



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:04 AM EDT

PDB ID : 1DCN / pdb_00001dcn
Title : INACTIVE MUTANT H162N OF DELTA 2 CRYSTALLIN WITH BOUND ARGININOSUCCINATE
Authors : Vallee, F.; Turner, M.A.; Lindley, P.; Howell, P.L.
Deposited on : 1998-10-29
Resolution : 2.30 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:

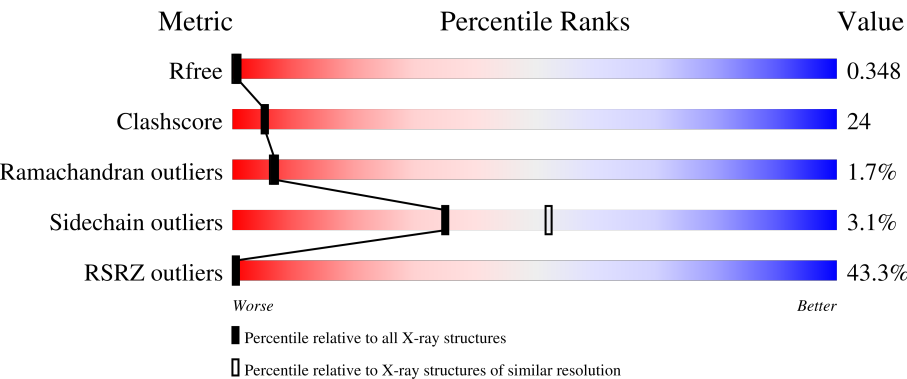
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	447	49% 54% 36% 5% 5%
1	B	447	30% 55% 36% . 6%
1	C	447	57% 50% 43% . .
1	D	447	30% 59% 36% . .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AS1	D	0	X	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13754 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.

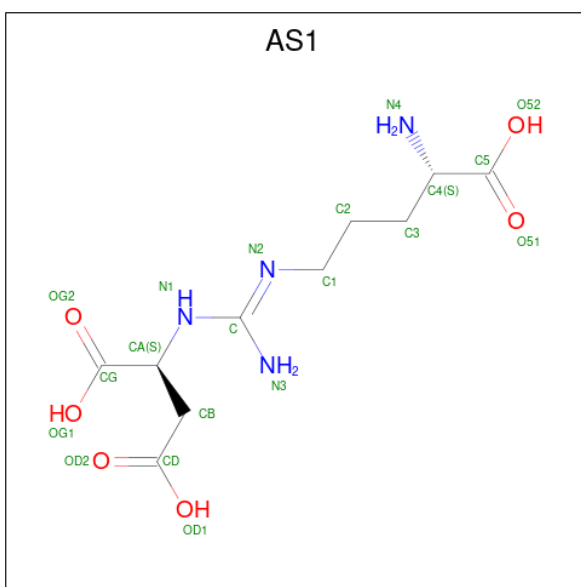
- Molecule 1 is a protein called DELTA 2 CRYSTALLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3287	2080	557	640	10			
1	B	418	Total	C	N	O	S	0	0	0
			3239	2050	549	629	11			
1	C	434	Total	C	N	O	S	0	0	0
			3360	2127	568	654	11			
1	D	436	Total	C	N	O	S	0	0	0
			3377	2139	571	656	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ASN	HIS	conflict	UNP P24058
A	162	ASN	HIS	engineered mutation	UNP P24058
A	302	SER	ALA	conflict	UNP P24058
A	409	ASN	LYS	conflict	UNP P24058
B	110	ASN	HIS	conflict	UNP P24058
B	162	ASN	HIS	engineered mutation	UNP P24058
B	302	SER	ALA	conflict	UNP P24058
B	409	ASN	LYS	conflict	UNP P24058
C	110	ASN	HIS	conflict	UNP P24058
C	162	ASN	HIS	engineered mutation	UNP P24058
C	302	SER	ALA	conflict	UNP P24058
C	409	ASN	LYS	conflict	UNP P24058
D	110	ASN	HIS	conflict	UNP P24058
D	162	ASN	HIS	engineered mutation	UNP P24058
D	302	SER	ALA	conflict	UNP P24058
D	409	ASN	LYS	conflict	UNP P24058

- Molecule 2 is ARGININOSUCCINATE (CCD ID: AS1) (formula: C₁₀H₁₈N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			20	10	4	6		

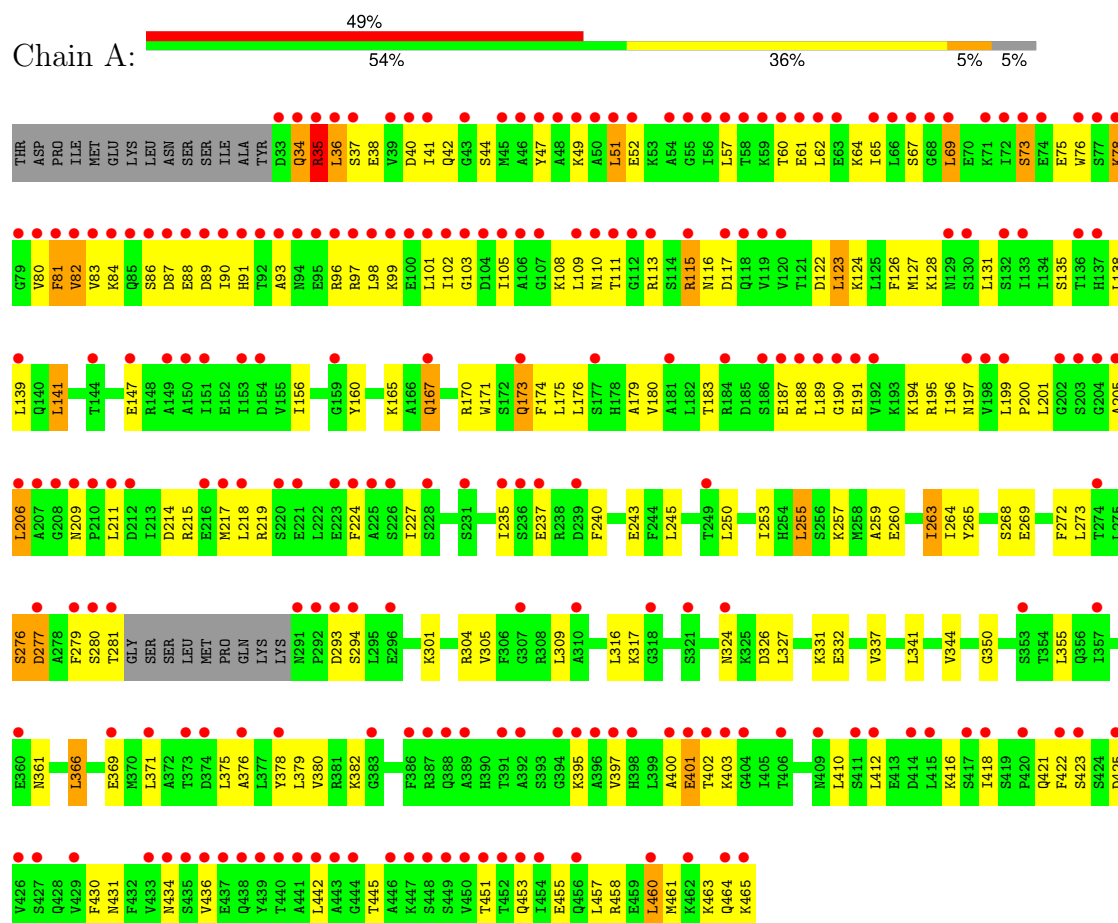
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	123	Total O 123 123	0	0
3	B	126	Total O 126 126	0	0
3	C	110	Total O 110 110	0	0
3	D	112	Total O 112 112	0	0

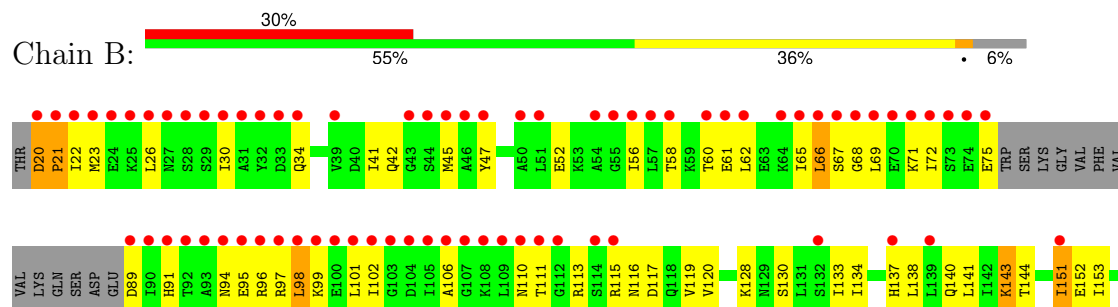
3 Residue-property plots

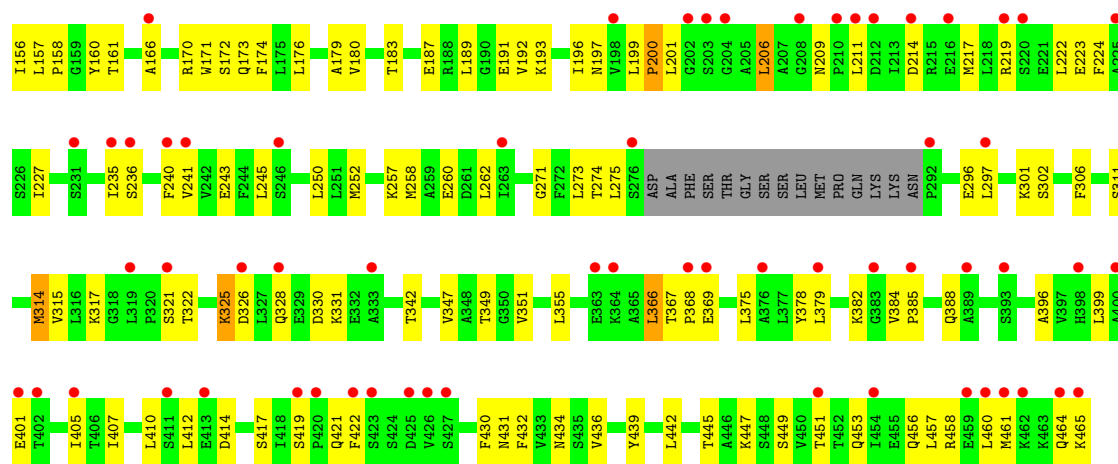
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DELTA 2 CRYSTALLIN

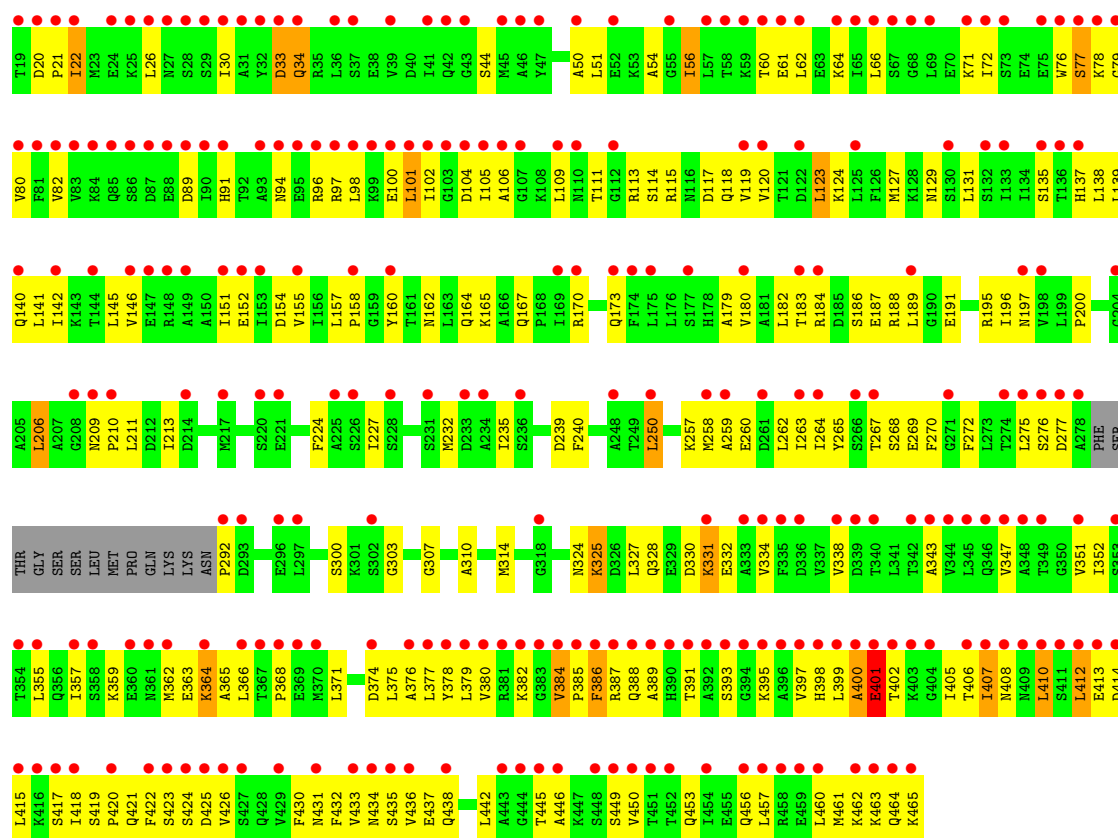


• Molecule 1: DELTA 2 CRYSTALLIN

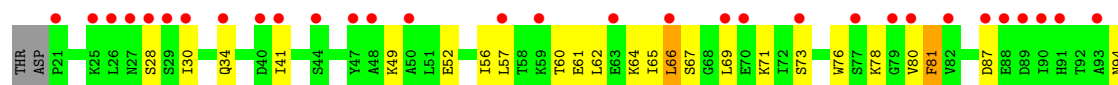


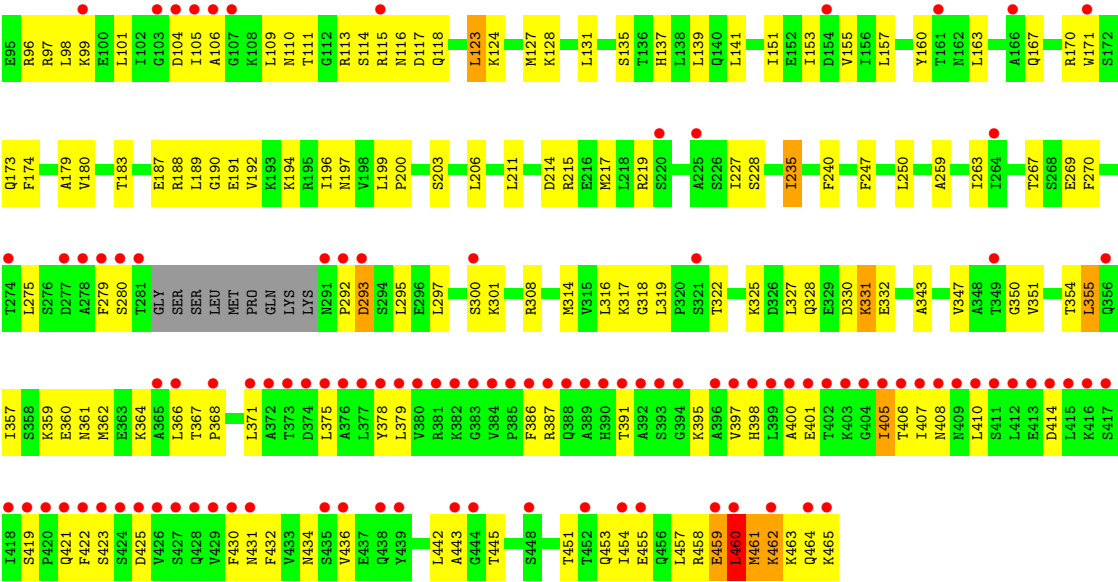


• Molecule 1: DELTA 2 CRYSTALLIN



• Molecule 1: DELTA 2 CRYSTALLIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.58Å 99.59Å 107.14Å 90.00° 101.68° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	82.8 (20.00-2.30) 75.8 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.27Å)	Xtriage
Refinement program	CNS 0.3C	Depositor
R, R_{free}	0.229 , 0.290 0.350 , 0.348	Depositor DCC
R_{free} test set	6682 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	13754	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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: AS1

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	0/3326	0.97	18/4484 (0.4%)
1	B	0.41	0/3275	0.94	11/4413 (0.2%)
1	C	0.41	0/3400	0.95	11/4584 (0.2%)
1	D	0.42	0/3418	0.93	10/4608 (0.2%)
All	All	0.41	0/13419	0.95	50/18089 (0.3%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	SER	N-CA-C	-8.90	102.55	113.41
1	D	461	MET	N-CA-C	-8.78	98.12	110.50
1	B	20	ASP	CA-C-N	8.53	130.50	119.84
1	B	20	ASP	C-N-CA	8.53	130.50	119.84
1	C	401	GLU	N-CA-C	-8.24	103.23	113.20
1	B	209	ASN	CA-C-N	7.50	127.13	119.56
1	B	209	ASN	C-N-CA	7.50	127.13	119.56
1	A	209	ASN	CA-C-N	7.43	127.07	119.56
1	A	209	ASN	C-N-CA	7.43	127.07	119.56
1	D	151	ILE	N-CA-C	7.30	117.43	110.42
1	D	331	LYS	N-CA-C	7.29	119.92	111.02
1	C	400	ALA	N-CA-C	-7.05	103.35	112.23
1	D	463	LYS	N-CA-C	-6.99	103.74	111.36
1	A	331	LYS	N-CA-C	6.88	119.37	111.11
1	B	151	ILE	N-CA-C	6.53	117.32	110.72
1	A	167	GLN	N-CA-C	6.33	113.82	108.13
1	C	209	ASN	CA-C-N	6.24	126.78	120.04
1	C	209	ASN	C-N-CA	6.24	126.78	120.04
1	A	160	TYR	N-CA-C	6.22	119.68	109.72
1	B	67	SER	N-CA-C	-6.15	105.27	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	TYR	N-CA-C	6.02	118.65	109.62
1	B	160	TYR	N-CA-C	5.85	119.26	109.95
1	D	354	THR	N-CA-C	5.82	120.00	113.02
1	A	276	SER	N-CA-C	5.81	119.84	112.87
1	D	160	TYR	N-CA-C	5.78	118.97	109.72
1	C	384	VAL	CA-C-N	5.73	126.05	119.92
1	C	384	VAL	C-N-CA	5.73	126.05	119.92
1	A	263	ILE	N-CA-C	-5.56	105.08	110.42
1	C	331	LYS	N-CA-C	5.55	117.79	111.02
1	A	83	VAL	N-CA-C	5.53	116.14	108.23
1	C	160	TYR	N-CA-C	5.49	118.53	109.85
1	D	460	LEU	N-CA-C	-5.49	104.52	111.11
1	A	224	PHE	N-CA-C	-5.46	102.38	110.46
1	C	413	GLU	N-CA-C	-5.44	106.49	113.02
1	A	173	GLN	N-CA-C	-5.43	105.44	111.36
1	A	253	ILE	N-CA-C	-5.37	105.26	110.42
1	A	73	SER	N-CA-C	-5.32	105.59	111.71
1	B	417	SER	N-CA-C	-5.31	106.76	113.18
1	D	115	ARG	N-CA-C	-5.22	106.17	112.54
1	C	268	SER	N-CA-C	-5.21	105.49	111.07
1	D	367	THR	CA-C-N	5.21	125.01	119.28
1	D	367	THR	C-N-CA	5.21	125.01	119.28
1	A	51	LEU	N-CA-C	-5.13	105.77	112.23
1	A	69	LEU	N-CA-C	-5.13	105.58	111.07
1	A	401	GLU	N-CA-C	-5.10	105.90	111.82
1	C	162	ASN	N-CA-C	-5.08	104.30	111.56
1	A	35	ARG	N-CA-C	5.06	121.57	110.80
1	B	236	SER	N-CA-C	5.06	119.72	113.50
1	B	396	ALA	N-CA-C	-5.05	105.86	111.36
1	A	268	SER	N-CA-C	-5.01	105.71	111.07

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	3287	0	3391	175	0
1	B	3239	0	3357	144	0
1	C	3360	0	3470	212	0
1	D	3377	0	3486	151	0
2	D	20	0	13	9	0
3	A	123	0	0	11	0
3	B	126	0	0	10	0
3	C	110	0	0	12	0
3	D	112	0	0	7	0
All	All	13754	0	13717	654	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 24.

All (654) 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)
2:D:0:AS1:CB	2:D:0:AS1:CA	1.79	1.60
2:D:0:AS1:N2	2:D:0:AS1:C1	1.69	1.53
1:B:456:GLN:O	1:B:460:LEU:HD23	1.66	0.95
1:A:403:LYS:HE2	1:A:403:LYS:HA	1.48	0.92
1:C:131:LEU:HD22	1:C:189:LEU:HD11	1.51	0.90
1:C:61:GLU:HG2	1:C:105:ILE:HD11	1.53	0.90
1:A:431:ASN:HB3	1:A:434:ASN:HD22	1.42	0.85
1:D:436:VAL:HG13	1:D:445:THR:HG23	1.60	0.83
1:B:173:GLN:HE22	1:B:453:GLN:HE22	1.24	0.83
1:D:366:LEU:HB3	1:D:432:PHE:CE2	2.14	0.83
1:D:155:VAL:HG22	1:D:359:LYS:HE3	1.59	0.82
1:B:458:ARG:HA	1:B:461:MET:HE2	1.62	0.81
1:B:140:GLN:O	1:B:144:THR:HG23	1.81	0.81
1:C:123:LEU:HD12	3:C:514:HOH:O	1.80	0.81
1:D:275:LEU:HB2	1:D:280:SER:HB3	1.61	0.80
1:A:397:VAL:O	1:A:401:GLU:HB2	1.80	0.79
1:C:415:LEU:HD23	1:C:418:ILE:HD12	1.64	0.79
1:B:193:LYS:HE3	3:B:523:HOH:O	1.83	0.78
1:D:464:GLN:O	1:D:465:LYS:HB2	1.83	0.77
1:A:80:VAL:O	1:A:81:PHE:HB2	1.83	0.77
1:D:397:VAL:O	1:D:401:GLU:HB2	1.85	0.77
1:A:379:LEU:HD11	1:A:422:PHE:CE1	2.19	0.76
1:D:215:ARG:HH22	1:D:228:SER:HB2	1.50	0.76
1:C:374:ASP:HA	1:C:377:LEU:HD12	1.66	0.76
1:C:378:TYR:O	1:C:382:LYS:HG2	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ILE:HD11	1:B:106:ALA:HB2	1.69	0.74
1:B:206:LEU:HD21	1:D:167:GLN:HG2	1.68	0.74
1:A:110:ASN:HD22	1:A:113:ARG:HB3	1.53	0.73
1:D:60:THR:HG22	1:D:64:LYS:HE2	1.70	0.73
1:D:200:PRO:HA	1:D:228:SER:OG	1.87	0.73
1:A:111:THR:HG22	1:A:211:LEU:HD11	1.70	0.73
1:C:131:LEU:HD22	1:C:189:LEU:CD1	2.19	0.72
1:D:173:GLN:HE22	1:D:453:GLN:HE22	1.35	0.72
2:D:0:AS1:N2	2:D:0:AS1:H12	1.99	0.72
1:D:170:ARG:HG3	1:D:436:VAL:HG11	1.72	0.71
1:A:102:ILE:HG13	1:A:103:GLY:H	1.55	0.71
1:B:143:LYS:NZ	1:B:143:LYS:HB2	2.06	0.71
1:A:332:GLU:HG3	3:A:480:HOH:O	1.90	0.71
1:A:369:GLU:HG3	3:A:574:HOH:O	1.91	0.71
1:C:405:ILE:HD11	1:C:410:LEU:HD23	1.73	0.71
1:A:199:LEU:HD11	1:A:201:LEU:HB3	1.74	0.70
1:D:196:ILE:HG12	1:D:240:PHE:HB2	1.73	0.70
1:C:400:ALA:HB1	1:C:405:ILE:O	1.91	0.70
1:C:398:HIS:O	1:C:401:GLU:HG3	1.92	0.69
1:C:332:GLU:HG3	3:C:529:HOH:O	1.92	0.69
1:A:78:LYS:NZ	1:A:78:LYS:HB3	2.07	0.69
1:B:314:MET:HG2	1:C:303:GLY:HA2	1.74	0.69
1:B:111:THR:OG1	1:D:386:PHE:HB2	1.93	0.69
1:B:436:VAL:HG13	1:B:445:THR:HG23	1.75	0.69
1:B:144:THR:HG21	1:B:349:THR:HG23	1.74	0.69
1:C:386:PHE:HE2	1:C:387:ARG:HH21	1.41	0.69
1:C:173:GLN:HE22	1:C:453:GLN:HE22	1.40	0.68
1:C:460:LEU:O	1:C:464:GLN:HG2	1.94	0.68
1:A:382:LYS:HE2	1:A:421:GLN:O	1.93	0.68
1:A:395:LYS:HD2	1:A:418:ILE:HG23	1.75	0.68
1:D:135:SER:O	1:D:139:LEU:HD13	1.94	0.68
1:C:257:LYS:HD3	3:C:479:HOH:O	1.93	0.67
1:A:87:ASP:HB3	1:A:96:ARG:HH21	1.59	0.67
1:C:379:LEU:HB3	1:C:384:VAL:HB	1.76	0.67
1:D:131:LEU:HD22	1:D:189:LEU:HD11	1.75	0.67
1:B:179:ALA:O	1:B:183:THR:HG23	1.94	0.67
1:A:127:MET:O	1:A:131:LEU:HG	1.95	0.67
1:D:398:HIS:O	1:D:401:GLU:HB3	1.94	0.66
1:A:190:GLY:O	1:A:194:LYS:HG2	1.96	0.66
1:A:378:TYR:HD2	1:A:379:LEU:HD12	1.61	0.66
1:C:374:ASP:CG	1:C:438:GLN:HE22	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:SER:HB3	1:C:109:LEU:HD21	1.77	0.66
1:C:154:ASP:HB2	3:C:558:HOH:O	1.94	0.66
1:A:115:ARG:NH1	1:A:116:ASN:HD21	1.94	0.66
1:B:219:ARG:HG2	1:B:219:ARG:HH11	1.60	0.66
1:D:461:MET:O	1:D:462:LYS:HB3	1.95	0.65
1:B:274:THR:HG23	3:B:568:HOH:O	1.95	0.65
1:A:277:ASP:HA	1:A:280:SER:OG	1.97	0.65
1:C:22:ILE:N	1:C:22:ILE:HD12	2.11	0.65
1:D:400:ALA:HB2	1:D:410:LEU:HD21	1.78	0.65
1:A:173:GLN:HA	1:A:173:GLN:HE21	1.61	0.65
1:B:41:ILE:HD11	1:B:72:ILE:HG22	1.79	0.65
1:C:435:SER:HA	1:C:438:GLN:HE21	1.61	0.64
2:D:0:AS1:CB	2:D:0:AS1:CG	2.72	0.64
1:C:414:ASP:O	1:C:417:SER:N	2.25	0.64
1:B:111:THR:HG22	1:B:211:LEU:HD11	1.79	0.64
1:D:111:THR:HG22	1:D:211:LEU:HD11	1.78	0.64
1:A:101:LEU:HD22	1:A:101:LEU:H	1.60	0.64
1:B:52:GLU:HG3	1:B:62:LEU:HD22	1.80	0.64
1:A:90:ILE:HD12	1:A:93:ALA:HB3	1.79	0.64
1:A:173:GLN:HE22	1:A:453:GLN:HE22	1.46	0.64
1:C:431:ASN:HB3	1:C:434:ASN:HD22	1.61	0.63
1:D:461:MET:O	1:D:462:LYS:CB	2.46	0.63
1:D:362:MET:O	1:D:366:LEU:HD13	1.95	0.63
1:B:98:LEU:HD22	1:B:106:ALA:HB2	1.78	0.63
1:C:357:ILE:HB	1:C:362:MET:HE3	1.81	0.63
1:D:49:LYS:NZ	1:D:66:LEU:HD21	2.14	0.63
1:D:361:ASN:HA	1:D:364:LYS:HE2	1.81	0.63
1:B:442:LEU:HB3	3:D:498:HOH:O	1.98	0.62
1:C:386:PHE:HE2	1:C:387:ARG:NH2	1.96	0.62
2:D:0:AS1:N2	2:D:0:AS1:H11	1.99	0.62
1:C:363:GLU:HA	1:C:366:LEU:HD13	1.79	0.62
1:C:393:SER:O	1:C:397:VAL:HG23	1.99	0.62
1:A:219:ARG:HH11	1:A:219:ARG:HG2	1.65	0.62
1:B:311:SER:O	1:B:315:VAL:HG23	1.99	0.62
1:A:102:ILE:HG13	1:A:103:GLY:N	2.15	0.61
1:A:131:LEU:HD11	1:A:196:ILE:HD12	1.80	0.61
1:A:214:ASP:OD2	1:A:217:MET:HB2	2.01	0.61
1:C:414:ASP:O	1:C:417:SER:OG	2.18	0.61
1:D:190:GLY:O	1:D:194:LYS:HG2	1.99	0.61
1:D:110:ASN:HD22	1:D:113:ARG:HB3	1.65	0.61
1:B:405:ILE:HD11	1:B:410:LEU:HD23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLU:O	1:A:191:GLU:HG3	2.01	0.61
1:B:214:ASP:OD2	1:B:217:MET:HB2	2.01	0.60
1:B:458:ARG:HA	1:B:461:MET:CE	2.30	0.60
1:B:379:LEU:HB3	1:B:384:VAL:HB	1.83	0.60
1:B:378:TYR:O	1:B:382:LYS:HG2	2.02	0.60
1:A:460:LEU:O	1:A:464:GLN:HG2	2.01	0.60
1:A:170:ARG:HG3	1:A:436:VAL:HG11	1.82	0.60
1:D:49:LYS:HZ3	1:D:66:LEU:HD21	1.65	0.60
1:C:179:ALA:O	1:C:183:THR:HG23	2.02	0.60
1:C:56:ILE:HD12	1:C:56:ILE:N	2.16	0.60
1:A:176:LEU:O	1:A:180:VAL:HG23	2.01	0.60
1:B:98:LEU:HD22	1:B:106:ALA:CB	2.32	0.60
1:B:173:GLN:HE22	1:B:453:GLN:NE2	1.99	0.60
1:C:72:ILE:HD11	1:C:94:ASN:ND2	2.16	0.60
1:C:269:GLU:H	1:C:269:GLU:CD	2.10	0.60
1:D:459:GLU:OE1	1:D:462:LYS:HD3	2.02	0.60
1:D:173:GLN:HE21	1:D:173:GLN:HA	1.67	0.59
1:A:60:THR:O	1:A:64:LYS:HD3	2.03	0.59
1:A:276:SER:O	1:A:277:ASP:HB2	2.02	0.59
1:B:379:LEU:HD11	1:B:422:PHE:CE1	2.37	0.59
1:C:331:LYS:HD2	3:C:528:HOH:O	2.01	0.59
1:B:258:MET:O	1:B:262:LEU:HD13	2.03	0.59
1:C:456:GLN:O	1:C:460:LEU:HD23	2.02	0.59
1:A:227:ILE:HD11	1:C:442:LEU:HD13	1.84	0.59
1:C:60:THR:O	1:C:64:LYS:HD3	2.03	0.59
1:C:366:LEU:HD23	1:C:432:PHE:CD2	2.37	0.59
1:C:401:GLU:OE1	1:C:401:GLU:O	2.21	0.59
1:D:157:LEU:HA	1:D:366:LEU:HD11	1.84	0.59
1:C:275:LEU:HD22	1:C:351:VAL:HG13	1.84	0.59
1:B:117:ASP:HB3	1:B:235:ILE:HD11	1.85	0.58
1:C:155:VAL:HG22	1:C:359:LYS:HE3	1.86	0.58
1:C:364:LYS:NZ	1:C:364:LYS:HB2	2.18	0.58
1:D:431:ASN:HB3	1:D:434:ASN:ND2	2.18	0.58
1:A:81:PHE:HZ	1:A:93:ALA:O	1.86	0.58
1:B:199:LEU:HD11	1:B:201:LEU:HB3	1.86	0.58
1:D:454:ILE:O	1:D:458:ARG:HB2	2.04	0.58
1:B:399:LEU:HD21	1:B:414:ASP:HB3	1.85	0.58
1:B:297:LEU:HD11	1:C:26:LEU:HD13	1.85	0.58
1:C:387:ARG:O	1:C:391:THR:HG23	2.04	0.58
1:D:60:THR:CG2	1:D:64:LYS:HE2	2.34	0.58
1:A:199:LEU:HD21	1:A:218:LEU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:HD3	1:A:317:LYS:C	2.28	0.57
1:D:187:GLU:O	1:D:191:GLU:HG3	2.03	0.57
1:D:360:GLU:O	1:D:364:LYS:HG3	2.04	0.57
1:C:22:ILE:HD12	1:C:22:ILE:H	1.69	0.57
1:C:117:ASP:HB3	1:C:235:ILE:HD11	1.85	0.57
1:A:87:ASP:CB	1:A:96:ARG:HH21	2.17	0.57
1:B:314:MET:HG2	1:C:303:GLY:CA	2.33	0.57
1:B:375:LEU:O	1:B:378:TYR:HB3	2.04	0.57
1:C:20:ASP:OD1	1:C:22:ILE:HD13	2.04	0.57
1:D:421:GLN:HA	1:D:421:GLN:HE21	1.69	0.57
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.69	0.57
1:B:196:ILE:HG12	1:B:240:PHE:HB2	1.87	0.57
1:B:385:PRO:HB2	1:B:388:GLN:HG2	1.85	0.57
1:B:388:GLN:HE21	1:B:388:GLN:HA	1.70	0.57
1:C:366:LEU:HB3	1:C:432:PHE:CE2	2.39	0.57
1:C:422:PHE:CD1	1:C:426:VAL:HG21	2.40	0.57
1:B:187:GLU:O	1:B:191:GLU:HG3	2.06	0.56
3:B:483:HOH:O	1:D:442:LEU:HB3	2.04	0.56
1:A:89:ASP:OD2	1:A:91:HIS:HB2	2.05	0.56
1:A:276:SER:O	1:A:277:ASP:CB	2.54	0.56
1:A:451:THR:O	1:A:455:GLU:HG3	2.05	0.56
1:B:115:ARG:HH21	1:B:115:ARG:HG3	1.70	0.56
1:C:408:ASN:HB3	1:C:430:PHE:CD2	2.40	0.56
1:C:412:LEU:HD12	1:C:412:LEU:N	2.20	0.56
1:C:21:PRO:HG2	1:C:22:ILE:HD12	1.87	0.56
1:A:309:LEU:HD21	3:A:499:HOH:O	2.05	0.56
1:A:324:ASN:O	1:A:327:LEU:HD13	2.06	0.56
1:C:78:LYS:C	1:C:80:VAL:H	2.11	0.56
1:C:379:LEU:HD12	1:C:379:LEU:N	2.19	0.56
1:B:116:ASN:HB3	1:B:235:ILE:HG23	1.87	0.56
1:B:133:ILE:HD13	3:B:535:HOH:O	2.05	0.56
1:C:20:ASP:OD2	1:C:22:ILE:HB	2.06	0.56
1:C:399:LEU:O	1:C:402:THR:HB	2.06	0.56
1:A:102:ILE:HD12	1:A:105:ILE:HG23	1.87	0.56
1:C:98:LEU:HD11	1:C:102:ILE:HD11	1.87	0.56
1:A:101:LEU:H	1:A:101:LEU:CD2	2.18	0.56
1:A:110:ASN:ND2	1:A:113:ARG:HB3	2.20	0.56
1:A:141:LEU:C	1:A:141:LEU:HD23	2.31	0.56
1:B:378:TYR:CD2	1:B:379:LEU:HD12	2.41	0.55
1:C:137:HIS:HE1	3:C:475:HOH:O	1.90	0.55
1:C:368:PRO:O	1:C:407:ILE:HD11	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ASP:OD1	1:C:331:LYS:N	2.39	0.55
1:D:297:LEU:O	1:D:297:LEU:HD13	2.06	0.55
1:A:189:LEU:HD23	1:A:189:LEU:C	2.32	0.55
1:B:199:LEU:HB3	1:B:227:ILE:HG22	1.88	0.55
1:C:180:VAL:HG12	1:C:184:ARG:HH12	1.72	0.55
1:B:151:ILE:HG13	1:B:152:GLU:HG3	1.88	0.55
1:A:52:GLU:HG3	1:A:62:LEU:HD22	1.88	0.55
1:A:139:LEU:HD21	1:A:464:GLN:CB	2.36	0.55
1:A:99:LYS:H	1:A:99:LYS:HD2	1.71	0.55
1:C:391:THR:O	1:C:395:LYS:HG3	2.07	0.55
1:C:119:VAL:HG21	1:C:331:LYS:HZ1	1.72	0.55
1:C:123:LEU:HD22	1:C:127:MET:SD	2.47	0.55
1:D:371:LEU:HD13	1:D:430:PHE:HA	1.89	0.55
1:C:379:LEU:HB3	1:C:384:VAL:CB	2.37	0.54
1:A:101:LEU:HD22	1:A:101:LEU:N	2.21	0.54
1:B:128:LYS:NZ	1:B:197:ASN:ND2	2.55	0.54
1:C:164:GLN:HE22	1:D:267:THR:HA	1.73	0.54
1:B:96:ARG:HG2	1:B:96:ARG:HH11	1.73	0.54
1:D:96:ARG:O	1:D:99:LYS:HB3	2.08	0.54
1:C:139:LEU:HD11	1:C:186:SER:OG	2.07	0.54
1:C:173:GLN:HE22	1:C:453:GLN:NE2	2.05	0.54
1:A:34:GLN:HG3	1:A:35:ARG:N	2.22	0.54
1:A:81:PHE:HE2	1:A:93:ALA:HB1	1.72	0.54
1:C:412:LEU:HD12	1:C:412:LEU:H	1.72	0.54
1:A:76:TRP:C	1:A:78:LYS:H	2.15	0.54
1:C:117:ASP:HA	1:C:120:VAL:HG12	1.90	0.54
1:C:364:LYS:HB2	1:C:364:LYS:HZ3	1.71	0.54
1:B:326:ASP:HA	1:C:300:SER:HB3	1.89	0.54
1:C:141:LEU:C	1:C:141:LEU:HD23	2.33	0.54
1:D:67:SER:O	1:D:71:LYS:HG3	2.08	0.54
1:A:171:TRP:O	1:A:174:PHE:HB3	2.08	0.54
1:A:259:ALA:O	1:A:263:ILE:HG13	2.07	0.54
1:C:119:VAL:HG22	3:C:528:HOH:O	2.07	0.54
1:B:219:ARG:HG2	1:B:219:ARG:NH1	2.23	0.54
1:A:176:LEU:HD22	1:A:457:LEU:CD1	2.38	0.53
1:A:195:ARG:NH1	1:C:187:GLU:OE2	2.41	0.53
1:D:355:LEU:HD12	1:D:355:LEU:C	2.33	0.53
1:B:42:GLN:HA	1:B:42:GLN:NE2	2.23	0.53
1:B:170:ARG:HG3	1:B:436:VAL:HG11	1.90	0.53
1:C:366:LEU:HD23	1:C:432:PHE:CG	2.43	0.53
1:B:325:LYS:HE2	1:B:328:GLN:OE1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:ASN:O	1:C:327:LEU:HD23	2.09	0.53
1:B:41:ILE:O	1:B:45:MET:HG3	2.09	0.53
1:C:98:LEU:HD12	1:C:106:ALA:HB1	1.91	0.53
1:B:41:ILE:HG23	1:B:69:LEU:HB3	1.90	0.53
1:B:117:ASP:HA	1:B:120:VAL:HG12	1.91	0.53
1:B:192:VAL:HG22	1:B:243:GLU:HB3	1.90	0.53
1:B:378:TYR:HD2	1:B:379:LEU:HD12	1.72	0.53
1:D:279:PHE:CZ	1:D:350:GLY:HA3	2.43	0.53
1:D:292:PRO:HB3	1:D:295:LEU:HD12	1.89	0.53
1:B:71:LYS:HD3	1:B:101:LEU:HD21	1.90	0.53
1:B:137:HIS:CE1	1:B:342:THR:HG23	2.44	0.53
1:C:124:LYS:HE2	1:C:240:PHE:CD2	2.44	0.53
1:B:191:GLU:HA	3:B:511:HOH:O	2.09	0.53
1:B:260:GLU:HG2	1:D:318:GLY:O	2.09	0.53
1:C:419:SER:C	1:C:421:GLN:H	2.16	0.53
1:C:431:ASN:CB	1:C:434:ASN:HD22	2.21	0.53
1:A:97:ARG:HG2	1:A:97:ARG:HH11	1.75	0.52
1:C:188:ARG:NH2	1:C:250:LEU:HD13	2.24	0.52
1:C:61:GLU:CG	1:C:105:ILE:HD11	2.33	0.52
1:C:371:LEU:HD13	1:C:430:PHE:HA	1.92	0.52
1:D:297:LEU:O	1:D:301:LYS:HD3	2.09	0.52
1:D:407:ILE:HG13	1:D:430:PHE:HE2	1.74	0.52
1:D:61:GLU:HG2	1:D:105:ILE:HD11	1.89	0.52
1:D:328:GLN:HE21	2:D:0:AS1:HN41	1.58	0.52
1:A:97:ARG:HG3	1:A:101:LEU:HD21	1.90	0.52
1:A:442:LEU:HD13	1:C:227:ILE:HD11	1.91	0.52
1:D:61:GLU:CG	1:D:105:ILE:HD11	2.39	0.52
1:B:367:THR:OG1	1:B:369:GLU:HG2	2.10	0.52
1:D:116:ASN:ND2	2:D:0:AS1:H11	2.25	0.52
1:A:375:LEU:O	1:A:378:TYR:HB3	2.10	0.52
1:A:403:LYS:HE2	1:A:403:LYS:CA	2.32	0.52
1:C:170:ARG:HG3	1:C:436:VAL:HG11	1.92	0.52
1:A:191:GLU:HB3	1:C:191:GLU:OE2	2.10	0.52
1:A:355:LEU:HD12	1:A:355:LEU:O	2.09	0.52
1:B:65:ILE:HG22	1:B:65:ILE:O	2.10	0.52
1:D:214:ASP:OD2	1:D:217:MET:HB2	2.10	0.52
1:C:146:VAL:HG22	1:C:457:LEU:HD13	1.92	0.52
1:D:219:ARG:HG2	1:D:219:ARG:HH11	1.75	0.52
1:A:78:LYS:HB3	1:A:78:LYS:HZ2	1.75	0.51
1:A:167:GLN:HG2	3:A:568:HOH:O	2.10	0.51
1:A:219:ARG:HG2	1:A:219:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:VAL:O	1:A:341:LEU:HD13	2.10	0.51
1:B:176:LEU:O	1:B:180:VAL:HG23	2.10	0.51
1:D:387:ARG:NE	1:D:387:ARG:HA	2.25	0.51
1:B:197:ASN:ND2	1:B:224:PHE:HA	2.25	0.51
1:D:110:ASN:ND2	1:D:113:ARG:HB3	2.24	0.51
1:A:36:LEU:HD22	1:A:122:ASP:HB3	1.93	0.51
1:C:334:VAL:O	1:C:338:VAL:HG23	2.11	0.51
1:C:415:LEU:C	1:C:417:SER:N	2.69	0.51
1:D:61:GLU:HG2	1:D:105:ILE:CD1	2.41	0.51
1:D:61:GLU:CD	1:D:105:ILE:HD11	2.35	0.51
1:C:265:TYR:HB3	1:C:272:PHE:HB2	1.93	0.51
1:D:97:ARG:NE	1:D:101:LEU:HD11	2.26	0.51
1:B:56:ILE:N	1:B:56:ILE:HD12	2.26	0.51
1:C:355:LEU:O	1:C:355:LEU:HD12	2.11	0.51
1:D:459:GLU:OE1	1:D:459:GLU:HA	2.11	0.51
1:A:423:SER:HB3	1:A:425:ASP:OD2	2.11	0.51
1:B:41:ILE:HD11	1:B:72:ILE:CG2	2.41	0.51
1:D:400:ALA:HB2	1:D:410:LEU:CD2	2.40	0.51
1:A:139:LEU:HD21	1:A:464:GLN:HB3	1.92	0.51
1:A:464:GLN:HE21	1:A:464:GLN:HA	1.76	0.51
1:C:77:SER:O	1:C:78:LYS:HD3	2.11	0.51
1:C:78:LYS:HB2	1:C:80:VAL:HG23	1.91	0.51
1:C:91:HIS:CD2	1:C:118:GLN:NE2	2.79	0.51
1:D:259:ALA:O	1:D:263:ILE:HG13	2.11	0.51
1:C:96:ARG:HG2	1:C:96:ARG:HH11	1.76	0.51
1:C:97:ARG:O	1:C:101:LEU:HB2	2.11	0.51
1:B:176:LEU:HD22	1:B:457:LEU:HD12	1.93	0.51
1:C:259:ALA:O	1:C:263:ILE:HG13	2.11	0.51
1:A:327:LEU:N	1:A:327:LEU:HD12	2.25	0.50
1:A:436:VAL:HG13	1:A:445:THR:HG23	1.93	0.50
1:B:143:LYS:HB2	1:B:143:LYS:HZ2	1.74	0.50
1:D:431:ASN:HB3	1:D:434:ASN:HD22	1.74	0.50
1:A:227:ILE:HG12	3:A:472:HOH:O	2.11	0.50
1:A:304:ARG:NH1	3:A:555:HOH:O	2.44	0.50
1:B:119:VAL:HG22	3:B:570:HOH:O	2.10	0.50
1:C:76:TRP:C	1:C:78:LYS:H	2.20	0.50
1:C:196:ILE:HG12	1:C:240:PHE:HB2	1.92	0.50
1:A:61:GLU:CD	1:A:105:ILE:HD11	2.36	0.50
1:B:66:LEU:C	1:B:66:LEU:HD23	2.36	0.50
1:D:98:LEU:HB3	1:D:106:ALA:HB1	1.94	0.50
1:A:65:ILE:C	1:A:67:SER:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HG3	1:A:101:LEU:CD2	2.41	0.50
1:A:403:LYS:HA	1:A:403:LYS:CE	2.32	0.50
1:B:297:LEU:HD13	1:B:297:LEU:C	2.37	0.50
1:C:111:THR:HG22	1:C:211:LEU:HD11	1.94	0.50
1:D:423:SER:HB3	1:D:425:ASP:OD2	2.12	0.50
1:A:188:ARG:CZ	1:A:250:LEU:HD23	2.42	0.50
1:C:33:ASP:OD1	1:C:33:ASP:O	2.30	0.50
1:C:364:LYS:HZ3	1:C:364:LYS:CB	2.25	0.50
1:C:141:LEU:HD22	1:C:182:LEU:HD13	1.93	0.50
1:D:431:ASN:HD22	1:D:432:PHE:N	2.09	0.50
1:A:81:PHE:CE2	1:A:93:ALA:HB1	2.47	0.49
1:B:161:THR:HG21	2:D:0:AS1:HB1	1.93	0.49
1:C:142:ILE:O	1:C:146:VAL:HG23	2.12	0.49
1:C:270:PHE:CE1	1:D:269:GLU:HG2	2.48	0.49
1:B:271:GLY:HA2	3:B:585:HOH:O	2.11	0.49
1:B:401:GLU:C	1:B:401:GLU:OE2	2.55	0.49
1:C:269:GLU:HG2	1:D:270:PHE:CD2	2.48	0.49
1:D:357:ILE:HB	1:D:362:MET:HE3	1.95	0.49
1:D:375:LEU:O	1:D:378:TYR:HB3	2.12	0.49
1:D:408:ASN:HB3	1:D:430:PHE:CD2	2.47	0.49
1:A:35:ARG:C	1:A:37:SER:H	2.21	0.49
1:A:257:LYS:HB2	3:C:500:HOH:O	2.13	0.49
1:A:431:ASN:HB3	1:A:434:ASN:ND2	2.19	0.49
1:C:379:LEU:H	1:C:379:LEU:CD1	2.26	0.49
1:D:379:LEU:HD11	1:D:422:PHE:CE1	2.48	0.49
1:C:157:LEU:HB3	1:C:362:MET:HB3	1.93	0.49
1:A:196:ILE:HG12	1:A:240:PHE:HB2	1.95	0.49
1:C:423:SER:C	1:C:425:ASP:H	2.19	0.49
1:D:330:ASP:OD1	1:D:331:LYS:N	2.46	0.49
1:D:436:VAL:HG13	1:D:445:THR:CG2	2.36	0.49
1:B:176:LEU:HD22	1:B:457:LEU:CD1	2.43	0.49
1:D:292:PRO:O	1:D:293:ASP:C	2.56	0.49
1:C:119:VAL:CG2	1:C:331:LYS:HZ1	2.26	0.48
1:C:415:LEU:C	1:C:417:SER:H	2.21	0.48
1:A:47:TYR:O	1:A:51:LEU:HB2	2.13	0.48
1:A:205:ALA:O	1:A:206:LEU:HB3	2.12	0.48
1:A:327:LEU:H	1:A:327:LEU:CD1	2.26	0.48
1:A:355:LEU:HD12	1:A:355:LEU:C	2.37	0.48
1:B:94:ASN:O	1:B:98:LEU:HB2	2.13	0.48
1:A:402:THR:HG22	1:A:403:LYS:HE3	1.94	0.48
1:D:199:LEU:HB3	1:D:227:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:MET:HA	1:D:314:MET:HE2	1.96	0.48
1:A:135:SER:O	1:A:139:LEU:HD13	2.14	0.48
1:A:260:GLU:O	1:A:264:ILE:HG13	2.13	0.48
1:C:135:SER:O	1:C:139:LEU:HD13	2.12	0.48
1:C:270:PHE:CD1	1:D:269:GLU:HG2	2.49	0.48
1:D:173:GLN:HA	1:D:173:GLN:NE2	2.27	0.48
1:A:102:ILE:HD12	1:A:105:ILE:CG2	2.44	0.48
1:B:20:ASP:CG	1:B:21:PRO:HD2	2.39	0.48
1:C:465:LYS:NZ	1:C:465:LYS:HB3	2.29	0.48
1:A:61:GLU:O	1:A:65:ILE:HG13	2.13	0.48
1:A:379:LEU:HD12	1:A:379:LEU:N	2.29	0.48
1:B:66:LEU:HD23	1:B:66:LEU:O	2.13	0.48
1:C:50:ALA:CB	1:C:213:ILE:HD11	2.44	0.48
1:C:78:LYS:C	1:C:80:VAL:N	2.71	0.48
1:C:104:ASP:C	1:C:106:ALA:H	2.20	0.48
1:C:206:LEU:HD12	1:C:232:MET:HG2	1.96	0.48
1:C:400:ALA:C	1:C:402:THR:H	2.22	0.48
1:A:35:ARG:O	1:A:37:SER:N	2.47	0.48
1:C:362:MET:O	1:C:366:LEU:CD1	2.61	0.48
1:B:464:GLN:O	1:B:465:LYS:HB2	2.14	0.48
1:D:292:PRO:CB	1:D:295:LEU:HD12	2.44	0.48
1:B:419:SER:C	1:B:421:GLN:H	2.22	0.47
1:C:343:ALA:O	1:C:347:VAL:HG23	2.14	0.47
1:A:141:LEU:HD23	1:A:141:LEU:O	2.15	0.47
1:B:97:ARG:O	1:B:97:ARG:HD3	2.14	0.47
1:B:421:GLN:HA	1:B:421:GLN:NE2	2.30	0.47
1:A:115:ARG:NH1	1:A:116:ASN:ND2	2.60	0.47
1:B:128:LYS:NZ	1:B:197:ASN:HD21	2.12	0.47
1:D:87:ASP:CG	1:D:96:ARG:HH21	2.22	0.47
1:C:197:ASN:ND2	1:C:224:PHE:HA	2.29	0.47
1:A:416:LYS:NZ	3:A:533:HOH:O	2.48	0.47
1:B:189:LEU:C	1:B:189:LEU:HD23	2.40	0.47
1:A:87:ASP:CG	1:A:96:ARG:HH21	2.23	0.47
1:A:117:ASP:HB3	1:A:235:ILE:HD11	1.97	0.47
1:B:447:LYS:O	1:B:451:THR:HG23	2.14	0.47
1:C:188:ARG:CZ	1:C:250:LEU:HD13	2.45	0.47
1:B:30:ILE:O	1:B:34:GLN:HG3	2.15	0.47
1:B:407:ILE:HG13	1:B:430:PHE:CE2	2.50	0.47
1:C:258:MET:O	1:C:262:LEU:HD13	2.15	0.47
1:C:398:HIS:O	1:C:398:HIS:CG	2.68	0.47
1:C:50:ALA:HB1	1:C:213:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LYS:O	1:C:80:VAL:N	2.48	0.47
1:C:197:ASN:HD21	1:C:224:PHE:HA	1.80	0.47
1:C:357:ILE:HB	1:C:362:MET:CE	2.45	0.47
1:D:30:ILE:O	1:D:34:GLN:HG3	2.15	0.47
1:A:82:VAL:HG13	1:A:82:VAL:O	2.15	0.47
1:B:26:LEU:HD11	1:C:343:ALA:HB1	1.96	0.47
1:B:222:LEU:O	1:B:223:GLU:HB2	2.15	0.47
1:C:446:ALA:O	1:C:450:VAL:HG23	2.15	0.47
1:B:317:LYS:HD3	1:B:317:LYS:C	2.40	0.46
1:C:105:ILE:HG12	1:C:105:ILE:O	2.14	0.46
1:C:355:LEU:HD12	1:C:355:LEU:C	2.40	0.46
1:A:139:LEU:HD21	1:A:464:GLN:HB2	1.98	0.46
1:B:30:ILE:HB	1:B:89:ASP:HA	1.97	0.46
1:C:352:ILE:HG22	1:C:352:ILE:O	2.16	0.46
1:D:203:SER:HB2	1:D:235:ILE:HD13	1.98	0.46
1:A:273:LEU:C	1:A:273:LEU:HD12	2.40	0.46
1:B:189:LEU:HD23	1:B:189:LEU:O	2.14	0.46
1:D:52:GLU:HG3	1:D:62:LEU:HD22	1.97	0.46
1:D:131:LEU:HD22	1:D:189:LEU:CD1	2.43	0.46
1:D:317:LYS:C	1:D:317:LYS:HD3	2.41	0.46
1:D:366:LEU:HB3	1:D:432:PHE:CD2	2.50	0.46
1:D:421:GLN:HA	1:D:421:GLN:NE2	2.31	0.46
1:A:179:ALA:O	1:A:183:THR:HG23	2.15	0.46
1:B:89:ASP:OD1	1:B:91:HIS:HB2	2.16	0.46
1:B:275:LEU:CD1	1:B:351:VAL:HG13	2.46	0.46
1:B:431:ASN:HB3	1:B:434:ASN:HD22	1.81	0.46
3:A:490:HOH:O	1:C:239:ASP:HB3	2.14	0.46
1:C:384:VAL:HG12	1:C:389:ALA:HB2	1.97	0.46
1:D:52:GLU:HA	1:D:57:LEU:HB2	1.98	0.46
1:D:80:VAL:O	1:D:81:PHE:C	2.58	0.46
1:D:124:LYS:NZ	3:D:569:HOH:O	2.48	0.46
1:A:69:LEU:HD23	1:A:98:LEU:HD11	1.97	0.46
1:A:376:ALA:O	1:A:380:VAL:HG23	2.16	0.46
1:D:371:LEU:CD1	1:D:430:PHE:HA	2.46	0.46
1:D:117:ASP:HB3	1:D:235:ILE:HD11	1.97	0.46
1:D:316:LEU:HA	1:D:319:LEU:HD12	1.98	0.46
1:A:34:GLN:HG3	1:A:35:ARG:HG3	1.98	0.46
1:C:379:LEU:N	1:C:379:LEU:CD1	2.79	0.46
1:D:368:PRO:O	1:D:407:ILE:HD11	2.16	0.46
1:A:99:LYS:HD2	1:A:99:LYS:N	2.31	0.45
1:A:293:ASP:OD1	1:D:325:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:VAL:HA	1:C:384:VAL:O	2.16	0.45
1:D:123:LEU:HD22	1:D:127:MET:SD	2.56	0.45
1:D:179:ALA:O	1:D:183:THR:HG23	2.16	0.45
1:D:203:SER:CB	1:D:235:ILE:HD13	2.46	0.45
1:A:110:ASN:ND2	1:A:110:ASN:O	2.50	0.45
1:A:176:LEU:HD22	1:A:457:LEU:HD12	1.97	0.45
1:D:173:GLN:HE22	1:D:453:GLN:NE2	2.08	0.45
1:A:47:TYR:CE2	1:A:113:ARG:HB2	2.51	0.45
1:A:327:LEU:N	1:A:327:LEU:CD1	2.80	0.45
1:B:94:ASN:C	1:B:96:ARG:H	2.24	0.45
1:C:180:VAL:HG12	1:C:184:ARG:NH1	2.30	0.45
1:D:41:ILE:CD1	1:D:73:SER:HA	2.46	0.45
1:D:219:ARG:HG2	1:D:219:ARG:NH1	2.31	0.45
1:B:58:THR:OG1	1:B:61:GLU:HG3	2.17	0.45
1:B:200:PRO:HB3	3:B:493:HOH:O	2.16	0.45
1:C:54:ALA:HB3	1:C:56:ILE:HD13	1.97	0.45
1:D:391:THR:O	1:D:395:LYS:HG3	2.16	0.45
1:A:141:LEU:C	1:A:141:LEU:CD2	2.90	0.45
1:B:99:LYS:C	1:B:101:LEU:H	2.24	0.45
1:B:275:LEU:HD11	1:B:351:VAL:HG13	1.99	0.45
1:C:91:HIS:CD2	1:C:115:ARG:HD2	2.51	0.45
1:C:140:GLN:HG2	3:C:544:HOH:O	2.15	0.45
1:D:170:ARG:HB3	3:D:540:HOH:O	2.17	0.45
1:A:165:LYS:HE2	3:B:466:HOH:O	2.17	0.45
1:C:206:LEU:CD1	1:C:232:MET:HG2	2.47	0.45
1:A:124:LYS:HE2	3:A:519:HOH:O	2.17	0.45
1:B:331:LYS:HE3	3:B:570:HOH:O	2.15	0.45
1:D:131:LEU:HD11	1:D:196:ILE:HD12	1.99	0.45
1:D:188:ARG:O	1:D:192:VAL:HG23	2.16	0.45
1:A:173:GLN:HA	1:A:173:GLN:NE2	2.28	0.45
1:C:82:VAL:O	1:C:82:VAL:HG13	2.15	0.45
1:C:173:GLN:NE2	1:C:453:GLN:HE22	2.09	0.45
1:A:44:SER:HB3	1:A:109:LEU:HD21	1.98	0.45
1:B:197:ASN:HD21	1:B:224:PHE:HA	1.80	0.45
1:B:368:PRO:O	1:B:407:ILE:HD11	2.17	0.45
1:C:20:ASP:HA	1:C:21:PRO:HD2	1.87	0.45
1:C:267:THR:HB	1:C:269:GLU:OE1	2.17	0.45
1:D:153:ILE:HG12	1:D:153:ILE:O	2.16	0.45
1:D:419:SER:C	1:D:421:GLN:H	2.25	0.45
1:C:22:ILE:N	1:C:22:ILE:CD1	2.80	0.45
1:C:412:LEU:H	1:C:412:LEU:CD1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:LYS:HE2	1:D:197:ASN:ND2	2.31	0.45
1:D:347:VAL:O	1:D:351:VAL:HG23	2.17	0.45
1:A:123:LEU:HD12	3:A:572:HOH:O	2.17	0.44
1:B:153:ILE:HA	1:B:172:SER:OG	2.17	0.44
1:B:431:ASN:HB3	1:B:434:ASN:ND2	2.32	0.44
1:A:80:VAL:O	1:A:81:PHE:CB	2.61	0.44
1:D:332:GLU:HG3	3:D:494:HOH:O	2.17	0.44
1:A:269:GLU:CD	1:A:269:GLU:H	2.26	0.44
1:B:366:LEU:HB3	1:B:432:PHE:CZ	2.53	0.44
1:C:76:TRP:C	1:C:78:LYS:N	2.75	0.44
1:C:407:ILE:HG13	1:C:430:PHE:HE2	1.81	0.44
1:D:189:LEU:HD13	1:D:247:PHE:CE2	2.52	0.44
1:C:374:ASP:O	1:C:377:LEU:HB2	2.17	0.44
1:D:117:ASP:CB	1:D:235:ILE:HD11	2.47	0.44
1:A:38:GLU:O	1:A:42:GLN:HG3	2.18	0.44
1:A:243:GLU:CD	1:C:188:ARG:HH11	2.25	0.44
1:D:76:TRP:HE1	1:D:94:ASN:HD21	1.65	0.44
1:D:183:THR:HG21	1:D:457:LEU:HD22	2.00	0.44
1:A:52:GLU:HA	1:A:57:LEU:HB2	1.98	0.44
1:A:245:LEU:CD2	1:A:337:VAL:HG21	2.48	0.44
1:A:371:LEU:HD13	1:A:430:PHE:HA	1.99	0.44
1:A:416:LYS:C	1:A:418:ILE:H	2.26	0.44
1:B:141:LEU:HD23	1:B:141:LEU:C	2.42	0.44
1:C:61:GLU:HG2	1:C:105:ILE:CD1	2.35	0.44
1:C:89:ASP:OD2	1:C:91:HIS:HB2	2.18	0.44
1:C:433:VAL:O	1:C:437:GLU:HG2	2.17	0.44
1:D:235:ILE:HG22	1:D:322:THR:HG22	2.00	0.44
1:D:275:LEU:HD11	1:D:295:LEU:HG	1.99	0.44
1:A:108:LYS:HE2	1:C:385:PRO:HG3	1.99	0.44
1:B:311:SER:HB3	1:C:307:GLY:HA3	1.99	0.44
1:B:366:LEU:HD23	1:B:432:PHE:CG	2.53	0.44
1:B:384:VAL:CG1	1:B:388:GLN:HB2	2.47	0.44
1:C:314:MET:HE2	1:D:314:MET:HA	2.00	0.44
1:C:398:HIS:HA	1:C:401:GLU:HG2	1.99	0.44
1:C:406:THR:O	1:C:408:ASN:N	2.51	0.44
1:C:419:SER:C	1:C:421:GLN:N	2.76	0.44
1:B:273:LEU:HD12	1:B:273:LEU:C	2.43	0.43
1:C:98:LEU:HD13	1:C:98:LEU:O	2.18	0.43
1:C:100:GLU:O	1:C:100:GLU:HG3	2.17	0.43
1:C:164:GLN:O	1:C:165:LYS:C	2.62	0.43
1:D:28:SER:OG	1:D:30:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LYS:H	1:A:99:LYS:CD	2.31	0.43
1:C:98:LEU:HD13	1:C:98:LEU:C	2.43	0.43
1:D:97:ARG:CZ	1:D:101:LEU:HD11	2.47	0.43
1:D:400:ALA:HB2	1:D:410:LEU:CG	2.48	0.43
1:C:22:ILE:O	1:C:26:LEU:HG	2.18	0.43
1:C:400:ALA:C	1:C:402:THR:N	2.75	0.43
1:C:431:ASN:CG	1:C:434:ASN:ND2	2.77	0.43
1:A:369:GLU:CD	3:A:544:HOH:O	2.61	0.43
1:B:60:THR:C	1:B:62:LEU:N	2.76	0.43
1:B:296:GLU:HB3	1:C:325:LYS:HB3	2.00	0.43
1:B:412:LEU:HD11	1:B:422:PHE:O	2.18	0.43
1:C:260:GLU:O	1:C:264:ILE:HG12	2.18	0.43
1:C:422:PHE:HD1	1:C:426:VAL:HG21	1.81	0.43
1:B:110:ASN:ND2	1:B:113:ARG:HH21	2.16	0.43
1:A:412:LEU:HG	1:A:416:LYS:HE2	2.01	0.43
1:B:141:LEU:HD23	1:B:141:LEU:O	2.19	0.43
1:C:30:ILE:O	1:C:34:GLN:HG3	2.18	0.43
1:C:463:LYS:C	1:C:465:LYS:H	2.26	0.43
1:D:56:ILE:HG12	1:D:211:LEU:HD13	2.01	0.43
1:D:180:VAL:HG22	1:D:457:LEU:HD21	2.00	0.43
1:A:123:LEU:O	1:A:127:MET:HG3	2.19	0.43
1:A:128:LYS:HE3	1:A:197:ASN:ND2	2.34	0.43
1:A:265:TYR:HB3	1:A:272:PHE:HB2	2.00	0.43
1:A:75:GLU:O	1:A:78:LYS:HB2	2.18	0.43
1:A:400:ALA:HB2	1:A:410:LEU:HD21	2.01	0.43
1:A:464:GLN:O	1:A:465:LYS:HG2	2.19	0.43
1:D:405:ILE:HG13	1:D:406:THR:N	2.34	0.43
1:A:206:LEU:HD21	1:C:167:GLN:HG2	2.01	0.42
1:A:279:PHE:CZ	1:A:350:GLY:HA3	2.55	0.42
1:C:62:LEU:O	1:C:66:LEU:HD13	2.19	0.42
1:C:129:ASN:HB3	3:C:546:HOH:O	2.18	0.42
1:C:206:LEU:HD12	1:C:206:LEU:O	2.19	0.42
1:D:379:LEU:N	1:D:379:LEU:HD12	2.34	0.42
1:A:206:LEU:HD21	1:C:167:GLN:CG	2.49	0.42
1:A:255:LEU:HD23	1:A:344:VAL:HG11	2.00	0.42
1:A:281:THR:HB	1:A:293:ASP:OD1	2.19	0.42
1:B:115:ARG:HG3	1:B:115:ARG:NH2	2.34	0.42
1:C:419:SER:HA	1:C:420:PRO:HD3	1.88	0.42
1:A:442:LEU:HB3	3:C:491:HOH:O	2.18	0.42
1:C:158:PRO:HG2	1:C:365:ALA:HB1	2.01	0.42
1:C:376:ALA:O	1:C:380:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:HIS:HD2	3:D:475:HOH:O	2.02	0.42
1:A:35:ARG:HD2	1:A:126:PHE:CE1	2.54	0.42
1:B:449:SER:O	1:B:453:GLN:HG3	2.19	0.42
1:C:71:LYS:HD3	1:C:71:LYS:C	2.44	0.42
1:C:375:LEU:HD23	1:C:393:SER:HA	2.01	0.42
1:A:36:LEU:O	1:A:40:ASP:HB2	2.19	0.42
1:D:431:ASN:HD22	1:D:431:ASN:C	2.27	0.42
1:A:41:ILE:HG21	1:A:73:SER:OG	2.19	0.42
1:A:371:LEU:CD1	1:A:430:PHE:HA	2.49	0.42
1:A:458:ARG:HA	1:A:461:MET:HE3	2.02	0.42
1:B:68:GLY:O	1:B:72:ILE:HG13	2.19	0.42
1:B:407:ILE:HG13	1:B:430:PHE:HE2	1.85	0.42
1:C:97:ARG:O	1:C:97:ARG:HD3	2.20	0.42
1:C:325:LYS:HE3	1:C:325:LYS:HA	2.01	0.42
1:D:114:SER:O	1:D:118:GLN:HB2	2.20	0.42
1:A:115:ARG:HH11	1:A:116:ASN:ND2	2.18	0.42
1:B:96:ARG:HG2	1:B:96:ARG:NH1	2.34	0.42
1:C:414:ASP:O	1:C:417:SER:CB	2.67	0.42
1:D:203:SER:HB2	1:D:235:ILE:CD1	2.50	0.42
1:A:187:GLU:OE2	1:C:195:ARG:NH1	2.51	0.42
1:B:306:PHE:CE2	1:C:310:ALA:HB1	2.55	0.42
1:C:325:LYS:HE2	1:C:328:GLN:OE1	2.18	0.42
1:C:463:LYS:C	1:C:465:LYS:N	2.77	0.42
1:D:419:SER:C	1:D:421:GLN:N	2.77	0.42
1:A:464:GLN:HA	1:A:464:GLN:NE2	2.34	0.42
1:B:42:GLN:HA	1:B:42:GLN:HE21	1.83	0.42
1:D:78:LYS:NZ	1:D:78:LYS:HB3	2.35	0.42
1:A:215:ARG:HA	1:A:218:LEU:HD12	2.02	0.42
1:A:316:LEU:O	1:A:317:LYS:C	2.63	0.42
1:A:326:ASP:HA	1:D:300:SER:HB3	2.01	0.42
1:C:22:ILE:H	1:C:22:ILE:CD1	2.32	0.42
1:C:113:ARG:HG2	1:C:114:SER:N	2.35	0.42
1:D:297:LEU:HD13	1:D:297:LEU:C	2.45	0.42
1:D:199:LEU:HD23	1:D:227:ILE:HG22	2.02	0.41
1:D:99:LYS:NZ	1:D:104:ASP:HA	2.35	0.41
1:A:65:ILE:C	1:A:67:SER:N	2.77	0.41
1:A:301:LYS:O	1:A:305:VAL:HG23	2.20	0.41
1:A:317:LYS:C	1:A:317:LYS:CD	2.93	0.41
1:A:431:ASN:CB	1:A:434:ASN:HD22	2.21	0.41
1:B:23:MET:HE2	1:C:292:PRO:HB3	2.02	0.41
1:B:330:ASP:OD1	1:B:331:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:LEU:C	1:C:414:ASP:H	2.27	0.41
1:C:151:ILE:HG13	1:C:152:GLU:HG3	2.02	0.41
1:D:215:ARG:HH22	1:D:228:SER:CB	2.28	0.41
1:A:147:GLU:HA	1:A:147:GLU:OE1	2.20	0.41
1:B:347:VAL:O	1:B:351:VAL:HG23	2.21	0.41
1:C:269:GLU:HG2	1:D:270:PHE:CG	2.55	0.41
1:C:449:SER:O	1:C:453:GLN:HG3	2.21	0.41
1:D:407:ILE:HG13	1:D:430:PHE:CE2	2.53	0.41
1:D:460:LEU:HD22	1:D:460:LEU:HA	1.91	0.41
1:B:257:LYS:HB2	3:D:572:HOH:O	2.20	0.41
1:D:98:LEU:HB3	1:D:106:ALA:CB	2.51	0.41
1:D:215:ARG:NH2	1:D:228:SER:HB2	2.27	0.41
1:D:292:PRO:O	1:D:295:LEU:N	2.50	0.41
1:A:49:LYS:HB3	1:A:217:MET:CE	2.50	0.41
1:A:156:ILE:HG22	1:A:366:LEU:HD21	2.02	0.41
1:A:171:TRP:NE1	1:A:175:LEU:HD11	2.36	0.41
1:B:252:MET:HB3	1:B:302:SER:HA	2.03	0.41
1:B:321:SER:HB2	1:B:322:THR:HA	2.03	0.41
1:A:96:ARG:HG2	1:A:96:ARG:NH1	2.35	0.41
1:B:47:TYR:CE2	1:B:113:ARG:HB2	2.55	0.41
1:B:166:ALA:HB1	2:D:0:AS1:OD1	2.21	0.41
1:B:171:TRP:O	1:B:174:PHE:HB3	2.21	0.41
1:B:241:VAL:O	1:B:245:LEU:HG	2.21	0.41
1:B:355:LEU:HD12	1:B:355:LEU:O	2.21	0.41
1:C:263:ILE:HG22	1:D:163:LEU:HD12	2.03	0.41
1:C:414:ASP:HB2	1:C:415:LEU:H	1.77	0.41
1:D:65:ILE:O	1:D:69:LEU:HG	2.21	0.41
1:D:171:TRP:O	1:D:174:PHE:HB3	2.21	0.41
1:D:343:ALA:O	1:D:347:VAL:HG23	2.21	0.41
1:A:191:GLU:OE2	1:C:191:GLU:HB3	2.21	0.41
1:B:388:GLN:HE21	1:B:388:GLN:CA	2.32	0.41
1:C:359:LYS:NZ	3:C:558:HOH:O	2.54	0.41
1:A:442:LEU:CD1	1:C:227:ILE:HD11	2.51	0.40
1:B:20:ASP:C	1:B:22:ILE:H	2.29	0.40
1:D:308:ARG:HD2	3:D:467:HOH:O	2.21	0.40
1:D:400:ALA:CB	1:D:410:LEU:HD21	2.50	0.40
1:D:407:ILE:CG1	1:D:430:PHE:HE2	2.33	0.40
1:A:279:PHE:HB3	1:A:294:SER:CB	2.51	0.40
1:A:361:ASN:N	1:A:361:ASN:HD22	2.19	0.40
1:A:463:LYS:C	1:A:465:LYS:H	2.29	0.40
1:B:156:ILE:HG22	1:B:366:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:GLN:HA	1:B:388:GLN:NE2	2.36	0.40
1:B:421:GLN:HA	1:B:421:GLN:HE21	1.84	0.40
1:C:366:LEU:N	1:C:366:LEU:HD12	2.37	0.40
1:D:451:THR:O	1:D:455:GLU:HG3	2.22	0.40
1:B:252:MET:HE2	1:B:301:LYS:HB2	2.03	0.40
1:C:145:LEU:HD23	1:C:352:ILE:HG21	2.03	0.40
1:C:461:MET:C	1:C:463:LYS:N	2.79	0.40
1:D:113:ARG:HG2	1:D:114:SER:N	2.37	0.40
1:B:130:SER:O	1:B:134:ILE:HG13	2.22	0.40
1:C:436:VAL:HG13	1:C:445:THR:HG23	2.03	0.40
1:A:379:LEU:HD11	1:A:422:PHE:CZ	2.56	0.40
1:B:157:LEU:HB2	1:B:158:PRO:CD	2.51	0.40
1:C:114:SER:O	1:C:118:GLN:HB2	2.22	0.40
1:C:123:LEU:O	1:C:127:MET:HG3	2.22	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	420/447 (94%)	379 (90%)	32 (8%)	9 (2%)	5	4
1	B	412/447 (92%)	382 (93%)	27 (7%)	3 (1%)	18	23
1	C	430/447 (96%)	389 (90%)	30 (7%)	11 (3%)	4	3
1	D	432/447 (97%)	397 (92%)	29 (7%)	6 (1%)	9	9
All	All	1694/1788 (95%)	1547 (91%)	118 (7%)	29 (2%)	7	7

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PHE

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Mol	Chain	Res	Type
1	A	82	VAL
1	A	84	LYS
1	A	88	GLU
1	A	206	LEU
1	C	276	SER
1	C	386	PHE
1	D	206	LEU
1	D	462	LYS
1	A	36	LEU
1	A	277	ASP
1	B	66	LEU
1	B	206	LEU
1	C	407	ILE
1	C	410	LEU
1	D	293	ASP
1	A	34	GLN
1	C	79	GLY
1	C	206	LEU
1	D	443	ALA
1	B	21	PRO
1	C	277	ASP
1	D	81	PHE
1	A	35	ARG
1	C	34	GLN
1	C	77	SER
1	C	101	LEU
1	C	424	SER
1	D	405	ILE

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	369/392 (94%)	359 (97%)	10 (3%)	39	58
1	B	364/392 (93%)	354 (97%)	10 (3%)	39	58
1	C	377/392 (96%)	362 (96%)	15 (4%)	28	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	379/392 (97%)	368 (97%)	11 (3%)	37 55
All	All	1489/1568 (95%)	1443 (97%)	46 (3%)	35 52

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LYS
1	A	115	ARG
1	A	123	LEU
1	A	138	LEU
1	A	141	LEU
1	A	200	PRO
1	A	237	GLU
1	A	255	LEU
1	A	366	LEU
1	A	460	LEU
1	B	75	GLU
1	B	95	GLU
1	B	98	LEU
1	B	138	LEU
1	B	143	LYS
1	B	200	PRO
1	B	250	LEU
1	B	314	MET
1	B	325	LYS
1	B	366	LEU
1	C	22	ILE
1	C	33	ASP
1	C	51	LEU
1	C	56	ILE
1	C	123	LEU
1	C	138	LEU
1	C	200	PRO
1	C	210	PRO
1	C	250	LEU
1	C	325	LYS
1	C	364	LYS
1	C	388	GLN
1	C	401	GLU
1	C	412	LEU
1	C	462	LYS
1	D	66	LEU

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Mol	Chain	Res	Type
1	D	109	LEU
1	D	123	LEU
1	D	141	LEU
1	D	235	ILE
1	D	250	LEU
1	D	327	LEU
1	D	355	LEU
1	D	414	ASP
1	D	459	GLU
1	D	460	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	110	ASN
1	A	116	ASN
1	A	129	ASN
1	A	137	HIS
1	A	173	GLN
1	A	197	ASN
1	A	361	ASN
1	A	421	GLN
1	A	434	ASN
1	A	464	GLN
1	B	34	GLN
1	B	42	GLN
1	B	110	ASN
1	B	118	GLN
1	B	129	ASN
1	B	137	HIS
1	B	167	GLN
1	B	173	GLN
1	B	197	ASN
1	B	324	ASN
1	B	388	GLN
1	B	409	ASN
1	B	421	GLN
1	B	434	ASN
1	C	42	GLN
1	C	91	HIS
1	C	94	ASN

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Mol	Chain	Res	Type
1	C	116	ASN
1	C	118	GLN
1	C	129	ASN
1	C	137	HIS
1	C	162	ASN
1	C	164	GLN
1	C	173	GLN
1	C	197	ASN
1	C	409	ASN
1	C	434	ASN
1	C	438	GLN
1	C	464	GLN
1	D	27	ASN
1	D	94	ASN
1	D	110	ASN
1	D	116	ASN
1	D	118	GLN
1	D	129	ASN
1	D	137	HIS
1	D	173	GLN
1	D	197	ASN
1	D	291	ASN
1	D	328	GLN
1	D	356	GLN
1	D	409	ASN
1	D	421	GLN
1	D	431	ASN
1	D	434	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AS1	D	0	-	18,19,19	4.08	8 (44%)	19,24,24	8.73	11 (57%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AS1	D	0	-	1/1/6/7	7/21/23/23	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	0	AS1	CB-CA	12.42	1.79	1.53
2	D	0	AS1	C1-N2	8.32	1.69	1.46
2	D	0	AS1	CB-CD	3.83	1.61	1.51
2	D	0	AS1	CA-N1	-3.77	1.38	1.45
2	D	0	AS1	C-N3	3.57	1.42	1.34
2	D	0	AS1	OD2-CD	2.51	1.30	1.22
2	D	0	AS1	C-N2	2.43	1.34	1.28
2	D	0	AS1	C-N1	2.18	1.39	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	0	AS1	C2-C1-N2	34.06	170.98	110.67
2	D	0	AS1	C1-N2-C	12.09	149.61	121.86
2	D	0	AS1	CA-CB-CD	5.35	127.78	112.75
2	D	0	AS1	N1-C-N2	4.73	136.45	125.00
2	D	0	AS1	N3-C-N2	-3.99	109.01	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	0	AS1	CB-CA-N1	3.90	118.08	110.64
2	D	0	AS1	OG1-CG-OG2	-3.75	115.56	124.08
2	D	0	AS1	CG-CA-N1	-3.49	102.48	110.57
2	D	0	AS1	C3-C4-N4	3.10	118.21	110.12
2	D	0	AS1	N3-C-N1	-2.25	114.55	118.86
2	D	0	AS1	OG1-CG-CA	2.04	120.41	113.51

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	0	AS1	C4

All (7) torsion outliers are listed below:

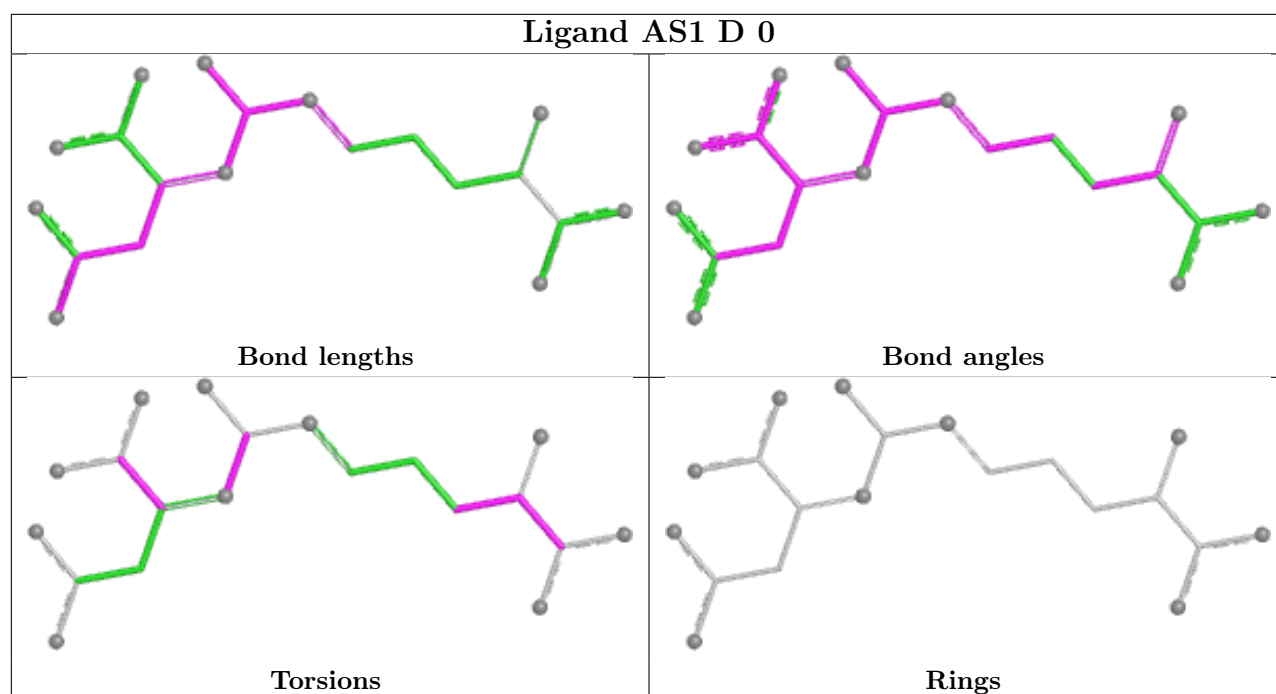
Mol	Chain	Res	Type	Atoms
2	D	0	AS1	C2-C3-C4-C5
2	D	0	AS1	CB-CA-CG-OG2
2	D	0	AS1	CB-CA-CG-OG1
2	D	0	AS1	C3-C4-C5-O52
2	D	0	AS1	N2-C-N1-CA
2	D	0	AS1	N1-CA-CG-OG2
2	D	0	AS1	C3-C4-C5-O51

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	0	AS1	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	424/447 (94%)	2.20	217 (51%) 0 0	17, 37, 85, 95	0
1	B	418/447 (93%)	1.57	134 (32%) 1 1	14, 35, 76, 98	0
1	C	434/447 (97%)	2.41	255 (58%) 0 0	18, 42, 95, 100	0
1	D	436/447 (97%)	1.58	136 (31%) 1 1	17, 36, 87, 99	0
All	All	1712/1788 (95%)	1.94	742 (43%) 0 0	14, 38, 87, 100	0

All (742) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	PRO	9.0
1	D	404	GLY	8.7
1	A	383	GLY	8.6
1	D	29	SER	6.6
1	A	402	THR	6.4
1	C	103	GLY	6.4
1	A	449	SER	6.3
1	B	29	SER	6.3
1	A	83	VAL	6.2
1	A	35	ARG	6.2
1	C	452	THR	6.2
1	A	82	VAL	6.1
1	D	378	TYR	6.0
1	D	409	ASN	6.0
1	A	37	SER	5.8
1	D	30	ILE	5.8
1	C	391	THR	5.7
1	C	31	ALA	5.7
1	C	414	ASP	5.6
1	C	398	HIS	5.6
1	D	420	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	451	THR	5.5
1	C	411	SER	5.4
1	C	67	SER	5.4
1	A	186	SER	5.4
1	C	79	GLY	5.3
1	C	393	SER	5.3
1	B	402	THR	5.3
1	D	414	ASP	5.3
1	C	89	ASP	5.3
1	B	68	GLY	5.3
1	A	415	LEU	5.2
1	D	281	THR	5.2
1	B	54	ALA	5.2
1	C	29	SER	5.1
1	A	386	PHE	5.1
1	A	460	LEU	5.1
1	D	389	ALA	5.0
1	A	46	ALA	5.0
1	A	103	GLY	5.0
1	B	400	ALA	5.0
1	A	85	GLN	4.9
1	C	60	THR	4.9
1	C	93	ALA	4.9
1	C	46	ALA	4.9
1	C	106	ALA	4.9
1	D	425	ASP	4.9
1	C	423	SER	4.8
1	A	80	VAL	4.8
1	C	80	VAL	4.8
1	D	397	VAL	4.8
1	A	400	ALA	4.8
1	A	73	SER	4.7
1	C	358	SER	4.7
1	C	77	SER	4.7
1	A	104	ASP	4.7
1	A	406	THR	4.7
1	D	394	GLY	4.7
1	C	424	SER	4.7
1	B	106	ALA	4.6
1	D	439	TYR	4.6
1	C	413	GLU	4.6
1	C	415	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	376	ALA	4.6
1	D	392	ALA	4.6
1	A	411	SER	4.5
1	D	278	ALA	4.5
1	A	110	ASN	4.5
1	A	81	PHE	4.5
1	B	24	GLU	4.5
1	A	98	LEU	4.5
1	A	97	ARG	4.5
1	C	57	LEU	4.4
1	C	101	LEU	4.4
1	C	366	LEU	4.4
1	C	86	SER	4.4
1	D	277	ASP	4.4
1	D	391	THR	4.4
1	C	73	SER	4.4
1	C	278	ALA	4.4
1	C	342	THR	4.3
1	C	90	ILE	4.3
1	D	380	VAL	4.3
1	B	21	PRO	4.3
1	B	93	ALA	4.3
1	A	36	LEU	4.3
1	B	103	GLY	4.3
1	C	425	ASP	4.2
1	C	422	PHE	4.2
1	C	368	PRO	4.2
1	C	68	GLY	4.2
1	C	83	VAL	4.2
1	D	427	SER	4.2
1	C	20	ASP	4.2
1	A	374	ASP	4.2
1	C	109	LEU	4.2
1	B	411	SER	4.2
1	A	436	VAL	4.1
1	C	449	SER	4.1
1	A	136	THR	4.1
1	A	34	GLN	4.1
1	C	385	PRO	4.1
1	A	66	LEU	4.1
1	A	87	ASP	4.1
1	C	434	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	151	ILE	4.1
1	B	95	GLU	4.1
1	A	225	ALA	4.0
1	D	388	GLN	4.0
1	A	209	ASN	4.0
1	D	89	ASP	4.0
1	D	390	HIS	4.0
1	C	343	ALA	4.0
1	A	398	HIS	4.0
1	C	225	ALA	4.0
1	C	399	LEU	4.0
1	D	279	PHE	4.0
1	C	277	ASP	4.0
1	C	293	ASP	4.0
1	D	417	SER	4.0
1	C	400	ALA	3.9
1	A	69	LEU	3.9
1	A	191	GLU	3.9
1	A	221	GLU	3.9
1	A	50	ALA	3.9
1	A	79	GLY	3.9
1	C	19	THR	3.9
1	C	102	ILE	3.9
1	A	388	GLN	3.9
1	C	389	ALA	3.9
1	D	396	ALA	3.9
1	D	21	PRO	3.9
1	A	39	VAL	3.9
1	B	98	LEU	3.9
1	C	62	LEU	3.8
1	C	91	HIS	3.8
1	A	84	LYS	3.8
1	B	208	GLY	3.8
1	D	406	THR	3.8
1	B	464	GLN	3.8
1	A	226	SER	3.8
1	D	423	SER	3.8
1	A	68	GLY	3.8
1	A	109	LEU	3.8
1	D	426	VAL	3.8
1	C	274	THR	3.8
1	C	84	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	65	ILE	3.8
1	B	56	ILE	3.8
1	D	407	ILE	3.8
1	B	91	HIS	3.8
1	A	378	TYR	3.7
1	C	402	THR	3.7
1	A	441	ALA	3.7
1	C	348	ALA	3.7
1	D	411	SER	3.7
1	C	99	LYS	3.7
1	A	33	ASP	3.7
1	A	389	ALA	3.7
1	A	72	ILE	3.7
1	A	112	GLY	3.7
1	C	426	VAL	3.7
1	A	417	SER	3.7
1	C	72	ILE	3.7
1	C	105	ILE	3.7
1	A	100	GLU	3.7
1	B	110	ASN	3.7
1	A	465	LYS	3.7
1	C	88	GLU	3.6
1	C	297	LEU	3.6
1	C	412	LEU	3.6
1	A	391	THR	3.6
1	D	161	THR	3.6
1	D	382	LYS	3.6
1	B	235	ILE	3.6
1	D	385	PRO	3.6
1	D	416	LYS	3.6
1	C	427	SER	3.6
1	C	65	ILE	3.6
1	D	418	ILE	3.6
1	C	82	VAL	3.6
1	B	46	ALA	3.6
1	A	95	GLU	3.6
1	B	101	LEU	3.6
1	B	111	THR	3.6
1	C	338	VAL	3.6
1	C	380	VAL	3.6
1	A	106	ALA	3.6
1	B	220	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	448	SER	3.5
1	C	362	MET	3.5
1	C	30	ILE	3.5
1	B	94	ASN	3.5
1	C	361	ASN	3.5
1	C	95	GLU	3.5
1	D	401	GLU	3.5
1	A	90	ILE	3.5
1	A	208	GLY	3.5
1	D	460	LEU	3.5
1	B	89	ASP	3.5
1	A	118	GLN	3.5
1	A	86	SER	3.5
1	A	280	SER	3.5
1	C	76	TRP	3.5
1	A	55	GLY	3.5
1	C	394	GLY	3.5
1	D	103	GLY	3.5
1	D	386	PHE	3.5
1	B	58	THR	3.5
1	D	384	VAL	3.5
1	A	78	LYS	3.5
1	B	71	LYS	3.5
1	A	394	GLY	3.5
1	B	90	ILE	3.5
1	A	437	GLU	3.5
1	B	51	LEU	3.5
1	B	139	LEU	3.5
1	D	399	LEU	3.5
1	D	402	THR	3.4
1	A	150	ALA	3.4
1	B	67	SER	3.4
1	C	409	ASN	3.4
1	C	85	GLN	3.4
1	C	386	PHE	3.4
1	A	220	SER	3.4
1	C	369	GLU	3.4
1	D	455	GLU	3.4
1	B	105	ILE	3.4
1	C	417	SER	3.4
1	C	459	GLU	3.4
1	B	30	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	420	PRO	3.4
1	B	70	GLU	3.4
1	D	393	SER	3.4
1	C	133	ILE	3.3
1	C	275	LEU	3.3
1	D	69	LEU	3.3
1	A	96	ARG	3.3
1	C	296	GLU	3.3
1	D	381	ARG	3.3
1	A	231	SER	3.3
1	A	40	ASP	3.3
1	C	26	LEU	3.3
1	D	412	LEU	3.3
1	B	92	THR	3.3
1	D	452	THR	3.3
1	B	74	GLU	3.3
1	C	360	GLU	3.3
1	A	130	SER	3.3
1	B	73	SER	3.3
1	C	130	SER	3.3
1	C	416	LYS	3.3
1	A	464	GLN	3.3
1	C	259	ALA	3.3
1	A	129	ASN	3.3
1	A	217	MET	3.3
1	D	375	LEU	3.3
1	C	22	ILE	3.3
1	C	184	ARG	3.3
1	B	231	SER	3.3
1	C	353	SER	3.3
1	A	120	VAL	3.3
1	D	444	GLY	3.3
1	B	33	ASP	3.3
1	A	139	LEU	3.3
1	C	377	LEU	3.3
1	A	41	ILE	3.3
1	D	413	GLU	3.3
1	A	111	THR	3.3
1	A	93	ALA	3.2
1	C	180	VAL	3.3
1	A	277	ASP	3.2
1	B	326	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	27	ASN	3.2
1	D	104	ASP	3.2
1	C	387	ARG	3.2
1	A	57	LEU	3.2
1	C	98	LEU	3.2
1	A	147	GLU	3.2
1	C	75	GLU	3.2
1	C	401	GLU	3.2
1	C	71	LYS	3.2
1	C	217	MET	3.2
1	C	383	GLY	3.2
1	A	89	ASP	3.2
1	A	369	GLU	3.2
1	A	403	LYS	3.2
1	C	175	LEU	3.2
1	A	452	THR	3.2
1	A	149	ALA	3.2
1	A	443	ALA	3.2
1	D	107	GLY	3.2
1	D	398	HIS	3.2
1	B	379	LEU	3.2
1	B	72	ILE	3.2
1	C	132	SER	3.2
1	C	214	ASP	3.2
1	B	26	LEU	3.2
1	D	421	GLN	3.2
1	C	41	ILE	3.2
1	C	183	THR	3.2
1	C	340	THR	3.2
1	C	37	SER	3.1
1	C	276	SER	3.1
1	A	181	ALA	3.1
1	B	20	ASP	3.1
1	B	57	LEU	3.1
1	C	438	GLN	3.1
1	A	373	THR	3.1
1	A	52	GLU	3.1
1	B	216	GLU	3.1
1	C	100	GLU	3.1
1	C	28	SER	3.1
1	A	197	ASN	3.1
1	C	410	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	133	ILE	3.1
1	C	357	ILE	3.1
1	A	216	GLU	3.1
1	A	177	SER	3.1
1	D	91	HIS	3.1
1	D	379	LEU	3.1
1	C	112	GLY	3.1
1	C	392	ALA	3.1
1	A	210	PRO	3.1
1	D	82	VAL	3.1
1	A	62	LEU	3.1
1	A	101	LEU	3.1
1	A	63	GLU	3.0
1	C	435	SER	3.0
1	C	464	GLN	3.0
1	B	214	ASP	3.0
1	C	81	PHE	3.0
1	A	397	VAL	3.0
1	A	412	LEU	3.0
1	C	397	VAL	3.0
1	C	378	TYR	3.0
1	B	65	ILE	3.0
1	C	418	ILE	3.0
1	A	435	SER	3.0
1	C	231	SER	3.0
1	A	190	GLY	3.0
1	C	408	ASN	3.0
1	A	224	PHE	3.0
1	B	389	ALA	3.0
1	D	372	ALA	3.0
1	A	192	VAL	3.0
1	B	460	LEU	3.0
1	C	39	VAL	3.0
1	C	436	VAL	3.0
1	D	436	VAL	3.0
1	A	56	ILE	3.0
1	B	102	ILE	3.0
1	B	64	LYS	3.0
1	C	97	ARG	3.0
1	D	403	LYS	3.0
1	A	448	SER	3.0
1	B	236	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	266	SER	3.0
1	A	202	GLY	3.0
1	A	318	GLY	3.0
1	D	422	PHE	3.0
1	D	430	PHE	3.0
1	A	446	ALA	3.0
1	C	149	ALA	3.0
1	C	454	ILE	3.0
1	B	219	ARG	3.0
1	C	456	GLN	3.0
1	D	438	GLN	3.0
1	C	451	THR	3.0
1	B	132	SER	3.0
1	A	239	ASP	3.0
1	A	414	ASP	3.0
1	B	27	ASN	3.0
1	C	250	LEU	2.9
1	C	64	LYS	2.9
1	C	382	LYS	2.9
1	D	435	SER	2.9
1	C	52	GLU	2.9
1	C	94	ASN	2.9
1	C	355	LEU	2.9
1	C	390	HIS	2.9
1	C	78	LYS	2.9
1	B	104	ASP	2.9
1	C	122	ASP	2.9
1	D	424	SER	2.9
1	A	137	HIS	2.9
1	B	25	LYS	2.9
1	C	146	VAL	2.9
1	C	367	THR	2.9
1	A	132	SER	2.9
1	C	32	TYR	2.9
1	B	210	PRO	2.9
1	D	25	LYS	2.9
1	A	54	ALA	2.9
1	B	66	LEU	2.9
1	B	69	LEU	2.9
1	A	281	THR	2.9
1	B	246	SER	2.8
1	B	321	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	419	SER	2.8
1	D	448	SER	2.8
1	C	292	PRO	2.8
1	C	388	GLN	2.8
1	A	392	ALA	2.8
1	A	401	GLU	2.8
1	A	151	ILE	2.8
1	D	274	THR	2.8
1	B	425	ASP	2.8
1	D	40	ASP	2.8
1	C	177	SER	2.8
1	A	292	PRO	2.8
1	A	88	GLU	2.8
1	B	369	GLU	2.8
1	A	198	VAL	2.8
1	C	155	VAL	2.8
1	A	60	THR	2.8
1	C	339	ASP	2.8
1	D	291	ASN	2.8
1	A	43	GLY	2.8
1	B	100	GLU	2.8
1	B	401	GLU	2.8
1	C	24	GLU	2.8
1	D	376	ALA	2.8
1	D	465	LYS	2.8
1	C	450	VAL	2.8
1	C	96	ARG	2.8
1	C	58	THR	2.8
1	B	212	ASP	2.8
1	C	208	GLY	2.8
1	D	383	GLY	2.8
1	C	147	GLU	2.8
1	C	45	MET	2.8
1	C	50	ALA	2.8
1	C	334	VAL	2.8
1	A	434	ASN	2.7
1	C	87	ASP	2.7
1	B	44	SER	2.7
1	C	55	GLY	2.7
1	C	220	SER	2.7
1	C	226	SER	2.7
1	A	442	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	457	LEU	2.7
1	C	198	VAL	2.7
1	D	264	ILE	2.7
1	C	107	GLY	2.7
1	B	114	SER	2.7
1	C	236	SER	2.7
1	A	447	LYS	2.7
1	B	462	LYS	2.7
1	C	370	MET	2.7
1	D	57	LEU	2.7
1	D	410	LEU	2.7
1	B	32	TYR	2.7
1	B	240	PHE	2.7
1	B	34	GLN	2.7
1	C	384	VAL	2.7
1	C	404	GLY	2.7
1	B	276	SER	2.7
1	B	393	SER	2.7
1	A	199	LEU	2.7
1	D	26	LEU	2.7
1	D	377	LEU	2.7
1	B	166	ALA	2.7
1	D	428	GLN	2.7
1	B	451	THR	2.7
1	C	27	ASN	2.7
1	D	429	VAL	2.7
1	A	223	GLU	2.7
1	C	144	THR	2.7
1	C	395	LYS	2.7
1	C	302	SER	2.7
1	D	220	SER	2.7
1	A	211	LEU	2.7
1	D	464	GLN	2.6
1	B	465	LYS	2.6
1	A	450	VAL	2.6
1	D	90	ILE	2.6
1	D	419	SER	2.6
1	D	374	ASP	2.6
1	A	387	ARG	2.6
1	A	102	ILE	2.6
1	B	22	ILE	2.6
1	B	28	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	189	LEU	2.6
1	C	379	LEU	2.6
1	C	333	ALA	2.6
1	C	148	ARG	2.6
1	C	197	ASN	2.6
1	C	153	ILE	2.6
1	A	99	LYS	2.6
1	A	48	ALA	2.6
1	A	409	ASN	2.6
1	D	293	ASP	2.6
1	D	408	ASN	2.6
1	A	45	MET	2.6
1	A	204	GLY	2.6
1	B	55	GLY	2.6
1	B	112	GLY	2.6
1	A	228	SER	2.6
1	A	294	SER	2.6
1	C	142	ILE	2.6
1	A	396	ALA	2.5
1	B	376	ALA	2.5
1	A	144	THR	2.5
1	C	21	PRO	2.5
1	C	354	THR	2.5
1	A	77	SER	2.5
1	A	203	SER	2.5
1	C	25	LYS	2.5
1	C	137	HIS	2.5
1	C	351	VAL	2.5
1	C	263	ILE	2.5
1	C	34	GLN	2.5
1	C	104	ASP	2.5
1	C	43	GLY	2.5
1	D	368	PRO	2.5
1	A	76	TRP	2.5
1	D	105	ILE	2.5
1	B	75	GLU	2.5
1	C	47	TYR	2.5
1	C	431	ASN	2.5
1	A	91	HIS	2.5
1	C	406	THR	2.5
1	C	445	THR	2.5
1	C	335	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	429	VAL	2.5
1	D	77	SER	2.5
1	B	263	ILE	2.5
1	C	407	ILE	2.5
1	B	297	LEU	2.5
1	B	461	MET	2.5
1	A	49	LYS	2.5
1	C	364	LYS	2.5
1	D	431	ASN	2.5
1	A	310	ALA	2.5
1	B	333	ALA	2.5
1	A	404	GLY	2.5
1	C	204	GLY	2.5
1	A	61	GLU	2.4
1	B	61	GLU	2.4
1	A	67	SER	2.4
1	A	236	SER	2.4
1	A	427	SER	2.4
1	B	423	SER	2.4
1	A	429	VAL	2.4
1	A	206	LEU	2.4
1	A	462	LYS	2.4
1	C	403	LYS	2.4
1	A	74	GLU	2.4
1	A	188	ARG	2.4
1	B	43	GLY	2.4
1	B	368	PRO	2.4
1	C	318	GLY	2.4
1	D	88	GLU	2.4
1	D	321	SER	2.4
1	B	426	VAL	2.4
1	B	23	MET	2.4
1	C	258	MET	2.4
1	A	371	LEU	2.4
1	A	113	ARG	2.4
1	D	50	ALA	2.4
1	D	225	ALA	2.4
1	A	71	LYS	2.4
1	A	235	ILE	2.4
1	D	59	LYS	2.4
1	A	433	VAL	2.4
1	B	241	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	366	LEU	2.4
1	B	398	HIS	2.4
1	A	438	GLN	2.4
1	A	296	GLU	2.4
1	C	396	ALA	2.4
1	C	465	LYS	2.4
1	D	300	SER	2.4
1	A	418	ILE	2.4
1	C	169	ILE	2.4
1	C	221	GLU	2.4
1	A	94	ASN	2.3
1	A	376	ALA	2.3
1	C	248	ALA	2.3
1	D	93	ALA	2.3
1	A	321	SER	2.3
1	C	135	SER	2.3
1	A	105	ILE	2.3
1	C	347	VAL	2.3
1	D	405	ILE	2.3
1	D	63	GLU	2.3
1	C	336	ASP	2.3
1	A	59	LYS	2.3
1	D	462	LYS	2.3
1	B	204	GLY	2.3
1	C	444	GLY	2.3
1	C	234	ALA	2.3
1	C	267	THR	2.3
1	A	184	ARG	2.3
1	B	97	ARG	2.3
1	A	153	ILE	2.3
1	D	41	ILE	2.3
1	A	279	PHE	2.3
1	B	39	VAL	2.3
1	C	119	VAL	2.3
1	B	108	LYS	2.3
1	C	210	PRO	2.3
1	A	439	TYR	2.3
1	D	171	TRP	2.3
1	C	446	ALA	2.3
1	A	92	THR	2.3
1	B	96	ARG	2.3
1	C	228	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	28	SER	2.3
1	A	456	GLN	2.3
1	C	140	GLN	2.3
1	D	356	GLN	2.3
1	D	454	ILE	2.3
1	C	174	PHE	2.3
1	A	395	LYS	2.3
1	B	319	LEU	2.3
1	A	212	ASP	2.3
1	B	202	GLY	2.3
1	C	136	THR	2.3
1	B	427	SER	2.3
1	D	44	SER	2.3
1	C	42	GLN	2.3
1	B	364	LYS	2.3
1	A	218	LEU	2.2
1	C	33	ASP	2.2
1	A	115	ARG	2.2
1	D	47	TYR	2.2
1	D	400	ALA	2.2
1	C	349	THR	2.2
1	D	73	SER	2.2
1	B	62	LEU	2.2
1	C	120	VAL	2.2
1	C	189	LEU	2.2
1	A	117	ASP	2.2
1	C	209	ASN	2.2
1	C	381	ARG	2.2
1	C	458	ARG	2.2
1	A	58	THR	2.2
1	A	353	SER	2.2
1	D	280	SER	2.2
1	B	405	ILE	2.2
1	B	454	ILE	2.2
1	C	36	LEU	2.2
1	D	371	LEU	2.2
1	A	154	ASP	2.2
1	A	420	PRO	2.2
1	A	107	GLY	2.2
1	D	79	GLY	2.2
1	B	413	GLU	2.2
1	A	173	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	331	LYS	2.2
1	C	443	ALA	2.2
1	D	166	ALA	2.2
1	A	423	SER	2.2
1	C	69	LEU	2.2
1	D	80	VAL	2.2
1	A	422	PHE	2.2
1	D	87	ASP	2.2
1	B	385	PRO	2.2
1	C	158	PRO	2.2
1	D	292	PRO	2.2
1	B	459	GLU	2.2
1	C	59	LYS	2.2
1	B	383	GLY	2.2
1	C	173	GLN	2.2
1	A	274	THR	2.2
1	B	60	THR	2.2
1	D	106	ALA	2.2
1	D	365	ALA	2.2
1	D	373	THR	2.2
1	D	387	ARG	2.1
1	C	125	LEU	2.1
1	A	426	VAL	2.1
1	C	433	VAL	2.1
1	B	363	GLU	2.1
1	B	420	PRO	2.1
1	A	307	GLY	2.1
1	A	205	ALA	2.1
1	B	225	ALA	2.1
1	D	48	ALA	2.1
1	C	160	TYR	2.1
1	A	454	ILE	2.1
1	C	66	LEU	2.1
1	D	415	LEU	2.1
1	A	187	GLU	2.1
1	A	237	GLU	2.1
1	A	291	ASN	2.1
1	A	293	ASP	2.1
1	C	261	ASP	2.1
1	C	374	ASP	2.1
1	D	154	ASP	2.1
1	B	198	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	344	VAL	2.1
1	B	422	PHE	2.1
1	A	444	GLY	2.1
1	D	115	ARG	2.1
1	A	207	ALA	2.1
1	B	50	ALA	2.1
1	D	443	ALA	2.1
1	A	51	LEU	2.1
1	B	109	LEU	2.1
1	A	47	TYR	2.1
1	A	425	ASP	2.1
1	B	47	TYR	2.1
1	B	137	HIS	2.1
1	B	328	GLN	2.1
1	D	34	GLN	2.1
1	A	159	GLY	2.1
1	C	271	GLY	2.1
1	C	170	ARG	2.1
1	B	203	SER	2.1
1	B	99	LYS	2.1
1	A	360	GLU	2.1
1	D	70	GLU	2.1
1	C	345	LEU	2.1
1	C	346	GLN	2.1
1	C	460	LEU	2.1
1	A	324	ASN	2.1
1	B	151	ILE	2.1
1	A	119	VAL	2.1
1	C	463	LYS	2.0
1	A	249	THR	2.0
1	B	31	ALA	2.0
1	B	45	MET	2.0
1	C	61	GLU	2.0
1	C	152	GLU	2.0
1	D	459	GLU	2.0
1	A	167	GLN	2.0
1	A	453	GLN	2.0
1	C	110	ASN	2.0
1	C	233	ASP	2.0
1	A	357	ILE	2.0
1	B	107	GLY	2.0
1	C	462	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	440	THR	2.0
1	D	349	THR	2.0
1	B	211	LEU	2.0
1	D	66	LEU	2.0
1	B	115	ARG	2.0
1	C	264	ILE	2.0
1	D	99	LYS	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](#)

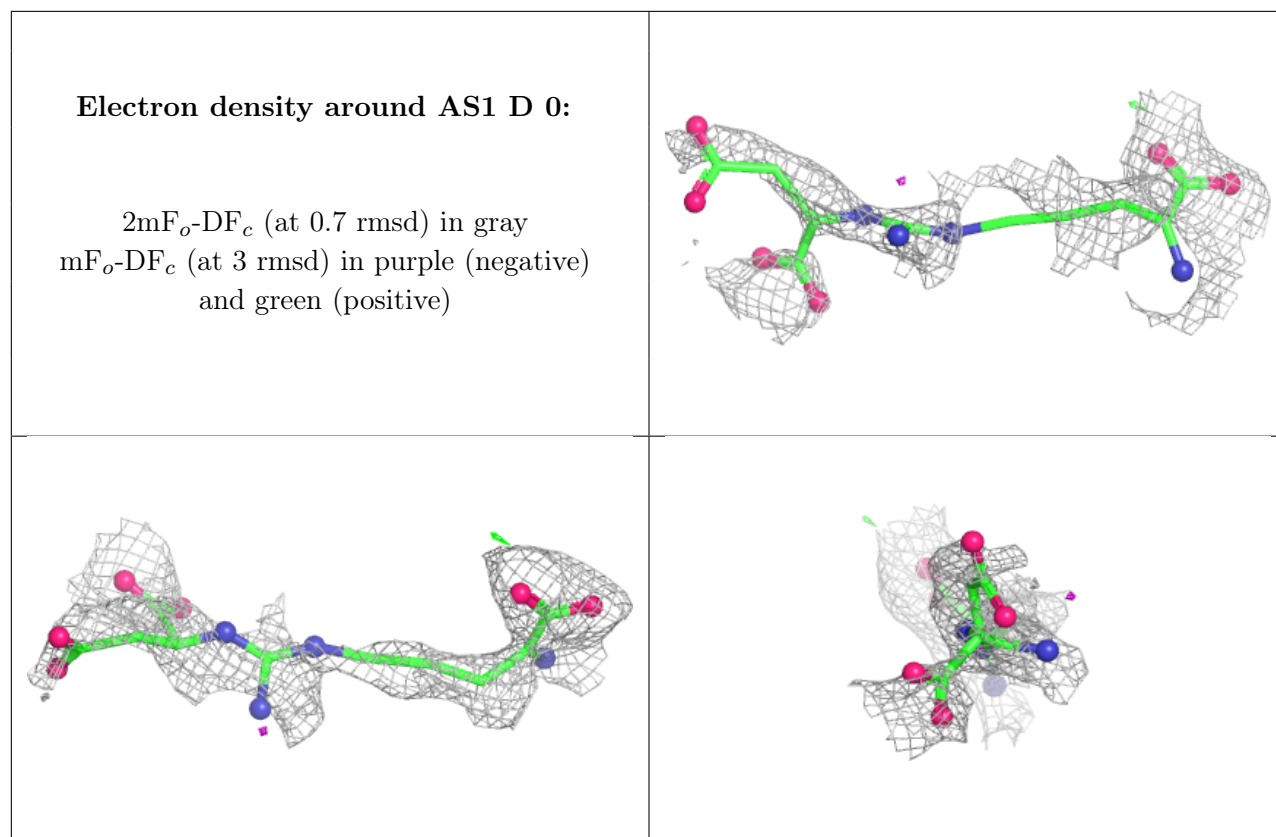
There are no oligosaccharides in this entry.

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	AS1	D	0	20/20	0.62	0.16	30,60,82,86	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.