TYR:CE2	1:D:241:LYS:HG2	2.54	0.42
1:A:201:PRO:CG	1:A:379:THR:HG21	2.46	0.42
1:B:349:LEU:O	1:B:353:VAL:HG13	2.19	0.42
1:C:74:PRO:O	1:C:78:VAL:HG23	2.19	0.42
1:D:265:LEU:HD13	1:D:265:LEU:O	2.20	0.42
1:A:393:ALA:CB	1:A:403:LEU:HD12	2.46	0.42
1:B:265:LEU:O	1:B:265:LEU:HD13	2.19	0.42
1:D:207:ALA:CA	1:D:212:LEU:HB2	2.47	0.42
1:A:45:VAL:O	1:A:49:ILE:HG12	2.19	0.42
1:A:93:ALA:HB2	1:B:93:ALA:HB2	2.00	0.42
1:A:303:LEU:O	1:A:308:VAL:HG12	2.19	0.42
1:B:47:LEU:HD11	1:B:80:PHE:CD1	2.54	0.42
1:B:71:ILE:O	1:B:74:PRO:HD2	2.19	0.42
1:B:106:LEU:HD12	1:B:303:LEU:HD11	2.00	0.42
1:B:277:PHE:O	1:B:280:PRO:HD2	2.19	0.42
1:B:346:ALA:CB	1:B:395:ALA:HB3	2.50	0.42
1:B:369:VAL:HG12	1:B:385:LEU:HD12	2.00	0.42
1:B:369:VAL:HG23	1:B:410:ALA:HB1	1.99	0.42
1:C:145:LEU:HD22	1:C:149:ILE:HD12	2.00	0.42
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.89	0.42
1:A:156:ALA:N	1:A:426:ILE:HD13	2.35	0.42
1:A:389:PHE:CG	1:A:407:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:TRP:C	1:D:461:TRP:HE3	2.27	0.42
1:B:131:MET:HA	1:B:134:ALA:HB3	2.01	0.42
1:C:274:LEU:O	1:C:278:SER:HB3	2.20	0.42
1:B:96:ILE:HG13	1:B:208:ALA:HA	2.02	0.42
1:B:352:MET:HB2	1:B:352:MET:HE3	1.81	0.42
1:B:393:ALA:HB2	1:B:403:LEU:HD12	2.01	0.42
1:B:418:PRO:HD3	1:B:438:MET:HE3	2.00	0.42
1:C:369:VAL:CG2	1:C:410:ALA:HB3	2.50	0.42
1:A:105:ALA:CB	1:A:300:ILE:HG12	2.49	0.42
1:B:74:PRO:HG2	1:B:92:PHE:CZ	2.55	0.42
1:C:241:LYS:O	1:C:241:LYS:CG	2.67	0.42
1:C:259:LYS:HE3	1:C:259:LYS:HB2	1.83	0.42
1:C:303:LEU:HB3	1:C:309:VAL:HG12	2.00	0.42
1:C:455:ALA:O	1:C:459:LEU:HG	2.18	0.42
1:D:149:ILE:HG22	1:D:150:SER:N	2.35	0.42
1:D:242:PRO:HD2	1:D:243:THR:HG23	2.01	0.42
1:D:365:VAL:HG22	1:D:389:PHE:CE1	2.55	0.42
1:D:186:ALA:HB2	1:D:427:VAL:HG11	2.01	0.42
1:D:393:ALA:O	1:D:398:MET:HB3	2.20	0.42
1:A:169:VAL:CG1	1:A:174:GLN:HG2	2.50	0.42
1:C:418:PRO:C	1:C:419:VAL:HG12	2.44	0.41
1:C:421:THR:HG22	1:C:422:PRO:HD2	2.01	0.41
1:D:421:THR:CG2	1:D:422:PRO:HD2	2.50	0.41
1:B:147:MET:HG2	1:B:195:ALA:HB3	2.01	0.41
1:B:179:VAL:HG23	1:B:433:ILE:HB	2.02	0.41
1:B:386:ILE:HB	1:B:387:PRO:HD3	2.02	0.41
1:D:105:ALA:HA	1:D:314:ILE:HG12	2.02	0.41
1:D:133:VAL:O	1:D:133:VAL:HG22	2.20	0.41
1:B:178:TYR:O	1:B:178:TYR:CG	2.74	0.41
1:B:197:LEU:HD21	1:B:204:ALA:HA	2.02	0.41
1:C:78:VAL:HG21	1:C:85:THR:HA	2.01	0.41
1:D:432:HIS:CG	1:D:433:ILE:N	2.88	0.41
1:A:418:PRO:C	1:A:419:VAL:HG12	2.45	0.41
1:B:65:HIS:HB3	1:B:68:VAL:HG23	2.02	0.41
1:B:71:ILE:HD11	1:B:324:LEU:HD23	2.02	0.41
1:B:360:VAL:O	1:B:364:VAL:HG23	2.20	0.41
1:C:418:PRO:N	1:C:438:MET:HE3	2.35	0.41
1:A:174:GLN:NE2	1:A:177:THR:OG1	2.46	0.41
1:A:418:PRO:O	1:A:420:ALA:N	2.53	0.41
1:B:42:GLU:OE1	1:B:44:ASN:HB2	2.21	0.41
1:C:149:ILE:HG22	1:C:150:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:ASP:C	1:D:174:GLN:N	2.78	0.41
1:B:202:PRO:HG3	1:B:379:THR:HA	2.01	0.41
1:C:369:VAL:HG23	1:C:410:ALA:CB	2.51	0.41
1:A:166:LEU:HD22	1:A:178:TYR:CD1	2.55	0.41
1:B:151:ASN:HD21	1:B:193:GLY:HA3	1.86	0.41
1:B:174:GLN:NE2	1:B:242:PRO:HB2	2.36	0.41
1:B:332:LEU:HD23	1:B:387:PRO:HG2	2.01	0.41
1:D:274:LEU:CD2	1:D:281:ILE:HD13	2.51	0.41
1:D:277:PHE:O	1:D:280:PRO:HD2	2.20	0.41
1:A:169:VAL:HG11	1:A:174:GLN:HG2	2.03	0.41
1:B:171:ALA:O	1:B:174:GLN:HB3	2.21	0.41
1:B:201:PRO:N	1:B:202:PRO:CD	2.83	0.41
1:C:452:LEU:HD11	1:C:456:ILE:HD11	2.03	0.41
1:A:356:MET:HE3	1:A:360:VAL:HG12	2.00	0.41
1:B:127:ALA:HB2	1:B:137:MET:SD	2.61	0.41
1:B:455:ALA:O	1:B:459:LEU:HG	2.21	0.41
1:D:110:MET:HE2	1:D:149:ILE:HG13	2.02	0.41
1:D:139:PHE:CZ	1:D:184:GLY:HA3	2.56	0.41
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.91	0.41
1:A:210:VAL:CG2	1:A:212:LEU:HG	2.50	0.41
1:A:304:SER:HB3	1:B:68:VAL:HG11	2.02	0.41
1:B:349:LEU:HB3	1:B:353:VAL:HG13	2.02	0.41
1:B:418:PRO:C	1:B:420:ALA:N	2.79	0.41
1:B:421:THR:HG22	1:B:422:PRO:HD2	2.03	0.41
1:C:201:PRO:N	1:C:202:PRO:CD	2.84	0.41
1:D:174:GLN:NE2	1:D:177:THR:OG1	2.49	0.41
1:D:212:LEU:HD13	1:D:217:TRP:HD1	1.85	0.41
1:D:264:THR:OG1	1:D:308:VAL:HG21	2.20	0.41
1:D:352:MET:HB2	1:D:352:MET:HE3	1.82	0.41
1:A:123:VAL:O	1:A:137:MET:CE	2.69	0.41
1:B:149:ILE:HG22	1:B:150:SER:N	2.35	0.41
1:B:233:ILE:HD13	1:B:233:ILE:HA	1.92	0.41
1:C:434:LYS:HB2	1:C:437:GLU:HG3	2.03	0.40
1:D:357:GLY:O	1:D:361:VAL:HG23	2.21	0.40
1:D:289:LYS:HD2	1:D:289:LYS:HA	1.87	0.40
1:A:186:ALA:HB2	1:A:427:VAL:HG21	2.03	0.40
1:B:174:GLN:HE22	1:B:242:PRO:HB2	1.85	0.40
1:B:175:ARG:HH12	1:B:434:LYS:HG3	1.85	0.40
1:D:28:ASP:OD2	1:D:57:VAL:HB	2.21	0.40
1:D:123:VAL:O	1:D:126:MET:HB2	2.21	0.40
1:D:228:MET:HG3	1:D:452:LEU:CD2	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:ILE:O	1:D:362:ILE:HG23	2.22	0.40
1:A:109:ALA:CB	1:A:303:LEU:HD22	2.51	0.40
1:A:351:ASP:HA	1:A:354:SER:OG	2.21	0.40
1:B:175:ARG:HH12	1:B:434:LYS:CD	2.34	0.40
1:B:369:VAL:HA	1:B:372:LEU:HB3	2.02	0.40
1:C:39:LEU:HA	1:C:40:PRO:HD3	1.96	0.40
1:D:267:ILE:HD13	1:D:303:LEU:HD23	2.03	0.40
1:A:175:ARG:HH12	1:A:434:LYS:CG	2.18	0.40
1:A:421:THR:CG2	1:A:422:PRO:HD2	2.51	0.40
1:C:141:VAL:HG12	1:C:158:MET:CE	2.52	0.40
1:C:421:THR:O	1:C:424:ASN:HB2	2.21	0.40
1:D:214:PHE:CD2	1:D:275:TRP:HB3	2.56	0.40
1:D:461:TRP:CE3	1:D:461:TRP:O	2.74	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	428/449 (95%)	393 (92%)	31 (7%)	4 (1%)	14	43
1	B	442/449 (98%)	403 (91%)	35 (8%)	4 (1%)	14	43
1	C	428/449 (95%)	389 (91%)	31 (7%)	8 (2%)	6	28
1	D	442/449 (98%)	403 (91%)	34 (8%)	5 (1%)	11	39
All	All	1740/1796 (97%)	1588 (91%)	131 (8%)	21 (1%)	10	37

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	242	PRO
1	D	240	LEU

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Mol	Chain	Res	Type
1	D	242	PRO
1	D	419	VAL
1	A	242	PRO
1	A	419	VAL
1	B	242	PRO
1	B	419	VAL
1	C	419	VAL
1	D	252	ARG
1	A	40	PRO
1	C	40	PRO
1	C	173	LYS
1	D	40	PRO
1	B	40	PRO
1	C	416	MET
1	C	150	SER
1	B	150	SER
1	C	418	PRO
1	C	129	GLY
1	A	129	GLY

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	339/357 (95%)	339 (100%)	0	100	100
1	B	347/357 (97%)	347 (100%)	0	100	100
1	C	339/357 (95%)	339 (100%)	0	100	100
1	D	347/357 (97%)	347 (100%)	0	100	100
All	All	1372/1428 (96%)	1372 (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	D	21	ASN
1	A	128	GLN
1	A	256	ASN
1	A	432	HIS
1	B	151	ASN
1	B	174	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FUM	C	503	-	7,7,7	1.17	0	8,8,8	0.95	0
3	FUM	B	502	-	7,7,7	1.20	1 (14%)	8,8,8	1.02	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
3	FUM	C	503	-	-	0/5/5/5	-
3	FUM	B	502	-	-	0/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	FUM	O-C	2.09	1.28	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	432/449 (96%)	0.83	77 (17%) 4 3	70, 115, 176, 200	0
1	B	444/449 (98%)	0.91	84 (18%) 3 3	64, 104, 160, 197	0
1	C	432/449 (96%)	0.83	71 (16%) 4 4	58, 101, 166, 243	0
1	D	444/449 (98%)	0.83	67 (15%) 5 5	59, 98, 147, 174	0
All	All	1752/1796 (97%)	0.85	299 (17%) 4 4	58, 104, 163, 243	0

All (299) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	462	GLN	14.8
1	D	461	TRP	12.9
1	C	163	LEU	11.0
1	C	460	PHE	10.8
1	C	178	TYR	10.5
1	B	168	LYS	10.2
1	C	167	SER	10.0
1	D	313	GLU	9.5
1	D	140	GLY	9.1
1	C	166	LEU	8.5
1	B	80	PHE	7.7
1	D	316	LYS	7.6
1	B	76	MET	7.6
1	C	164	GLY	7.5
1	C	170	ASP	7.4
1	A	118	VAL	7.3
1	B	78	VAL	7.1
1	D	156	ALA	7.1
1	B	79	PHE	7.1
1	D	315	GLN	7.0
1	B	77	ALA	6.7

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Mol	Chain	Res	Type	RSRZ
1	B	36	TYR	6.6
1	C	165	VAL	6.3
1	B	32	PHE	6.2
1	C	169	VAL	6.0
1	C	316	LYS	6.0
1	D	139	PHE	6.0
1	A	368	PHE	5.9
1	D	188	SER	5.8
1	B	33	LEU	5.8
1	C	81	GLY	5.7
1	C	221	GLY	5.7
1	B	75	VAL	5.7
1	D	155	ALA	5.6
1	B	87	ALA	5.6
1	A	312	LYS	5.6
1	B	169	VAL	5.5
1	B	198	VAL	5.4
1	A	149	ILE	5.2
1	C	176	SER	5.2
1	D	312	LYS	5.2
1	B	316	LYS	5.2
1	B	128	GLN	5.1
1	B	51	MET	5.1
1	C	220	PHE	5.0
1	B	371	PHE	5.0
1	D	141	VAL	5.0
1	B	37	HIS	4.8
1	A	358	ILE	4.8
1	B	83	PHE	4.7
1	D	84	GLU	4.7
1	D	444	TYR	4.7
1	D	423	PRO	4.7
1	B	375	PHE	4.6
1	B	103	GLY	4.6
1	B	389	PHE	4.5
1	A	310	HIS	4.5
1	A	375	PHE	4.4
1	A	461	TRP	4.4
1	C	377	SER	4.4
1	D	83	PHE	4.3
1	B	38	PHE	4.3
1	C	160	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	417	LEU	4.3
1	C	462	GLN	4.1
1	D	205	ILE	4.1
1	A	140	GLY	4.1
1	A	367	THR	4.1
1	A	257	TRP	4.1
1	B	385	LEU	4.1
1	D	426	ILE	4.1
1	A	412	SER	4.0
1	B	243	THR	4.0
1	B	244	LEU	4.0
1	B	104	PHE	4.0
1	C	338	GLN	4.0
1	C	44	ASN	4.0
1	C	162	VAL	3.9
1	A	193	GLY	3.9
1	D	157	MET	3.9
1	A	314	ILE	3.9
1	C	136	PHE	3.8
1	D	189	ALA	3.8
1	A	168	LYS	3.8
1	A	191	ILE	3.8
1	A	453	LEU	3.8
1	D	33	LEU	3.8
1	A	288	PHE	3.8
1	C	149	ILE	3.8
1	A	379	THR	3.8
1	D	422	PRO	3.7
1	A	380	ALA	3.7
1	A	121	ASP	3.7
1	D	187	TYR	3.7
1	C	174	GLN	3.7
1	C	168	LYS	3.7
1	C	312	LYS	3.7
1	B	102	GLY	3.7
1	A	462	GLN	3.7
1	D	326	PHE	3.7
1	D	154	THR	3.6
1	A	369	VAL	3.6
1	B	40	PRO	3.6
1	B	74	PRO	3.5
1	A	449	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	403	LEU	3.5
1	B	144	LEU	3.5
1	A	413	CYS	3.5
1	A	457	ALA	3.5
1	B	88	ALA	3.5
1	B	247	MET	3.5
1	D	460	PHE	3.4
1	B	90	ASN	3.4
1	B	197	LEU	3.4
1	D	398	MET	3.4
1	C	61	THR	3.4
1	C	376	ALA	3.4
1	A	200	SER	3.4
1	C	42	GLU	3.4
1	D	153	ALA	3.4
1	A	279	SER	3.4
1	D	197	LEU	3.4
1	C	124	LEU	3.3
1	B	72	LEU	3.3
1	D	190	SER	3.3
1	B	170	ASP	3.3
1	A	43	HIS	3.3
1	A	372	LEU	3.3
1	B	257	TRP	3.3
1	B	34	ALA	3.3
1	D	397	GLY	3.2
1	A	371	PHE	3.2
1	B	199	GLY	3.2
1	B	100	PHE	3.2
1	A	304	SER	3.2
1	A	397	GLY	3.2
1	D	152	THR	3.2
1	A	115	LEU	3.1
1	D	119	ILE	3.1
1	D	412	SER	3.1
1	D	81	GLY	3.1
1	A	311	TRP	3.1
1	B	152	THR	3.1
1	C	300	ILE	3.1
1	D	317	THR	3.0
1	B	368	PHE	3.0
1	B	381	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	97	ILE	3.0
1	B	99	LEU	3.0
1	A	195	ALA	3.0
1	D	198	VAL	3.0
1	B	54	PHE	3.0
1	C	371	PHE	3.0
1	B	374	GLU	3.0
1	B	53	ALA	3.0
1	D	323	LEU	2.9
1	C	103	GLY	2.9
1	C	227	MET	2.9
1	D	149	ILE	2.9
1	D	142	THR	2.9
1	B	35	LEU	2.9
1	A	354	SER	2.9
1	C	303	LEU	2.9
1	A	240	LEU	2.9
1	B	106	LEU	2.9
1	C	161	LEU	2.8
1	C	461	TRP	2.8
1	B	426	ILE	2.8
1	A	165	VAL	2.8
1	A	220	PHE	2.8
1	A	399	SER	2.8
1	D	82	ILE	2.8
1	C	286	GLY	2.8
1	A	383	ALA	2.8
1	B	73	VAL	2.8
1	C	106	LEU	2.8
1	A	145	LEU	2.8
1	A	350	SER	2.8
1	C	288	PHE	2.7
1	A	194	ILE	2.8
1	C	310	HIS	2.7
1	A	202	PRO	2.7
1	B	240	LEU	2.7
1	C	434	LYS	2.7
1	D	309	VAL	2.7
1	C	459	LEU	2.7
1	B	242	PRO	2.7
1	B	49	ILE	2.7
1	C	412	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	441	VAL	2.7
1	D	100	PHE	2.7
1	B	50	SER	2.7
1	C	105	ALA	2.7
1	D	143	ALA	2.7
1	A	119	ILE	2.7
1	C	137	MET	2.7
1	B	129	GLY	2.7
1	C	370	VAL	2.7
1	A	419	VAL	2.7
1	B	149	ILE	2.6
1	C	198	VAL	2.6
1	D	112	HIS	2.6
1	B	312	LYS	2.6
1	A	129	GLY	2.6
1	A	355	HIS	2.6
1	A	422	PRO	2.6
1	C	82	ILE	2.6
1	B	241	LYS	2.6
1	A	278	SER	2.6
1	C	223	PRO	2.6
1	A	309	VAL	2.6
1	C	379	THR	2.6
1	A	210	VAL	2.5
1	B	253	ALA	2.5
1	D	257	TRP	2.5
1	A	218	MET	2.5
1	B	361	VAL	2.5
1	C	43	HIS	2.5
1	C	219	LYS	2.5
1	A	114	GLY	2.5
1	C	107	ALA	2.5
1	B	64	LEU	2.5
1	D	123	VAL	2.5
1	B	364	VAL	2.5
1	A	395	ALA	2.5
1	B	250	LEU	2.4
1	D	111	HIS	2.4
1	D	262	VAL	2.4
1	C	299	ALA	2.4
1	A	410	ALA	2.4
1	B	315	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	417	LEU	2.4
1	D	256	ASN	2.4
1	C	292	ASP	2.4
1	C	140	GLY	2.4
1	D	169	VAL	2.4
1	A	167	SER	2.4
1	B	215	THR	2.4
1	D	78	VAL	2.4
1	A	164	GLY	2.4
1	D	96	ILE	2.4
1	D	356	MET	2.4
1	A	303	LEU	2.4
1	B	249	GLU	2.4
1	A	352	MET	2.4
1	A	396	PHE	2.4
1	C	40	PRO	2.4
1	C	117	LYS	2.3
1	C	109	ALA	2.3
1	C	318	ALA	2.3
1	C	366	ALA	2.3
1	B	131	MET	2.3
1	B	365	VAL	2.3
1	D	322	VAL	2.3
1	C	457	ALA	2.3
1	D	379	THR	2.3
1	C	144	LEU	2.3
1	D	419	VAL	2.3
1	B	422	PRO	2.3
1	D	243	THR	2.3
1	D	203	ASN	2.3
1	A	192	GLY	2.2
1	B	172	ASP	2.2
1	C	375	PHE	2.2
1	C	418	PRO	2.2
1	A	366	ALA	2.2
1	B	376	ALA	2.2
1	D	79	PHE	2.2
1	D	353	VAL	2.2
1	B	81	GLY	2.2
1	A	353	VAL	2.1
1	A	392	VAL	2.1
1	A	393	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	107	ALA	2.1
1	A	307	ARG	2.1
1	B	432	HIS	2.1
1	B	96	ILE	2.1
1	C	153	ALA	2.1
1	D	73	VAL	2.1
1	C	84	GLU	2.1
1	D	136	PHE	2.1
1	D	347	ASN	2.1
1	A	351	ASP	2.1
1	A	398	MET	2.1
1	A	460	PHE	2.1
1	B	42	GLU	2.1
1	B	377	SER	2.1
1	B	181	VAL	2.1
1	C	446	ASN	2.1
1	A	259	LYS	2.1
1	B	122	LYS	2.1
1	C	289	LYS	2.0
1	B	167	SER	2.0
1	C	382	ALA	2.0
1	A	23	LEU	2.0
1	A	349	LEU	2.0
1	B	386	ILE	2.0
1	D	98	PHE	2.0
1	D	236	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($\text{\AA}^2$)	Q<0.9
2	NA	A	502	1/1	0.57	0.21	179,179,179,179	0
3	FUM	C	503	8/8	0.83	0.15	103,123,146,154	0
2	NA	C	501	1/1	0.84	0.11	175,175,175,175	0
3	FUM	B	502	8/8	0.84	0.13	97,118,142,142	0
2	NA	D	502	1/1	0.93	0.07	164,164,164,164	0
2	NA	C	502	1/1	0.94	0.06	193,193,193,193	0
2	NA	D	501	1/1	0.96	0.11	146,146,146,146	0
2	NA	B	501	1/1	0.96	0.05	81,81,81,81	0
2	NA	A	501	1/1	0.98	0.03	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.