



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:19 PM UTC

PDB ID : 2HNE / pdb_00002hne
Title : Crystal structure of l-fuconate dehydratase from xanthomonas campestris pv. campestris str. ATCC 33913
Authors : Fedorov, A.A.; Fedorov, E.V.; Yew, W.S.; Gerlt, J.A.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-07-12
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

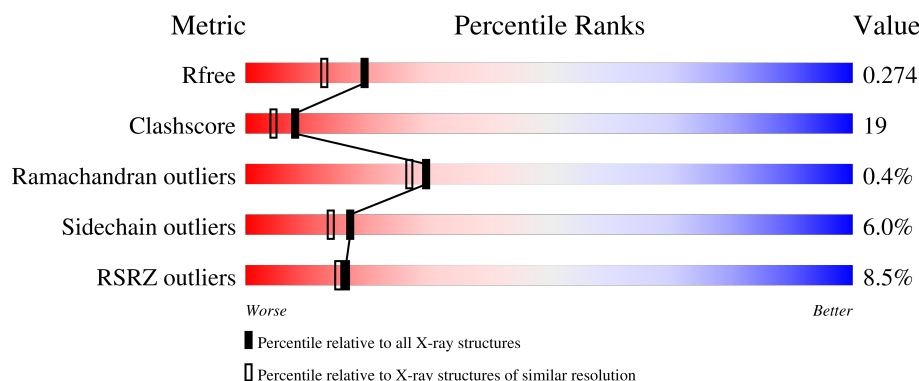
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	436	6% 63% 30% • •
1	B	436	6% 65% 29% • •
1	C	436	11% 59% 36% •
1	D	436	11% 68% 27% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13619 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L-fuconate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3295	2091	587	607	10			
1	B	432	Total	C	N	O	S	0	0	0
			3334	2112	594	617	11			
1	C	434	Total	C	N	O	S	0	0	0
			3350	2122	596	621	11			
1	D	433	Total	C	N	O	S	0	0	0
			3341	2116	595	619	11			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

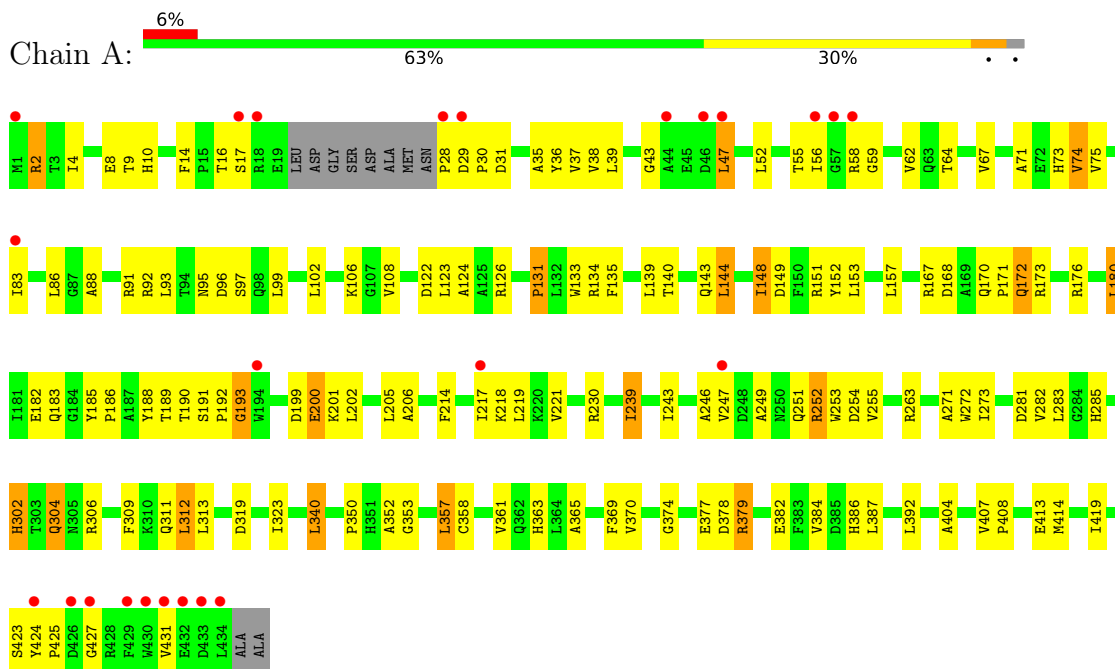
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	76	Total	O	0	0
			76	76		
3	B	91	Total	O	0	0
			91	91		
3	C	63	Total	O	0	0
			63	63		
3	D	65	Total	O	0	0
			65	65		

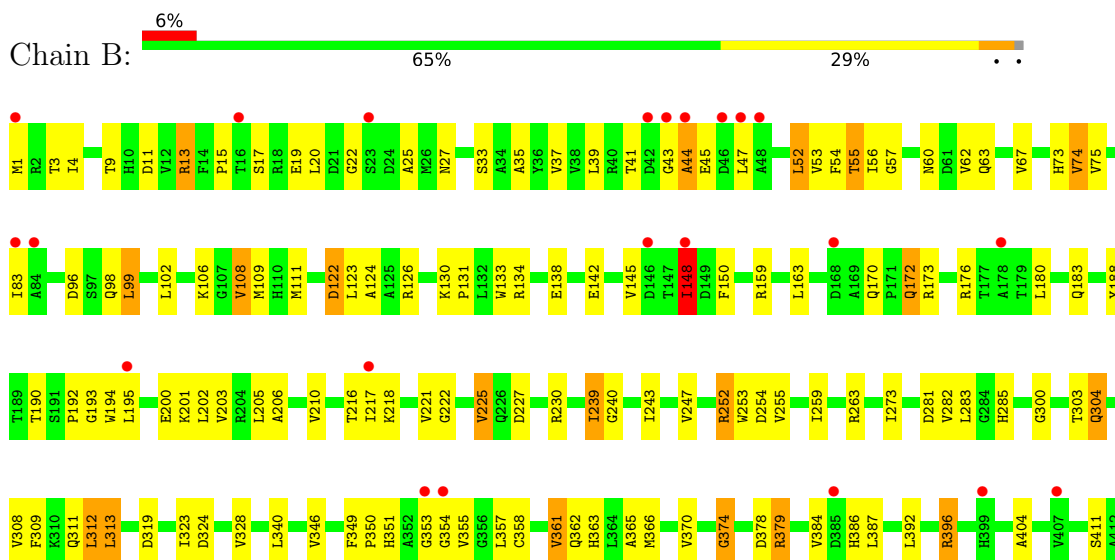
3 Residue-property plots [i](#)

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: L-fuconate dehydratase

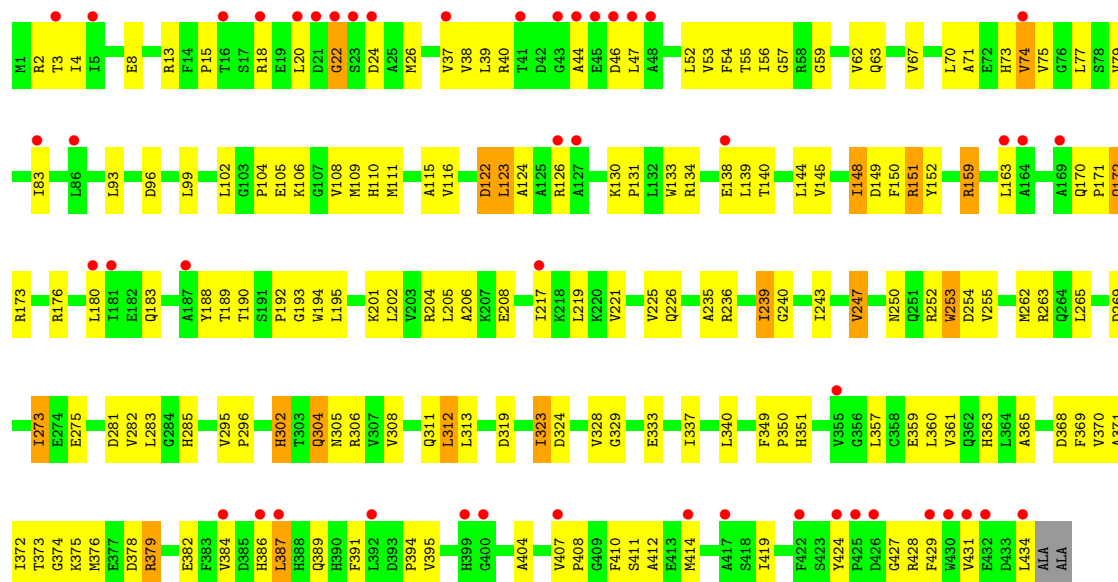


• Molecule 1: L-fuconate dehydratase

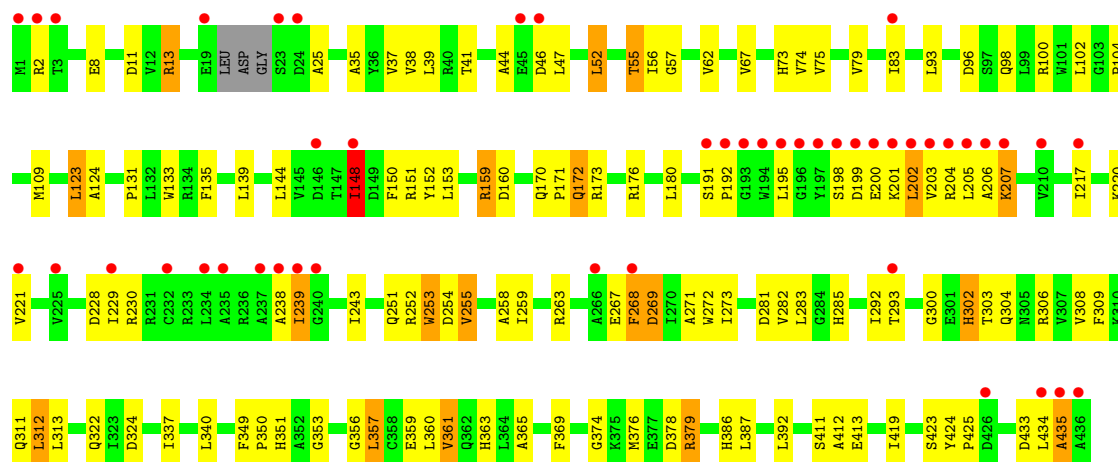




• Molecule 1: L-fuconate dehydratase



• Molecule 1: L-fuconate dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.63Å 130.63Å 195.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.68 – 2.00 24.68 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (24.68-2.00) 94.1 (24.68-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.274 0.241 , 0.274	Depositor DCC
R_{free} test set	7677 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13619	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/3367	0.93	12/4584 (0.3%)
1	B	0.44	0/3407	1.01	21/4640 (0.5%)
1	C	0.40	0/3423	0.96	13/4662 (0.3%)
1	D	0.40	0/3413	0.95	12/4646 (0.3%)
All	All	0.42	0/13610	0.96	58/18532 (0.3%)

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ARG	N-CA-C	9.85	122.02	111.28
1	A	304	GLN	N-CA-C	9.37	121.50	111.28
1	B	74	VAL	N-CA-C	8.72	118.96	111.90
1	B	304	GLN	N-CA-C	8.71	120.77	111.28
1	C	252	ARG	N-CA-C	8.39	120.50	111.36
1	A	252	ARG	N-CA-C	8.08	120.17	111.36
1	D	304	GLN	N-CA-C	7.73	120.60	111.71
1	B	195	LEU	N-CA-C	-7.46	101.24	110.41
1	B	253	TRP	N-CA-C	7.42	121.51	110.52
1	A	254	ASP	N-CA-C	-7.27	100.04	110.59
1	C	304	GLN	N-CA-C	7.01	118.93	111.28
1	D	253	TRP	N-CA-C	6.87	120.69	110.52
1	B	193	GLY	N-CA-C	6.78	126.52	115.46
1	D	252	ARG	N-CA-C	6.75	120.73	112.23
1	A	253	TRP	N-CA-C	6.74	120.50	110.52
1	C	253	TRP	N-CA-C	6.70	120.44	110.52
1	B	254	ASP	N-CA-C	-6.70	100.88	110.59
1	A	255	VAL	N-CA-C	6.42	116.90	110.23
1	A	74	VAL	N-CA-C	6.41	119.37	112.96
1	C	74	VAL	N-CA-C	6.35	117.45	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	254	ASP	N-CA-C	-6.30	100.65	110.42
1	C	254	ASP	N-CA-C	-6.29	101.47	110.59
1	C	370	VAL	N-CA-C	6.21	116.32	110.30
1	B	361	VAL	N-CA-C	6.04	118.60	111.05
1	D	255	VAL	N-CA-C	5.94	116.41	110.23
1	B	323	ILE	N-CA-C	-5.93	99.16	108.95
1	C	122	ASP	N-CA-C	-5.92	104.75	111.14
1	D	74	VAL	N-CA-C	5.89	118.85	112.96
1	B	374	GLY	N-CA-C	-5.87	107.15	115.30
1	B	108	VAL	N-CA-C	5.80	116.45	110.36
1	B	131	PRO	N-CA-C	-5.80	102.16	111.38
1	B	370	VAL	N-CA-C	5.77	115.95	110.53
1	C	371	ALA	N-CA-C	5.68	120.37	113.38
1	B	319	ASP	N-CA-C	-5.66	106.50	113.41
1	A	108	VAL	N-CA-C	5.56	116.20	110.36
1	B	255	VAL	N-CA-C	5.56	115.76	110.42
1	D	361	VAL	N-CA-C	5.44	117.85	111.05
1	A	131	PRO	N-CA-C	-5.38	102.83	111.38
1	A	35	ALA	N-CA-C	-5.34	98.59	107.99
1	B	422	PHE	N-CA-C	5.31	119.07	112.59
1	B	222	GLY	N-CA-C	5.29	122.04	114.64
1	A	319	ASP	N-CA-C	-5.28	106.97	113.41
1	B	183	GLN	N-CA-C	5.27	119.80	112.90
1	D	35	ALA	N-CA-C	-5.23	97.42	107.57
1	C	255	VAL	N-CA-C	5.18	115.39	110.42
1	D	292	ILE	N-CA-C	5.18	117.15	111.77
1	C	108	VAL	N-CA-C	5.17	115.79	110.36
1	B	148	ILE	N-CA-C	5.15	117.10	109.17
1	B	358	CYS	N-CA-C	-5.13	105.60	111.14
1	A	323	ILE	N-CA-C	-5.12	100.52	108.81
1	B	122	ASP	N-CA-C	-5.09	105.62	111.07
1	C	183	GLN	N-CA-C	5.08	119.55	112.90
1	D	435	ALA	N-CA-C	-5.06	105.42	112.30
1	C	275	GLU	CB-CA-C	-5.04	107.62	111.20
1	D	131	PRO	N-CA-C	-5.04	103.38	111.38
1	C	319	ASP	N-CA-C	-5.03	107.31	113.50
1	A	193	GLY	N-CA-C	5.02	123.72	115.34
1	D	148	ILE	N-CA-C	5.00	116.46	109.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3295	0	3265	126	0
1	B	3334	0	3297	140	0
1	C	3350	0	3312	167	0
1	D	3341	0	3303	119	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	76	0	0	1	0
3	B	91	0	0	2	0
3	C	63	0	0	2	0
3	D	65	0	0	5	0
All	All	13619	0	13177	514	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 19.

All (514) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:VAL:HG11	1:B:67:VAL:HG11	1.22	1.08
1:B:239:ILE:HG23	1:B:243:ILE:HB	1.39	1.05
1:D:170:GLN:HA	1:D:173:ARG:HD3	1.41	1.02
1:A:122:ASP:O	1:A:126:ARG:HG2	1.61	1.01
1:B:170:GLN:HA	1:B:173:ARG:HD3	1.44	1.00
1:C:239:ILE:HG23	1:C:243:ILE:HB	1.44	0.97
1:C:170:GLN:HA	1:C:173:ARG:HD3	1.52	0.90
1:C:134:ARG:O	1:C:138:GLU:HG2	1.73	0.88
1:C:262:MET:HE1	1:C:265:LEU:HD12	1.55	0.87
1:B:122:ASP:O	1:B:126:ARG:HG2	1.74	0.86
1:B:9:THR:HG22	1:B:37:VAL:HG12	1.56	0.85
1:D:198:SER:HB3	1:D:201:LYS:HB2	1.57	0.85
1:B:239:ILE:CG2	1:B:243:ILE:HB	2.08	0.84
1:C:239:ILE:CG2	1:C:243:ILE:HB	2.08	0.82
1:D:11:ASP:OD1	1:D:13:ARG:HD3	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:MET:HA	1:C:262:MET:HE2	1.62	0.82
1:B:206:ALA:HB1	1:B:239:ILE:CD1	2.12	0.79
1:D:192:PRO:HB2	1:D:217:ILE:HD11	1.67	0.77
1:A:151:ARG:HD3	1:A:152:TYR:CE2	2.19	0.77
1:C:133:TRP:H	1:C:363:HIS:HD2	1.35	0.75
1:D:151:ARG:HD3	1:D:152:TYR:CE2	2.21	0.74
1:D:55:THR:HG23	3:D:605:HOH:O	1.88	0.74
1:C:247:VAL:HG12	1:C:273:ILE:HD13	1.70	0.73
1:B:13:ARG:HB3	1:B:33:SER:OG	1.89	0.73
1:B:192:PRO:HB2	1:B:217:ILE:HD11	1.70	0.72
1:A:171:PRO:HB2	1:A:172:GLN:OE1	1.89	0.72
1:A:283:LEU:H	1:B:311:GLN:HE21	1.38	0.72
1:A:170:GLN:HB3	1:A:171:PRO:HD3	1.69	0.71
1:C:151:ARG:HD3	1:C:152:TYR:CE2	2.25	0.71
1:A:28:PRO:C	1:A:30:PRO:HD3	2.16	0.70
1:C:387:LEU:HA	1:C:389:GLN:HE22	1.55	0.70
1:A:83:ILE:HD11	1:A:123:LEU:HD22	1.72	0.70
1:C:378:ASP:OD1	1:C:379:ARG:HD2	1.92	0.70
1:D:239:ILE:HG23	1:D:243:ILE:HB	1.74	0.69
3:A:603:HOH:O	1:B:55:THR:HG23	1.90	0.69
1:C:253:TRP:CH2	1:C:262:MET:HE3	2.27	0.69
1:A:58:ARG:HG3	1:B:98:GLN:OE1	1.92	0.69
1:C:282:VAL:H	1:D:311:GLN:HE22	1.39	0.69
1:B:145:VAL:HG11	1:B:159:ARG:HG3	1.74	0.68
1:B:142:GLU:HG2	1:D:200:GLU:HG2	1.75	0.68
1:D:324:ASP:OD2	1:D:351:HIS:HD2	1.75	0.68
1:B:37:VAL:CG1	1:B:67:VAL:HG11	2.12	0.68
1:A:180:LEU:HD22	1:A:404:ALA:HB2	1.75	0.67
1:A:10:HIS:HB2	1:A:36:TYR:HB3	1.75	0.67
1:A:2:ARG:HB2	1:A:2:ARG:NH2	2.09	0.67
1:D:192:PRO:CB	1:D:217:ILE:HD11	2.25	0.66
1:B:225:VAL:HG23	3:B:657:HOH:O	1.94	0.66
1:A:239:ILE:HG23	1:A:243:ILE:HB	1.78	0.66
1:A:378:ASP:OD1	1:A:379:ARG:HD2	1.96	0.66
1:A:58:ARG:NH1	1:B:98:GLN:HG3	2.11	0.66
1:D:172:GLN:H	1:D:172:GLN:NE2	1.92	0.66
1:A:427:GLY:O	1:A:431:VAL:HG23	1.96	0.66
1:C:328:VAL:HG22	1:C:333:GLU:OE2	1.95	0.66
1:B:133:TRP:H	1:B:363:HIS:HD2	1.42	0.65
1:C:122:ASP:O	1:C:126:ARG:HG2	1.96	0.65
1:D:47:LEU:HD13	1:D:123:LEU:HD21	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ALA:HB1	1:D:239:ILE:HD13	1.79	0.65
1:C:13:ARG:HG3	1:C:424:TYR:HB2	1.78	0.65
1:B:15:PRO:HG3	1:B:429:PHE:CZ	2.31	0.65
1:D:52:LEU:CD2	1:D:360:LEU:HD11	2.27	0.65
1:D:52:LEU:HD21	1:D:360:LEU:HD11	1.79	0.65
1:D:433:ASP:C	1:D:435:ALA:H	2.04	0.65
1:C:133:TRP:H	1:C:363:HIS:CD2	2.15	0.65
1:D:13:ARG:HG3	1:D:424:TYR:HB2	1.79	0.65
1:B:239:ILE:HG22	1:B:240:GLY:O	1.97	0.65
1:C:170:GLN:HA	1:C:173:ARG:CD	2.26	0.64
1:B:172:GLN:H	1:B:172:GLN:HE21	1.44	0.64
1:C:54:PHE:HB2	1:C:357:LEU:HD21	1.78	0.64
1:D:2:ARG:HG3	1:D:79:VAL:HB	1.79	0.64
1:D:172:GLN:NE2	1:D:172:GLN:N	2.46	0.64
1:C:328:VAL:HG22	1:C:329:GLY:H	1.61	0.64
1:C:26:MET:HE1	3:D:621:HOH:O	1.98	0.64
1:C:59:GLY:O	1:C:62:VAL:HG22	1.98	0.64
1:C:225:VAL:HG23	3:C:653:HOH:O	1.96	0.64
1:D:83:ILE:HD12	1:D:124:ALA:CA	2.28	0.64
1:B:180:LEU:CD2	1:B:404:ALA:HB2	2.27	0.63
1:B:259:ILE:O	1:B:263:ARG:HG3	1.98	0.63
1:D:83:ILE:HD12	1:D:124:ALA:HA	1.80	0.63
1:B:145:VAL:CG1	1:B:159:ARG:HG3	2.28	0.63
1:C:2:ARG:NH2	1:C:47:LEU:HD11	2.14	0.63
1:A:133:TRP:H	1:A:363:HIS:HD2	1.45	0.63
1:B:201:LYS:O	1:B:205:LEU:HD13	1.99	0.63
1:A:414:MET:HB2	1:A:419:ILE:HD11	1.81	0.63
1:C:131:PRO:HG2	1:C:134:ARG:HB2	1.80	0.63
1:D:369:PHE:CZ	1:D:376:MET:HE2	2.33	0.63
1:B:130:LYS:HE3	1:B:138:GLU:OE2	1.98	0.62
1:C:206:ALA:HB1	1:C:239:ILE:CD1	2.29	0.62
1:A:283:LEU:H	1:B:311:GLN:NE2	1.96	0.62
1:A:282:VAL:H	1:B:311:GLN:HE22	1.47	0.62
1:C:37:VAL:HG22	1:C:67:VAL:HG11	1.81	0.62
1:C:386:HIS:HB3	1:C:387:LEU:HD22	1.81	0.62
1:B:148:ILE:HG12	1:B:150:PHE:CE1	2.34	0.62
1:A:88:ALA:O	1:A:92:ARG:HG3	2.00	0.62
1:B:102:LEU:HD12	1:B:109:MET:HE3	1.80	0.62
1:A:309:PHE:O	1:A:313:LEU:HD13	2.00	0.61
1:D:8:GLU:HB2	1:D:38:VAL:HB	1.82	0.61
1:A:59:GLY:O	1:A:62:VAL:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:O	1:A:171:PRO:HD2	2.00	0.61
1:B:227:ASP:OD2	1:B:230:ARG:NH1	2.34	0.61
1:B:428:ARG:O	1:B:431:VAL:HG12	2.00	0.61
1:C:311:GLN:HE22	1:D:282:VAL:H	1.48	0.61
1:D:133:TRP:H	1:D:363:HIS:HD2	1.46	0.61
1:A:206:ALA:HB1	1:A:239:ILE:HD13	1.82	0.60
1:C:283:LEU:H	1:D:311:GLN:HE21	1.49	0.60
1:A:311:GLN:HE22	1:B:282:VAL:H	1.50	0.60
1:B:180:LEU:HD22	1:B:404:ALA:HB2	1.84	0.60
1:C:37:VAL:CG2	1:C:67:VAL:HG11	2.32	0.60
1:D:353:GLY:O	1:D:357:LEU:HB2	2.02	0.60
1:A:193:GLY:HA3	1:A:219:LEU:HA	1.84	0.59
1:B:396:ARG:HG2	1:B:396:ARG:HH11	1.67	0.59
1:A:52:LEU:HD12	1:A:52:LEU:C	2.28	0.59
1:B:55:THR:HG22	1:B:57:GLY:H	1.67	0.59
1:C:311:GLN:HE21	1:D:283:LEU:H	1.50	0.58
1:C:282:VAL:N	1:D:311:GLN:HE22	2.01	0.58
1:D:203:VAL:O	1:D:207:LYS:HD3	2.03	0.58
1:A:282:VAL:N	1:B:311:GLN:HE22	2.01	0.58
1:C:360:LEU:HD21	1:C:412:ALA:HB2	1.86	0.58
1:B:313:LEU:HD11	1:B:346:VAL:HG21	1.85	0.58
1:D:207:LYS:HG3	1:D:238:ALA:HB1	1.86	0.58
1:C:201:LYS:HG2	1:C:205:LEU:HD23	1.86	0.57
1:C:130:LYS:NZ	1:C:138:GLU:HG3	2.19	0.57
1:C:407:VAL:HG13	1:C:408:PRO:HD2	1.85	0.57
1:A:131:PRO:HG2	1:A:134:ARG:HB2	1.87	0.57
1:C:145:VAL:O	1:C:148:ILE:HG23	2.05	0.57
1:A:37:VAL:HG22	1:A:67:VAL:HG11	1.86	0.57
1:A:170:GLN:HA	1:A:173:ARG:HD3	1.87	0.57
1:D:73:HIS:HE1	1:D:96:ASP:OD2	1.87	0.57
1:C:62:VAL:HG21	1:D:109:MET:CE	2.35	0.57
1:D:363:HIS:HE1	1:D:411:SER:OG	1.88	0.56
1:D:200:GLU:O	1:D:203:VAL:HG22	2.05	0.56
1:B:55:THR:HG21	1:B:60:ASN:HB2	1.87	0.56
1:C:55:THR:HG23	3:D:644:HOH:O	2.03	0.56
1:D:387:LEU:N	1:D:387:LEU:HD12	2.20	0.56
1:A:200:GLU:OE1	1:C:159:ARG:NH1	2.39	0.56
1:D:267:GLU:C	1:D:269:ASP:H	2.13	0.56
1:D:360:LEU:HD21	1:D:412:ALA:HB2	1.87	0.56
1:B:35:ALA:HB3	1:B:53:VAL:HB	1.88	0.56
1:C:180:LEU:CD2	1:C:404:ALA:HB2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:LEU:HD22	1:C:404:ALA:HB2	1.86	0.56
1:C:71:ALA:O	1:C:75:VAL:HG22	2.04	0.56
1:C:387:LEU:HA	1:C:389:GLN:NE2	2.20	0.56
1:B:428:ARG:HG2	1:B:428:ARG:HH11	1.70	0.56
1:B:172:GLN:H	1:B:172:GLN:NE2	2.04	0.56
1:A:17:SER:HB2	1:A:31:ASP:OD1	2.06	0.55
1:A:419:ILE:O	1:A:423:SER:HB2	2.06	0.55
1:C:204:ARG:O	1:C:208:GLU:HG3	2.06	0.55
1:D:172:GLN:H	1:D:172:GLN:HE21	1.53	0.55
1:D:386:HIS:HB3	1:D:387:LEU:HD13	1.88	0.55
1:B:148:ILE:HD11	1:B:150:PHE:CE2	2.41	0.55
1:D:201:LYS:O	1:D:201:LYS:HD3	2.06	0.55
1:C:368:ASP:OD2	1:C:372:ILE:HB	2.07	0.54
1:C:375:LYS:O	1:C:379:ARG:HD3	2.08	0.54
1:B:363:HIS:HE1	1:B:411:SER:OG	1.89	0.54
1:C:138:GLU:HB2	3:C:648:HOH:O	2.07	0.54
1:C:350:PRO:HB3	1:C:361:VAL:HG21	1.89	0.54
1:A:407:VAL:HG13	1:A:408:PRO:HD2	1.89	0.54
1:C:79:VAL:O	1:C:83:ILE:HD13	2.08	0.54
1:B:45:GLU:C	1:B:47:LEU:H	2.15	0.54
1:C:70:LEU:HD12	1:C:116:VAL:HG21	1.89	0.54
1:C:102:LEU:CD2	1:C:109:MET:HE3	2.38	0.54
1:B:324:ASP:OD2	1:B:351:HIS:HD2	1.91	0.54
1:D:202:LEU:HD12	1:D:202:LEU:C	2.32	0.54
1:A:172:GLN:O	1:A:176:ARG:HG3	2.08	0.54
1:C:189:THR:HG23	1:C:217:ILE:CD1	2.37	0.53
1:B:43:GLY:O	1:B:44:ALA:C	2.51	0.53
1:D:201:LYS:O	1:D:205:LEU:HD13	2.09	0.53
1:C:15:PRO:HG3	1:C:429:PHE:CZ	2.43	0.53
1:C:389:GLN:CD	1:C:389:GLN:H	2.15	0.53
1:D:37:VAL:HG22	1:D:67:VAL:HG11	1.90	0.53
1:B:378:ASP:OD1	1:B:379:ARG:HD2	2.08	0.53
1:C:145:VAL:HG13	1:C:150:PHE:CZ	2.44	0.53
1:C:239:ILE:HG22	1:C:240:GLY:O	2.08	0.53
1:B:180:LEU:O	1:B:180:LEU:HD23	2.09	0.53
1:B:387:LEU:N	1:B:387:LEU:HD12	2.24	0.53
1:C:20:LEU:N	1:C:20:LEU:HD12	2.24	0.53
1:D:206:ALA:HB1	1:D:239:ILE:CD1	2.38	0.53
1:B:145:VAL:HG13	1:B:150:PHE:CZ	2.43	0.53
1:A:8:GLU:CG	1:A:38:VAL:HB	2.39	0.53
1:A:139:LEU:HB2	1:A:144:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:THR:HG23	1:C:217:ILE:HD12	1.91	0.53
1:A:387:LEU:N	1:A:387:LEU:HD22	2.24	0.53
1:C:262:MET:HE1	1:C:265:LEU:CD1	2.32	0.53
1:D:419:ILE:O	1:D:423:SER:HB2	2.09	0.52
1:C:221:VAL:CG2	1:C:247:VAL:HG13	2.40	0.52
1:C:384:VAL:HG12	1:C:386:HIS:ND1	2.25	0.52
1:A:249:ALA:O	1:A:252:ARG:HG3	2.09	0.52
1:D:204:ARG:HA	1:D:207:LYS:HZ2	1.74	0.52
1:A:62:VAL:HG21	1:B:109:MET:CE	2.40	0.52
1:C:83:ILE:HG13	1:C:124:ALA:HA	1.90	0.52
1:C:311:GLN:NE2	1:D:283:LEU:H	2.07	0.52
1:A:206:ALA:HB1	1:A:239:ILE:CD1	2.40	0.52
1:B:206:ALA:HB1	1:B:239:ILE:HD11	1.90	0.52
1:B:392:LEU:HD13	1:B:413:GLU:HG2	1.92	0.52
1:A:353:GLY:O	1:A:357:LEU:HB2	2.09	0.52
1:A:423:SER:O	1:A:427:GLY:HA3	2.10	0.52
1:C:63:GLN:NE2	1:C:111:MET:HE3	2.25	0.52
1:C:145:VAL:HG21	1:C:163:LEU:HG	1.92	0.52
1:B:357:LEU:N	1:B:357:LEU:HD22	2.25	0.52
1:B:386:HIS:HB3	1:B:387:LEU:HD13	1.92	0.52
1:C:349:PHE:CZ	1:C:379:ARG:HA	2.44	0.52
1:B:172:GLN:NE2	1:B:172:GLN:N	2.58	0.52
1:B:349:PHE:CZ	1:B:379:ARG:HA	2.44	0.52
1:A:83:ILE:CD1	1:A:123:LEU:HD22	2.40	0.52
1:B:362:GLN:HB2	1:B:366:MET:HE3	1.91	0.52
1:A:55:THR:HG22	1:A:56:ILE:N	2.25	0.51
1:D:207:LYS:HB2	1:D:207:LYS:NZ	2.24	0.51
1:A:369:PHE:O	1:A:374:GLY:HA2	2.09	0.51
1:C:15:PRO:O	1:C:18:ARG:HG2	2.11	0.51
1:C:55:THR:HG22	1:C:57:GLY:H	1.75	0.51
1:C:56:ILE:HG13	1:D:98:GLN:HG2	1.91	0.51
1:C:311:GLN:HE22	1:D:282:VAL:N	2.08	0.51
1:C:226:GLN:H	1:C:226:GLN:NE2	2.08	0.51
1:B:54:PHE:HB2	1:B:357:LEU:HD21	1.92	0.51
1:C:206:ALA:HB1	1:C:239:ILE:HD13	1.93	0.51
1:C:62:VAL:HG21	1:D:109:MET:HE2	1.92	0.51
1:C:172:GLN:NE2	1:C:172:GLN:H	2.08	0.51
1:D:267:GLU:HG3	1:D:268:PHE:N	2.26	0.51
1:A:239:ILE:CG2	1:A:243:ILE:HB	2.39	0.51
1:B:221:VAL:HG22	1:B:247:VAL:HG13	1.93	0.51
1:C:139:LEU:HB2	1:C:144:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:SER:HA	3:B:649:HOH:O	2.11	0.50
1:C:283:LEU:H	1:D:311:GLN:NE2	2.09	0.50
1:B:392:LEU:HD22	1:B:413:GLU:CD	2.36	0.50
1:C:52:LEU:N	1:C:52:LEU:HD23	2.26	0.50
1:A:102:LEU:HD12	1:B:108:VAL:HG22	1.93	0.50
1:A:191:SER:OG	1:A:192:PRO:HD3	2.11	0.50
1:D:251:GLN:HE22	1:D:302:HIS:CD2	2.29	0.50
1:B:176:ARG:CD	1:B:374:GLY:HA2	2.41	0.50
1:B:221:VAL:CG2	1:B:247:VAL:CG1	2.89	0.50
1:B:353:GLY:O	1:B:354:GLY:C	2.54	0.50
1:C:105:GLU:HA	1:C:110:HIS:ND1	2.26	0.50
1:D:173:ARG:HD2	3:D:626:HOH:O	2.11	0.50
1:B:22:GLY:HA2	1:B:194:TRP:CZ3	2.46	0.50
1:B:221:VAL:CG2	1:B:247:VAL:HG13	2.42	0.50
1:B:384:VAL:HG12	1:B:386:HIS:HD1	1.77	0.50
1:D:83:ILE:HD11	1:D:123:LEU:HD13	1.93	0.50
1:C:102:LEU:HD23	1:C:109:MET:HE3	1.94	0.49
1:C:192:PRO:HB3	1:C:205:LEU:HB3	1.94	0.49
1:B:188:TYR:HB2	1:B:216:THR:HB	1.94	0.49
1:C:302:HIS:HD2	1:D:104:PRO:HD3	1.78	0.49
1:C:192:PRO:O	1:C:202:LEU:HD23	2.12	0.49
1:A:182:GLU:HG3	1:A:183:GLN:N	2.28	0.49
1:C:376:MET:HA	1:C:379:ARG:HD3	1.93	0.49
1:A:189:THR:HG23	1:A:214:PHE:CE2	2.48	0.49
1:B:172:GLN:HE21	1:B:172:GLN:N	2.10	0.49
1:D:159:ARG:HG3	1:D:160:ASP:N	2.28	0.49
1:B:19:GLU:O	1:B:20:LEU:HB2	2.13	0.49
1:C:83:ILE:HD11	1:C:123:LEU:HD22	1.95	0.49
1:C:104:PRO:HD3	1:D:302:HIS:HD2	1.78	0.49
1:C:130:LYS:HZ3	1:C:138:GLU:HG3	1.77	0.49
1:A:2:ARG:HB2	1:A:2:ARG:HH21	1.76	0.48
1:B:25:ALA:HB1	1:B:252:ARG:HG3	1.94	0.48
1:A:176:ARG:HD2	1:A:370:VAL:O	2.13	0.48
1:B:221:VAL:HG21	1:B:247:VAL:CG1	2.42	0.48
1:C:247:VAL:HG12	1:C:273:ILE:CD1	2.40	0.48
1:D:135:PHE:O	1:D:139:LEU:HG	2.13	0.48
1:B:45:GLU:HA	1:B:45:GLU:OE2	2.13	0.48
1:C:24:ASP:HB2	1:C:250:ASN:ND2	2.28	0.48
1:C:55:THR:CG2	1:C:56:ILE:N	2.77	0.48
1:C:73:HIS:HE1	1:C:96:ASP:OD2	1.96	0.48
1:C:236:ARG:HH21	1:C:269:ASP:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:GLY:HA2	1:C:194:TRP:CZ3	2.49	0.48
1:C:148:ILE:HG13	1:C:149:ASP:N	2.27	0.48
1:C:151:ARG:HD3	1:C:152:TYR:CZ	2.48	0.48
1:C:350:PRO:HB3	1:C:361:VAL:CG2	2.44	0.48
1:C:369:PHE:O	1:C:374:GLY:HA2	2.14	0.48
1:C:428:ARG:HG2	1:C:428:ARG:HH11	1.76	0.48
1:A:199:ASP:OD2	1:A:230:ARG:NH2	2.47	0.48
1:B:83:ILE:HG23	1:B:124:ALA:CB	2.43	0.48
1:C:8:GLU:HB2	1:C:38:VAL:HB	1.94	0.48
1:B:355:VAL:O	1:B:357:LEU:HD22	2.14	0.48
1:C:13:ARG:HG3	1:C:424:TYR:CB	2.43	0.48
1:B:180:LEU:HD23	1:B:180:LEU:C	2.38	0.48
1:B:200:GLU:O	1:B:203:VAL:HG22	2.13	0.48
1:C:359:GLU:CD	1:C:395:VAL:HG13	2.39	0.48
1:A:92:ARG:HB3	1:A:92:ARG:NH2	2.28	0.48
1:B:73:HIS:HE1	1:B:96:ASP:OD2	1.96	0.48
1:D:369:PHE:CD2	1:D:376:MET:HB3	2.49	0.48
1:A:200:GLU:CD	1:A:200:GLU:H	2.21	0.48
1:A:83:ILE:HG13	1:A:124:ALA:HA	1.96	0.48
1:D:387:LEU:N	1:D:387:LEU:CD1	2.77	0.47
1:C:139:LEU:HB2	1:C:144:LEU:CD2	2.45	0.47
1:C:176:ARG:HD3	1:C:374:GLY:HA2	1.94	0.47
1:B:96:ASP:OD1	1:B:96:ASP:C	2.58	0.47
1:D:392:LEU:HD22	1:D:413:GLU:CD	2.38	0.47
1:A:311:GLN:NE2	1:B:283:LEU:H	2.12	0.47
1:A:350:PRO:HG2	1:A:365:ALA:HB2	1.96	0.47
1:D:202:LEU:HD12	1:D:203:VAL:N	2.29	0.47
1:A:281:ASP:O	1:A:285:HIS:HD2	1.97	0.47
1:D:44:ALA:C	1:D:46:ASP:H	2.21	0.47
1:A:91:ARG:O	1:A:95:ASN:HB2	2.14	0.47
1:A:139:LEU:HD12	1:A:144:LEU:CD1	2.45	0.47
1:B:428:ARG:HG2	1:B:428:ARG:NH1	2.29	0.47
1:C:2:ARG:HH21	1:C:47:LEU:HD11	1.78	0.47
1:C:180:LEU:HD23	1:C:180:LEU:O	2.15	0.47
1:D:44:ALA:C	1:D:46:ASP:N	2.73	0.47
1:A:190:THR:HG21	1:A:382:GLU:OE2	2.15	0.47
1:D:433:ASP:C	1:D:435:ALA:N	2.72	0.47
1:A:47:LEU:HD11	1:A:123:LEU:HD21	1.97	0.47
1:B:308:VAL:O	1:B:312:LEU:CD2	2.63	0.47
1:D:207:LYS:CD	1:D:238:ALA:HB1	2.45	0.47
1:D:378:ASP:OD1	1:D:379:ARG:CD	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ALA:HB1	1:A:358:CYS:SG	2.55	0.47
1:A:378:ASP:OD1	1:A:379:ARG:CD	2.63	0.46
1:D:148:ILE:HG23	1:D:150:PHE:CE1	2.49	0.46
1:A:4:ILE:HG21	1:A:74:VAL:HG12	1.98	0.46
1:A:311:GLN:HE21	1:B:283:LEU:H	1.62	0.46
1:C:201:LYS:HG2	1:C:205:LEU:CD2	2.45	0.46
1:C:109:MET:HE1	1:D:62:VAL:HG21	1.98	0.46
1:C:262:MET:CE	1:C:265:LEU:HD12	2.35	0.46
1:D:153:LEU:HD11	1:D:306:ARG:HD2	1.97	0.46
1:C:4:ILE:HG21	1:C:74:VAL:HG12	1.97	0.46
1:C:40:ARG:HG2	1:C:40:ARG:HH21	1.80	0.46
1:C:54:PHE:CB	1:C:357:LEU:HD21	2.44	0.46
1:C:105:GLU:HA	1:C:110:HIS:CG	2.50	0.46
1:C:328:VAL:HG13	1:C:329:GLY:N	2.31	0.46
1:A:190:THR:HG22	1:A:218:LYS:HE2	1.97	0.46
1:A:192:PRO:HB2	1:A:217:ILE:HD11	1.97	0.46
1:D:2:ARG:HG2	1:D:2:ARG:HH21	1.80	0.46
1:A:58:ARG:HH12	1:B:98:GLN:HG3	1.81	0.46
1:B:145:VAL:HG13	1:B:150:PHE:CE1	2.51	0.46
1:A:140:THR:OG1	1:A:143:GLN:HG3	2.16	0.46
1:A:182:GLU:HG3	1:A:183:GLN:HG3	1.98	0.46
1:C:130:LYS:HB2	1:C:131:PRO:HD2	1.98	0.46
1:C:262:MET:HE2	1:C:262:MET:CA	2.39	0.46
1:D:83:ILE:HG23	1:D:124:ALA:CB	2.46	0.46
1:A:221:VAL:HG22	1:A:247:VAL:HG13	1.98	0.45
1:B:145:VAL:HG21	1:B:163:LEU:HG	1.98	0.45
1:D:41:THR:OG1	1:D:47:LEU:HD12	2.16	0.45
1:A:58:ARG:HB2	1:B:98:GLN:HB2	1.97	0.45
1:A:157:LEU:HD22	1:A:340:LEU:HD13	1.99	0.45
1:A:201:LYS:O	1:A:205:LEU:HD13	2.17	0.45
1:B:350:PRO:HG2	1:B:365:ALA:HB2	1.98	0.45
1:C:145:VAL:HG13	1:C:150:PHE:CE1	2.52	0.45
1:C:190:THR:O	1:C:190:THR:HG22	2.17	0.45
1:C:282:VAL:HG22	1:C:312:LEU:HD13	1.97	0.45
1:D:207:LYS:HZ2	1:D:207:LYS:HB2	1.81	0.45
1:B:133:TRP:H	1:B:363:HIS:CD2	2.28	0.45
1:B:190:THR:HG22	1:B:190:THR:O	2.16	0.45
1:B:217:ILE:HG12	1:B:218:LYS:N	2.32	0.45
1:C:55:THR:HG22	1:C:56:ILE:N	2.32	0.45
1:D:433:ASP:O	1:D:435:ALA:N	2.49	0.45
1:C:308:VAL:O	1:C:312:LEU:HD22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ILE:HG23	1:B:243:ILE:CB	2.28	0.45
1:D:55:THR:HG22	1:D:57:GLY:H	1.82	0.45
1:A:47:LEU:HD13	1:A:47:LEU:C	2.42	0.45
1:C:221:VAL:HG22	1:C:247:VAL:HG13	1.99	0.45
1:D:13:ARG:CG	1:D:424:TYR:HB2	2.47	0.45
1:D:221:VAL:HB	1:D:228:ASP:OD1	2.17	0.45
1:A:311:GLN:HE22	1:B:282:VAL:N	2.14	0.45
1:B:45:GLU:C	1:B:47:LEU:N	2.75	0.45
1:B:387:LEU:N	1:B:387:LEU:CD1	2.80	0.45
1:D:191:SER:N	1:D:192:PRO:CD	2.79	0.45
1:D:199:ASP:OD2	1:D:230:ARG:NH2	2.50	0.45
1:A:424:TYR:CD1	1:A:425:PRO:HA	2.51	0.45
1:B:11:ASP:OD1	1:B:13:ARG:HD3	2.16	0.45
1:B:176:ARG:HD2	1:B:374:GLY:HA2	1.98	0.45
1:C:140:THR:O	1:C:144:LEU:HD23	2.17	0.45
1:A:153:LEU:HD11	1:A:306:ARG:HD2	1.98	0.44
1:A:176:ARG:HD2	1:A:370:VAL:HA	1.98	0.44
1:B:188:TYR:CB	1:B:216:THR:HB	2.47	0.44
1:C:104:PRO:HD3	1:D:302:HIS:CD2	2.52	0.44
1:B:52:LEU:C	1:B:52:LEU:HD22	2.43	0.44
1:A:62:VAL:HG21	1:B:109:MET:HE2	1.98	0.44
1:A:123:LEU:HD23	1:A:123:LEU:O	2.17	0.44
1:C:93:LEU:HD22	1:C:93:LEU:N	2.32	0.44
1:A:386:HIS:HB3	1:A:387:LEU:CD2	2.47	0.44
1:B:41:THR:OG1	1:B:47:LEU:HD12	2.18	0.44
1:B:423:SER:O	1:B:427:GLY:HA3	2.17	0.44
1:A:106:LYS:NZ	1:B:304:GLN:HE21	2.16	0.44
1:A:135:PHE:O	1:A:139:LEU:HG	2.17	0.44
1:A:221:VAL:CG2	1:A:247:VAL:CG1	2.96	0.44
1:C:44:ALA:C	1:C:46:ASP:N	2.73	0.44
1:D:37:VAL:CG2	1:D:67:VAL:HG11	2.48	0.44
1:D:221:VAL:HB	1:D:228:ASP:CG	2.43	0.44
1:A:151:ARG:HD3	1:A:152:TYR:CZ	2.52	0.44
1:B:308:VAL:O	1:B:312:LEU:HD22	2.17	0.44
1:D:300:GLY:HA2	1:D:303:THR:OG1	2.18	0.44
1:A:83:ILE:HG13	1:A:124:ALA:CB	2.48	0.44
1:B:130:LYS:HE3	1:B:138:GLU:CD	2.43	0.44
1:B:281:ASP:O	1:B:285:HIS:HD2	2.00	0.44
1:B:378:ASP:OD1	1:B:379:ARG:CD	2.66	0.43
1:C:188:TYR:CZ	1:C:382:GLU:HB2	2.53	0.43
1:C:193:GLY:HA3	1:C:219:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:HG2	1:A:43:GLY:HA3	2.00	0.43
1:A:92:ARG:CB	1:A:92:ARG:HH21	2.31	0.43
1:B:44:ALA:O	1:B:47:LEU:N	2.48	0.43
1:C:26:MET:HE3	1:C:26:MET:O	2.18	0.43
1:C:221:VAL:HG21	1:C:247:VAL:CG1	2.48	0.43
1:C:428:ARG:HG2	1:C:428:ARG:NH1	2.31	0.43
1:D:229:ILE:HG13	1:D:268:PHE:CE1	2.53	0.43
1:A:123:LEU:HD23	1:A:123:LEU:C	2.43	0.43
1:D:271:ALA:O	1:D:272:TRP:HB3	2.19	0.43
1:D:322:GLN:HG3	1:D:349:PHE:O	2.19	0.43
1:A:97:SER:HB2	1:B:27:ASN:OD1	2.19	0.43
1:B:75:VAL:O	1:B:75:VAL:HG23	2.19	0.43
1:D:170:GLN:HB3	1:D:171:PRO:HD3	1.99	0.43
1:D:267:GLU:C	1:D:269:ASP:N	2.76	0.43
1:B:180:LEU:CD2	1:B:180:LEU:C	2.92	0.43
1:C:281:ASP:O	1:C:285:HIS:HD2	2.02	0.43
1:A:190:THR:HG22	1:A:218:LYS:HB3	2.01	0.43
1:A:419:ILE:N	1:A:419:ILE:HD12	2.33	0.43
1:B:148:ILE:HD11	1:B:150:PHE:CZ	2.53	0.43
1:A:392:LEU:HD22	1:A:413:GLU:CD	2.44	0.43
1:B:4:ILE:HG21	1:B:74:VAL:HG12	2.01	0.43
1:B:47:LEU:HD13	1:B:123:LEU:HD11	2.01	0.43
1:C:414:MET:CB	1:C:419:ILE:HD11	2.49	0.43
1:D:267:GLU:O	1:D:269:ASP:N	2.52	0.43
1:A:407:VAL:CG1	1:A:408:PRO:HD2	2.48	0.43
1:C:427:GLY:O	1:C:431:VAL:HG22	2.19	0.43
1:D:259:ILE:O	1:D:263:ARG:HG3	2.18	0.43
1:D:350:PRO:HG2	1:D:365:ALA:HB2	2.00	0.43
1:C:170:GLN:N	1:C:171:PRO:CD	2.82	0.42
1:A:39:LEU:HD11	1:A:74:VAL:HG11	1.99	0.42
1:A:189:THR:HG23	1:A:214:PHE:CD2	2.54	0.42
1:A:251:GLN:HE22	1:A:302:HIS:CD2	2.38	0.42
1:C:410:PHE:O	1:C:411:SER:HB2	2.19	0.42
1:B:47:LEU:CD1	1:B:123:LEU:HD11	2.48	0.42
1:C:201:LYS:O	1:C:205:LEU:HD23	2.19	0.42
1:C:391:PHE:O	1:C:394:PRO:HD3	2.19	0.42
1:D:2:ARG:HG2	1:D:2:ARG:NH2	2.35	0.42
1:D:378:ASP:OD1	1:D:379:ARG:HD2	2.19	0.42
1:A:92:ARG:NH2	1:A:92:ARG:CB	2.83	0.42
1:D:308:VAL:O	1:D:312:LEU:HD22	2.19	0.42
1:A:8:GLU:HG2	1:A:38:VAL:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:PHE:C	1:A:16:THR:H	2.28	0.42
1:C:236:ARG:NH2	1:C:269:ASP:HB3	2.35	0.42
1:C:295:VAL:HA	1:C:296:PRO:HD3	1.88	0.42
1:A:167:ARG:O	1:A:170:GLN:HB3	2.20	0.42
1:B:43:GLY:O	1:B:45:GLU:N	2.52	0.42
1:C:3:THR:HG23	1:C:77:LEU:O	2.19	0.42
1:A:282:VAL:HG22	1:A:312:LEU:HD13	2.02	0.42
1:A:304:GLN:HE21	1:B:106:LYS:NZ	2.17	0.42
1:B:1:MET:HE3	1:B:3:THR:OG1	2.19	0.42
1:C:150:PHE:CZ	1:C:159:ARG:HA	2.55	0.42
1:D:55:THR:CG2	1:D:56:ILE:N	2.82	0.42
1:D:176:ARG:CD	1:D:374:GLY:HA2	2.49	0.42
1:D:253:TRP:HB2	1:D:258:ALA:HB2	2.01	0.42
1:C:427:GLY:O	1:C:428:ARG:C	2.63	0.42
1:A:71:ALA:O	1:A:75:VAL:HG22	2.20	0.41
1:B:142:GLU:CG	1:D:200:GLU:HG2	2.48	0.41
1:B:210:VAL:CG2	1:B:239:ILE:HG13	2.50	0.41
1:C:304:GLN:HE21	1:C:304:GLN:HB3	1.70	0.41
1:C:305:ASN:HB2	1:C:333:GLU:OE1	2.20	0.41
1:B:55:THR:CG2	1:B:56:ILE:N	2.82	0.41
1:C:328:VAL:HG22	1:C:333:GLU:CD	2.44	0.41
1:C:414:MET:HB2	1:C:419:ILE:HD11	2.02	0.41
1:D:309:PHE:CE1	1:D:337:ILE:HD13	2.55	0.41
1:B:13:ARG:CG	1:B:424:TYR:HB2	2.51	0.41
1:B:47:LEU:HD13	1:B:47:LEU:C	2.45	0.41
1:C:26:MET:HE2	1:D:100:ARG:HD3	2.03	0.41
1:C:324:ASP:OD2	1:C:351:HIS:HD2	2.03	0.41
1:D:75:VAL:HG23	1:D:75:VAL:O	2.19	0.41
1:B:159:ARG:HG2	1:B:159:ARG:HH11	1.85	0.41
1:B:303:THR:HB	1:B:309:PHE:CE1	2.55	0.41
1:B:308:VAL:HG12	1:B:312:LEU:CD2	2.50	0.41
1:D:102:LEU:N	1:D:102:LEU:HD22	2.34	0.41
1:A:73:HIS:HE1	1:A:96:ASP:OD2	2.03	0.41
1:B:221:VAL:HG21	1:B:247:VAL:HG11	2.02	0.41
1:C:139:LEU:HD12	1:C:144:LEU:HD13	2.03	0.41
1:C:239:ILE:HG23	1:C:243:ILE:CB	2.32	0.41
1:C:350:PRO:HG2	1:C:365:ALA:HB2	2.02	0.41
1:A:83:ILE:HG13	1:A:124:ALA:HB2	2.02	0.41
1:C:387:LEU:HD22	1:C:387:LEU:N	2.35	0.41
1:C:419:ILE:HD12	1:C:419:ILE:N	2.36	0.41
1:B:99:LEU:HD12	1:B:99:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:VAL:N	1:D:311:GLN:NE2	2.67	0.41
1:C:323:ILE:HD11	1:C:337:ILE:HG22	2.02	0.41
1:D:255:VAL:O	1:D:259:ILE:HG13	2.21	0.41
1:D:281:ASP:O	1:D:285:HIS:HD2	2.04	0.41
1:A:9:THR:HB	1:A:64:THR:HG23	2.03	0.41
1:A:52:LEU:HD12	1:A:52:LEU:O	2.21	0.41
1:A:144:LEU:HD12	1:A:144:LEU:HA	1.97	0.41
1:A:148:ILE:HD12	1:A:149:ASP:N	2.36	0.41
1:A:188:TYR:CZ	1:A:382:GLU:HB2	2.56	0.41
1:A:230:ARG:HH21	1:A:230:ARG:HG2	1.86	0.41
1:A:271:ALA:O	1:A:272:TRP:HB3	2.21	0.41
1:B:55:THR:HG21	1:B:60:ASN:CB	2.50	0.41
1:B:63:GLN:NE2	1:B:111:MET:HE3	2.36	0.41
1:B:134:ARG:O	1:B:138:GLU:HG3	2.21	0.41
1:C:52:LEU:N	1:C:52:LEU:CD2	2.84	0.41
1:C:192:PRO:HG3	1:C:217:ILE:HD11	2.02	0.41
1:C:368:ASP:OD2	1:C:373:THR:HG23	2.20	0.41
1:C:434:LEU:N	1:C:434:LEU:HD22	2.36	0.41
1:A:47:LEU:HD22	1:A:47:LEU:HA	1.86	0.41
1:A:29:ASP:N	1:A:30:PRO:HD3	2.35	0.40
1:B:3:THR:CG2	1:B:4:ILE:N	2.84	0.40
1:C:130:LYS:C	1:C:408:PRO:HA	2.45	0.40
1:C:305:ASN:HA	1:C:328:VAL:HG23	2.03	0.40
1:A:2:ARG:HG2	1:A:43:GLY:CA	2.51	0.40
1:B:396:ARG:HH11	1:B:396:ARG:CG	2.33	0.40
1:C:219:LEU:HD11	1:C:235:ALA:CB	2.51	0.40
1:D:25:ALA:N	1:D:195:LEU:HD12	2.36	0.40
1:A:384:VAL:CG1	1:A:386:HIS:ND1	2.85	0.40
1:B:3:THR:HG22	1:B:4:ILE:N	2.37	0.40
1:B:55:THR:HB	1:B:60:ASN:OD1	2.22	0.40
1:B:300:GLY:HA2	1:B:303:THR:OG1	2.22	0.40
1:D:47:LEU:CD1	1:D:123:LEU:HD21	2.46	0.40
1:D:356:GLY:HA2	1:D:359:GLU:OE2	2.22	0.40
1:D:378:ASP:OD1	1:D:379:ARG:HD3	2.21	0.40
1:A:185:TYR:CD1	1:A:186:PRO:HD2	2.57	0.40
1:A:218:LYS:HA	1:A:246:ALA:O	2.22	0.40
1:C:53:VAL:CG2	1:C:115:ALA:HB2	2.51	0.40
1:C:407:VAL:CG1	1:C:408:PRO:HD2	2.49	0.40
1:D:200:GLU:C	1:D:203:VAL:HG22	2.46	0.40
1:D:207:LYS:CG	1:D:238:ALA:HB1	2.50	0.40
1:D:387:LEU:HD12	1:D:387:LEU:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLU:HG3	1:A:38:VAL:HB	2.01	0.40
1:A:28:PRO:O	1:A:30:PRO:HD3	2.20	0.40
1:B:102:LEU:HD12	1:B:109:MET:CE	2.51	0.40
1:C:104:PRO:O	1:C:106:LYS:HE3	2.21	0.40
1:C:306:ARG:HH11	1:C:306:ARG:HG2	1.86	0.40
1:D:2:ARG:HG2	1:D:2:ARG:H	1.49	0.40
1:D:220:LYS:NZ	3:D:668:HOH:O	2.55	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	422/436 (97%)	405 (96%)	17 (4%)	0	100	100
1	B	430/436 (99%)	412 (96%)	16 (4%)	2 (0%)	24	21
1	C	432/436 (99%)	405 (94%)	25 (6%)	2 (0%)	24	21
1	D	429/436 (98%)	407 (95%)	19 (4%)	3 (1%)	18	14
All	All	1713/1744 (98%)	1629 (95%)	77 (4%)	7 (0%)	30	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	ALA
1	D	268	PHE
1	D	434	LEU
1	D	269	ASP
1	C	22	GLY
1	C	387	LEU
1	B	328	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/340 (98%)	313 (94%)	21 (6%)	16	13
1	B	338/340 (99%)	320 (95%)	18 (5%)	20	18
1	C	340/340 (100%)	322 (95%)	18 (5%)	20	18
1	D	338/340 (99%)	314 (93%)	24 (7%)	13	10
All	All	1350/1360 (99%)	1269 (94%)	81 (6%)	17	14

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	47	LEU
1	A	86	LEU
1	A	93	LEU
1	A	99	LEU
1	A	144	LEU
1	A	148	ILE
1	A	172	GLN
1	A	180	LEU
1	A	200	GLU
1	A	202	LEU
1	A	239	ILE
1	A	263	ARG
1	A	273	ILE
1	A	302	HIS
1	A	312	LEU
1	A	340	LEU
1	A	357	LEU
1	A	361	VAL
1	A	377	GLU
1	A	379	ARG
1	B	13	ARG
1	B	39	LEU
1	B	52	LEU

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Mol	Chain	Res	Type
1	B	55	THR
1	B	62	VAL
1	B	99	LEU
1	B	148	ILE
1	B	172	GLN
1	B	202	LEU
1	B	225	VAL
1	B	239	ILE
1	B	273	ILE
1	B	312	LEU
1	B	313	LEU
1	B	340	LEU
1	B	361	VAL
1	B	379	ARG
1	B	396	ARG
1	C	39	LEU
1	C	99	LEU
1	C	123	LEU
1	C	148	ILE
1	C	151	ARG
1	C	159	ARG
1	C	172	GLN
1	C	195	LEU
1	C	239	ILE
1	C	247	VAL
1	C	263	ARG
1	C	273	ILE
1	C	302	HIS
1	C	312	LEU
1	C	313	LEU
1	C	323	ILE
1	C	340	LEU
1	C	379	ARG
1	D	13	ARG
1	D	39	LEU
1	D	52	LEU
1	D	55	THR
1	D	93	LEU
1	D	123	LEU
1	D	144	LEU
1	D	148	ILE
1	D	159	ARG

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Mol	Chain	Res	Type
1	D	172	GLN
1	D	180	LEU
1	D	202	LEU
1	D	207	LYS
1	D	239	ILE
1	D	273	ILE
1	D	293	THR
1	D	302	HIS
1	D	312	LEU
1	D	313	LEU
1	D	340	LEU
1	D	357	LEU
1	D	361	VAL
1	D	379	ARG
1	D	425	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	129	ASN
1	A	285	HIS
1	A	302	HIS
1	A	304	GLN
1	A	311	GLN
1	A	314	GLN
1	A	322	GLN
1	A	351	HIS
1	A	363	HIS
1	A	390	HIS
1	A	399	HIS
1	B	10	HIS
1	B	63	GLN
1	B	73	HIS
1	B	170	GLN
1	B	172	GLN
1	B	183	GLN
1	B	250	ASN
1	B	285	HIS
1	B	304	GLN
1	B	311	GLN
1	B	314	GLN

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Mol	Chain	Res	Type
1	B	322	GLN
1	B	351	HIS
1	B	363	HIS
1	B	390	HIS
1	C	63	GLN
1	C	73	HIS
1	C	95	ASN
1	C	170	GLN
1	C	172	GLN
1	C	226	GLN
1	C	250	ASN
1	C	285	HIS
1	C	302	HIS
1	C	304	GLN
1	C	311	GLN
1	C	314	GLN
1	C	351	HIS
1	C	363	HIS
1	C	389	GLN
1	C	399	HIS
1	D	63	GLN
1	D	73	HIS
1	D	170	GLN
1	D	172	GLN
1	D	183	GLN
1	D	250	ASN
1	D	251	GLN
1	D	285	HIS
1	D	302	HIS
1	D	304	GLN
1	D	311	GLN
1	D	314	GLN
1	D	351	HIS
1	D	363	HIS
1	D	390	HIS

5.3.3 RNA ⓘ

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	426/436 (97%)	0.52	24 (5%)	30	29	21, 34, 58, 84	0
1	B	432/436 (99%)	0.41	27 (6%)	26	24	21, 32, 55, 87	0
1	C	434/436 (99%)	0.83	49 (11%)	10	9	21, 39, 68, 88	0
1	D	433/436 (99%)	0.65	47 (10%)	10	9	24, 36, 59, 84	0
All	All	1725/1744 (98%)	0.60	147 (8%)	16	15	21, 35, 60, 88	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	ASP	6.0
1	A	28	PRO	5.7
1	D	434	LEU	5.6
1	A	434	LEU	5.3
1	D	202	LEU	5.3
1	B	44	ALA	5.2
1	C	20	LEU	5.1
1	C	44	ALA	5.0
1	A	47	LEU	4.9
1	C	47	LEU	4.8
1	D	234	LEU	4.7
1	C	434	LEU	4.4
1	D	1	MET	4.3
1	D	238	ALA	4.2
1	A	44	ALA	4.2
1	B	430	TRP	4.0
1	D	235	ALA	3.9
1	A	426	ASP	3.9
1	D	239	ILE	3.8
1	D	205	LEU	3.8
1	D	199	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	237	ALA	3.6
1	D	436	ALA	3.6
1	D	221	VAL	3.5
1	B	47	LEU	3.5
1	D	23	SER	3.4
1	D	435	ALA	3.4
1	D	45	GLU	3.4
1	A	424	TYR	3.4
1	D	192	PRO	3.4
1	A	217	ILE	3.4
1	C	43	GLY	3.4
1	B	431	VAL	3.4
1	D	195	LEU	3.3
1	C	46	ASP	3.3
1	D	203	VAL	3.3
1	D	46	ASP	3.3
1	C	430	TRP	3.2
1	D	268	PHE	3.2
1	D	197	TYR	3.2
1	C	180	LEU	3.1
1	D	2	ARG	3.1
1	C	399	HIS	3.1
1	B	432	GLU	3.1
1	C	127	ALA	3.1
1	D	146	ASP	3.0
1	D	229	ILE	3.0
1	D	193	GLY	3.0
1	D	194	TRP	3.0
1	C	422	PHE	3.0
1	C	386	HIS	3.0
1	D	198	SER	3.0
1	B	353	GLY	3.0
1	C	429	PHE	3.0
1	C	417	ALA	2.9
1	B	399	HIS	2.9
1	D	201	LYS	2.9
1	D	196	GLY	2.9
1	D	24	ASP	2.8
1	C	164	ALA	2.8
1	B	426	ASP	2.7
1	B	83	ILE	2.7
1	A	194	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.7
1	B	46	ASP	2.7
1	C	48	ALA	2.6
1	A	57	GLY	2.6
1	C	431	VAL	2.6
1	C	187	ALA	2.6
1	D	293	THR	2.6
1	B	385	ASP	2.6
1	D	240	GLY	2.6
1	B	42	ASP	2.5
1	D	83	ILE	2.5
1	C	45	GLU	2.5
1	A	429	PHE	2.5
1	C	181	ILE	2.5
1	C	426	ASP	2.4
1	C	424	TYR	2.4
1	B	195	LEU	2.4
1	B	429	PHE	2.4
1	C	22	GLY	2.4
1	D	217	ILE	2.4
1	D	191	SER	2.4
1	C	414	MET	2.4
1	C	425	PRO	2.4
1	C	21	ASP	2.4
1	C	355	VAL	2.4
1	D	225	VAL	2.4
1	D	3	THR	2.4
1	D	206	ALA	2.4
1	A	432	GLU	2.4
1	B	43	GLY	2.4
1	B	168	ASP	2.4
1	D	19	GLU	2.3
1	C	163	LEU	2.3
1	C	384	VAL	2.3
1	C	16	THR	2.3
1	C	392	LEU	2.3
1	B	217	ILE	2.3
1	A	431	VAL	2.3
1	A	29	ASP	2.3
1	C	24	ASP	2.3
1	B	407	VAL	2.3
1	A	18	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	232	CYS	2.3
1	C	86	LEU	2.3
1	C	83	ILE	2.2
1	C	3	THR	2.2
1	A	58	ARG	2.2
1	B	1	MET	2.2
1	C	169	ALA	2.2
1	D	200	GLU	2.2
1	A	430	TRP	2.2
1	A	17	SER	2.2
1	D	148	ILE	2.2
1	B	146	ASP	2.2
1	C	432	GLU	2.2
1	C	387	LEU	2.2
1	C	18	ARG	2.2
1	C	126	ARG	2.2
1	C	41	THR	2.2
1	D	426	ASP	2.2
1	C	138	GLU	2.2
1	C	400	GLY	2.2
1	B	48	ALA	2.2
1	A	83	ILE	2.1
1	B	354	GLY	2.1
1	B	148	ILE	2.1
1	C	37	VAL	2.1
1	D	204	ARG	2.1
1	B	84	ALA	2.1
1	A	56	ILE	2.1
1	C	217	ILE	2.1
1	A	247	VAL	2.1
1	C	407	VAL	2.1
1	A	433	ASP	2.1
1	B	16	THR	2.1
1	C	74	VAL	2.1
1	B	23	SER	2.1
1	D	266	ALA	2.1
1	D	207	LYS	2.0
1	C	5	ILE	2.0
1	D	210	VAL	2.0
1	C	23	SER	2.0
1	B	178	ALA	2.0
1	A	427	GLY	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	MG	D	604	1/1	0.85	0.16	56,56,56,56	0
2	MG	C	603	1/1	0.90	0.09	37,37,37,37	0
2	MG	B	602	1/1	0.92	0.07	31,31,31,31	0
2	MG	A	601	1/1	0.97	0.07	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.