



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:43 AM UTC

PDB ID : 3UKR / pdb_00003ukr
Title : Crystal structure of Bos taurus Arp2/3 complex with bound inhibitor CK-666
Authors : Nolen, B.J.; Han, M.
Deposited on : 2011-11-09
Resolution : 2.48 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

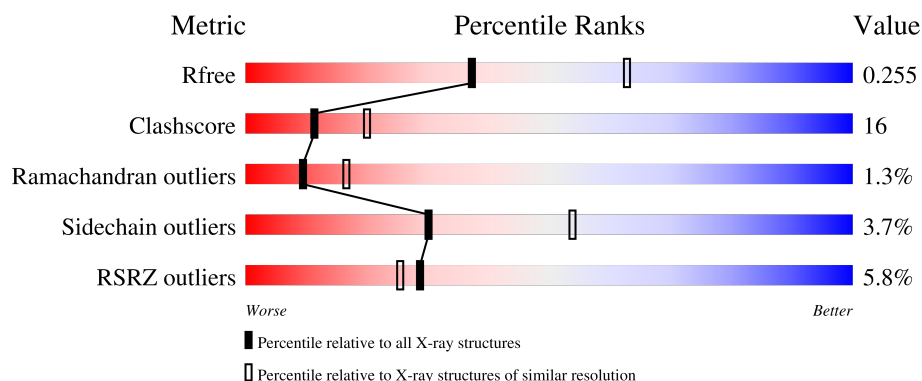
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	418	5% 68% 26% • •
2	B	394	7% 26% 19% • 51%
3	C	372	4% 64% 27% • 6%
4	D	300	2% 72% 21% • 6%
5	E	178	8% 57% 34% 6% •

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Mol	Chain	Length	Quality of chain
6	F	168	2% 74% 23% ••
7	G	151	10% 60% 26% • 10%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13746 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3187	2048	534	589	16			

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	0	0
			1527	982	257	284	4			

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	349	Total	C	N	O	S	0	0	0
			2716	1721	480	496	19			

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	282	Total	C	N	O	S	0	0	0
			2279	1449	395	427	8			

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	173	Total	C	N	O	S	0	0	0
			1401	902	235	255	9			

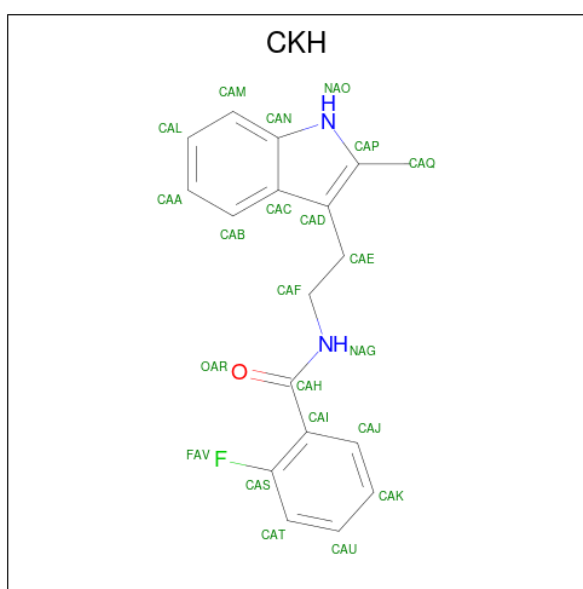
- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	167	Total	C	N	O	S	0	0	0
			1363	871	239	244	9			

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	136	Total	C	N	O	S	0	0	0
			1030	647	181	199	3			

- Molecule 8 is 2-fluoro-N-[2-(2-methyl-1H-indol-3-yl)ethyl]benzamide (CCD ID: CKH) (formula: C₁₈H₁₇FN₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	F	N	O	0	0
			22	18	1	2	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	45	Total	O	0	0
			45	45		
9	B	11	Total	O	0	0
			11	11		
9	C	51	Total	O	0	0
			51	51		
9	D	51	Total	O	0	0
			51	51		

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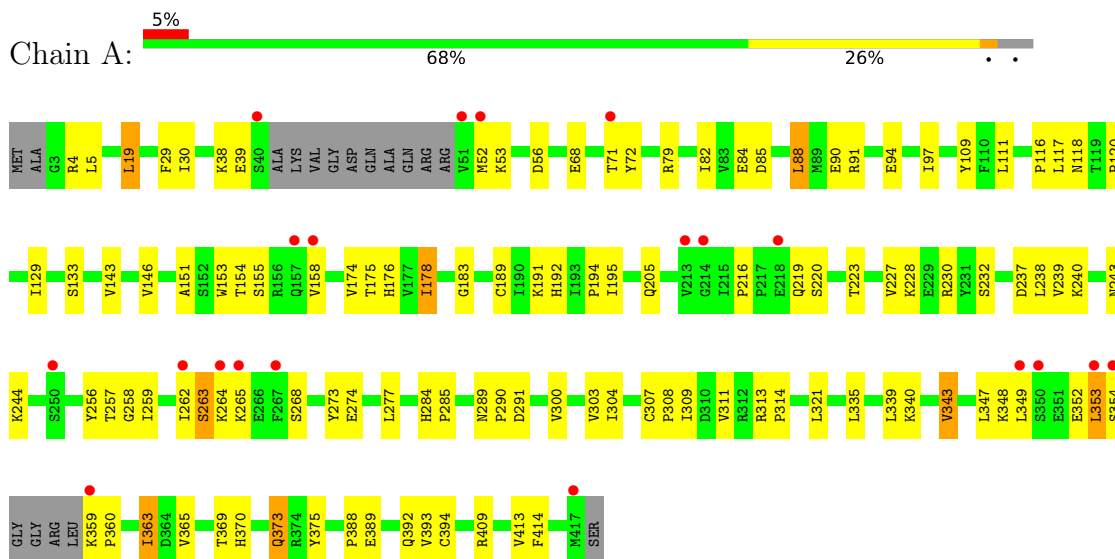
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	6	Total 6	O 6	0	0
9	F	46	Total 46	O 46	0	0
9	G	11	Total 11	O 11	0	0

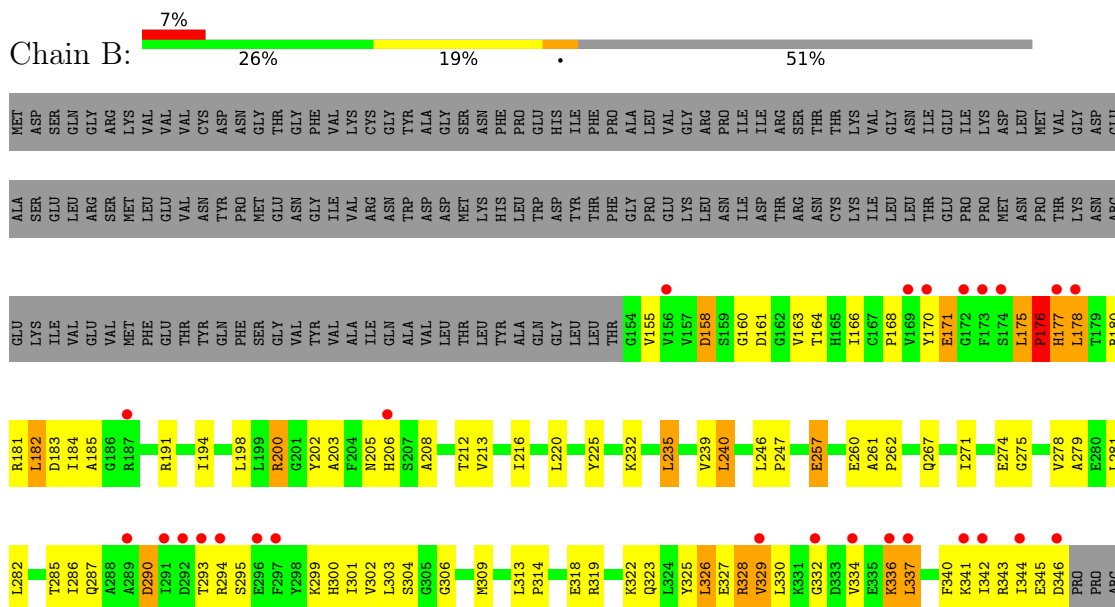
3 Residue-property plots [i](#)

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: Actin-related protein 3



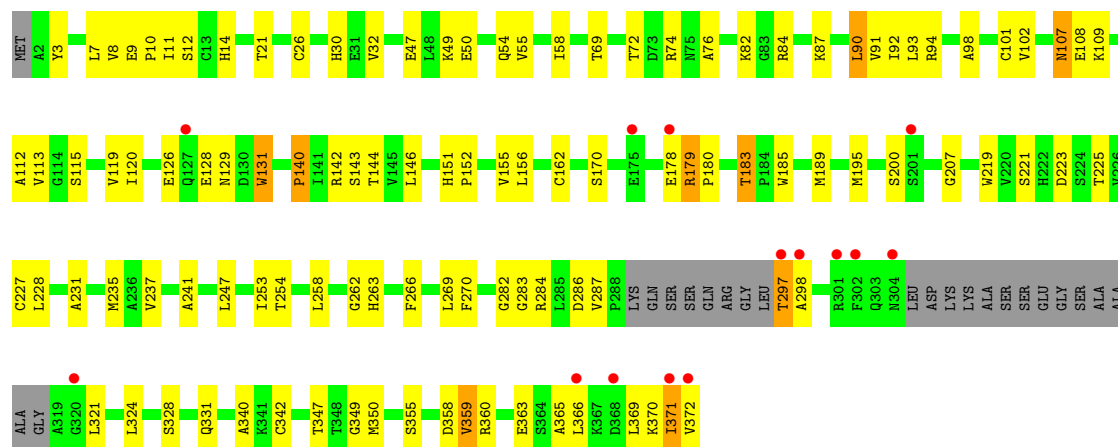
• Molecule 2: Actin-related protein 2



ARG
LYS
HIS
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PHE
LEU
GLY
GLY
ALA
VAL
LEU
ALA
ASP
ILE
MET
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ASP
LYS
ASP
ASN
TRP
PHE
MET
THR
THR
ARG
GLN
GLU
TYR
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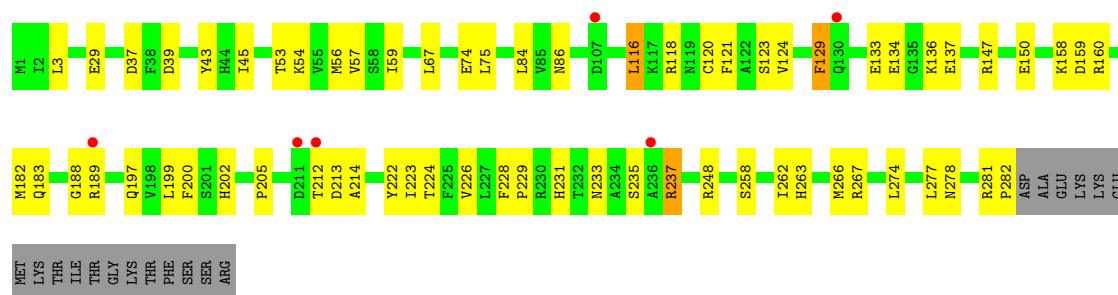
• Molecule 3: Actin-related protein 2/3 complex subunit 1B

Chain C: 4% 64% 27% 6%



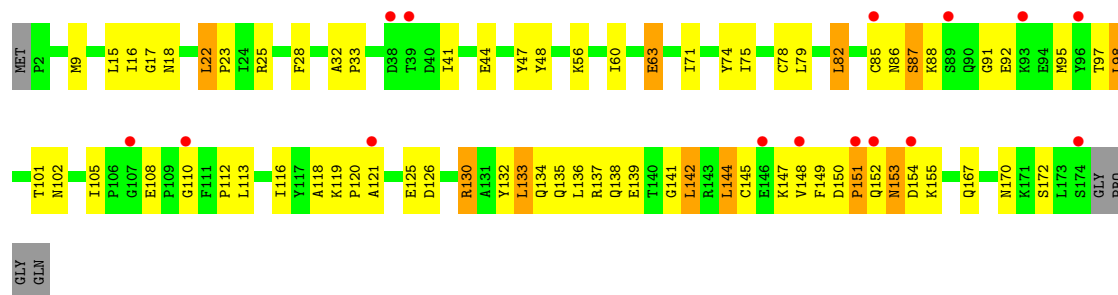
• Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain D: 2% 72% 21% 6%



• Molecule 5: Actin-related protein 2/3 complex subunit 3

Chain E: 8% 57% 34% 6%

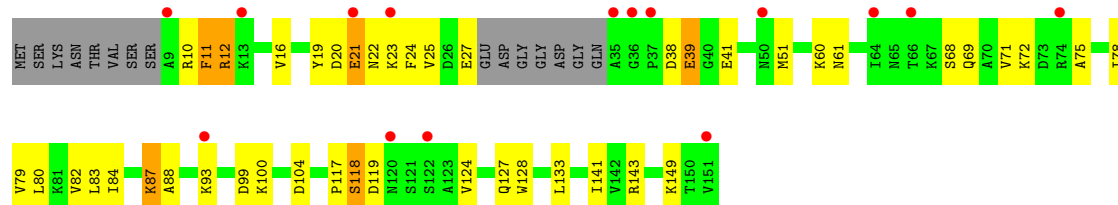


• Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F: 2% 74% 23% ..



• Molecule 7: Actin-related protein 2/3 complex subunit 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.19Å 129.69Å 205.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.48 20.00 – 2.48	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.48) 84.2 (20.00-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.261 0.212 , 0.255	Depositor DCC
R_{free} test set	4709 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13746	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 2.67% 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: CKH

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	0.46	0/3268	0.94	10/4437 (0.2%)
2	B	0.44	0/1554	0.88	4/2100 (0.2%)
3	C	0.45	0/2785	0.92	8/3777 (0.2%)
4	D	0.47	0/2328	0.90	4/3143 (0.1%)
5	E	0.37	0/1435	0.89	2/1936 (0.1%)
6	F	0.47	0/1385	0.94	4/1858 (0.2%)
7	G	0.38	0/1042	0.89	2/1401 (0.1%)
All	All	0.44	0/13797	0.91	34/18652 (0.2%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	337	LEU	N-CA-C	7.36	120.17	111.71
1	A	178	ILE	N-CA-C	7.25	115.36	107.60
1	A	373	GLN	N-CA-C	6.87	118.77	111.28
4	D	129	PHE	N-CA-C	-6.81	103.79	111.14
4	D	39	ASP	N-CA-C	6.74	120.95	111.52
3	C	11	ILE	N-CA-C	-6.64	97.37	107.73
1	A	238	LEU	N-CA-C	6.34	118.19	111.28
1	A	97	ILE	N-CA-C	6.33	117.34	111.45
6	F	81	GLU	N-CA-C	6.20	118.04	111.28
3	C	328	SER	N-CA-C	6.01	119.19	110.42
1	A	118	ASN	N-CA-C	-5.94	100.31	109.76
5	E	17	GLY	N-CA-C	-5.94	100.85	110.95
6	F	132	VAL	N-CA-C	-5.89	105.00	110.53
3	C	349	GLY	N-CA-C	5.88	119.88	111.12
1	A	109	TYR	N-CA-C	-5.66	101.26	110.20
1	A	68	GLU	N-CA-C	5.64	117.66	110.61
1	A	189	CYS	N-CA-C	5.60	119.81	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	110	GLY	N-CA-C	-5.40	107.47	113.79
6	F	109	VAL	N-CA-C	-5.34	102.69	109.58
1	A	273	TYR	N-CA-C	5.33	117.51	111.11
3	C	359	VAL	N-CA-C	5.33	116.05	110.62
3	C	287	VAL	N-CA-C	5.32	113.68	107.89
2	B	271	ILE	N-CA-C	-5.30	107.19	111.91
3	C	283	GLY	N-CA-C	5.29	116.98	111.95
7	G	12	ARG	N-CA-C	-5.28	106.61	113.16
6	F	79	ALA	N-CA-C	5.24	117.00	111.28
7	G	51	MET	N-CA-C	5.17	116.60	110.97
3	C	237	VAL	N-CA-C	5.13	115.25	107.75
2	B	177	HIS	N-CA-C	-5.09	101.01	109.46
1	A	5	LEU	N-CA-C	5.08	116.98	109.62
4	D	86	ASN	CA-C-N	5.04	125.28	119.83
4	D	86	ASN	C-N-CA	5.04	125.28	119.83
2	B	203	ALA	N-CA-C	5.02	117.37	109.39
3	C	115	SER	N-CA-C	5.02	115.67	108.74

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3187	0	3117	82	0
2	B	1527	0	1551	100	0
3	C	2716	0	2666	83	0
4	D	2279	0	2248	54	0
5	E	1401	0	1405	63	0
6	F	1363	0	1402	41	0
7	G	1030	0	1047	41	0
8	B	22	0	17	1	0
9	A	45	0	0	3	0
9	B	11	0	0	0	0
9	C	51	0	0	2	0
9	D	51	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	6	0	0	0	0
9	F	46	0	0	1	0
9	G	11	0	0	0	0
All	All	13746	0	13453	438	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 16.

All (438) 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)
3:C:183:THR:HG22	3:C:185:TRP:H	1.18	1.04
7:G:23:LYS:HG2	7:G:24:PHE:H	1.28	0.96
3:C:142:ARG:NH2	7:G:25:VAL:H	1.64	0.94
2:B:175:LEU:HD12	2:B:178:LEU:HD12	1.48	0.92
3:C:142:ARG:HH22	7:G:25:VAL:H	0.93	0.90
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.51	0.90
3:C:142:ARG:HH22	7:G:25:VAL:N	1.69	0.89
4:D:197:GLN:HE21	4:D:199:LEU:HD11	1.34	0.89
7:G:87:LYS:HE3	7:G:87:LYS:H	1.37	0.89
2:B:205:ASN:HD22	2:B:208:ALA:H	1.17	0.88
2:B:158:ASP:OD1	2:B:304:SER:HB3	1.75	0.86
2:B:330:LEU:HG	2:B:336:LYS:NZ	1.89	0.86
5:E:82:LEU:HD23	5:E:148:VAL:HG21	1.56	0.86
5:E:95:MET:HE3	5:E:95:MET:HA	1.57	0.85
5:E:15:LEU:HD21	5:E:63:GLU:HG3	1.61	0.82
2:B:267:GLN:HG2	7:G:12:ARG:HH12	1.45	0.81
2:B:177:HIS:O	2:B:178:LEU:HB2	1.81	0.79
3:C:107:ASN:ND2	3:C:109:LYS:H	1.80	0.79
3:C:183:THR:HG22	3:C:185:TRP:N	1.98	0.79
3:C:185:TRP:HE3	3:C:235:MET:HE2	1.47	0.79
6:F:31:GLU:OE2	6:F:32:ARG:HG3	1.82	0.79
1:A:243:ASN:ND2	5:E:47:TYR:HE1	1.81	0.78
3:C:284:ARG:HD3	3:C:286:ASP:O	1.84	0.78
7:G:10:ARG:O	7:G:11:PHE:HB3	1.84	0.78
2:B:194:ILE:HG12	2:B:213:VAL:HG21	1.66	0.77
1:A:39:GLU:HG3	1:A:39:GLU:O	1.84	0.76
4:D:228:PHE:H	4:D:231:HIS:HD2	1.31	0.76
1:A:289:ASN:ND2	1:A:291:ASP:H	1.86	0.74
2:B:327:GLU:HG3	2:B:328:ARG:N	2.02	0.74
2:B:163:VAL:HG22	2:B:164:THR:H	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:ASN:C	3:C:107:ASN:HD22	1.96	0.74
2:B:180:ARG:HH12	2:B:285:THR:HA	1.52	0.73
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.70	0.73
1:A:191:LYS:HE2	1:A:303:VAL:HG22	1.71	0.73
6:F:4:THR:HG23	6:F:55:ARG:HE	1.54	0.72
2:B:329:VAL:HG13	2:B:330:LEU:HD22	1.72	0.72
5:E:28:PHE:HE1	5:E:142:LEU:HD22	1.55	0.71
5:E:18:ASN:ND2	5:E:118:ALA:H	1.88	0.71
5:E:60:ILE:HD11	5:E:116:ILE:HD13	1.72	0.71
7:G:68:SER:O	7:G:71:VAL:HG12	1.90	0.71
6:F:158:ARG:O	6:F:162:GLU:HG3	1.91	0.70
2:B:329:VAL:HG13	2:B:330:LEU:CD2	2.21	0.70
1:A:79:ARG:HG3	1:A:84:GLU:OE1	1.92	0.70
2:B:340:PHE:CE2	2:B:342:ILE:HD11	2.27	0.69
4:D:189:ARG:NH2	4:D:197:GLN:HG3	2.07	0.69
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.58	0.69
7:G:87:LYS:HE3	7:G:87:LYS:N	2.07	0.69
2:B:329:VAL:C	2:B:330:LEU:HD22	2.18	0.69
5:E:18:ASN:HD21	5:E:118:ALA:H	1.41	0.69
2:B:336:LYS:HE2	2:B:336:LYS:C	2.18	0.68
2:B:327:GLU:HG3	2:B:328:ARG:H	1.56	0.68
2:B:336:LYS:HE2	2:B:337:LEU:N	2.07	0.68
2:B:345:GLU:HG3	2:B:346:ASP:N	2.08	0.68
1:A:274:GLU:N	1:A:274:GLU:OE1	2.27	0.68
3:C:297:THR:HG22	3:C:298:ALA:H	1.58	0.67
1:A:194:PRO:C	1:A:195:ILE:HD12	2.20	0.67
7:G:75:ALA:O	7:G:79:VAL:HG23	1.95	0.67
5:E:86:ASN:C	5:E:154:ASP:HA	2.20	0.66
2:B:282:LEU:HD21	2:B:301:ILE:HD13	1.76	0.66
3:C:183:THR:CG2	3:C:185:TRP:H	2.02	0.66
2:B:290:ASP:HB2	2:B:293:THR:OG1	1.95	0.66
2:B:163:VAL:HG22	2:B:164:THR:N	2.10	0.65
6:F:58:LYS:HE2	6:F:58:LYS:HA	1.77	0.65
2:B:175:LEU:HD23	2:B:175:LEU:N	2.11	0.65
4:D:278:ASN:HB3	9:D:427:HOH:O	1.96	0.65
2:B:274:GLU:OE1	2:B:275:GLY:N	2.23	0.65
2:B:330:LEU:HG	2:B:336:LYS:HZ2	1.60	0.65
1:A:289:ASN:HD22	1:A:291:ASP:H	1.44	0.64
3:C:131:TRP:HE3	3:C:131:TRP:O	1.80	0.64
5:E:56:LYS:HG3	5:E:170:ASN:ND2	2.13	0.64
5:E:152:GLN:HB2	5:E:155:LYS:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.80	0.64
6:F:86:LEU:HB3	6:F:149:MET:CE	2.28	0.64
1:A:262:ILE:O	1:A:263:SER:HB3	1.96	0.64
2:B:205:ASN:ND2	2:B:208:ALA:H	1.91	0.63
5:E:119:LYS:HB2	5:E:120:PRO:HD2	1.81	0.63
3:C:72:THR:HA	3:C:98:ALA:HB1	1.81	0.63
4:D:121:PHE:O	4:D:124:VAL:HG12	1.98	0.63
1:A:223:THR:O	1:A:227:VAL:HG23	1.98	0.63
1:A:389:GLU:HA	1:A:392:GLN:OE1	1.98	0.63
7:G:23:LYS:HG2	7:G:24:PHE:N	2.09	0.63
5:E:18:ASN:HD21	5:E:118:ALA:N	1.96	0.63
7:G:38:ASP:HB3	7:G:41:GLU:HB3	1.80	0.63
3:C:189:MET:HA	3:C:195:MET:HE1	1.81	0.62
1:A:321:LEU:HD12	1:A:369:THR:HG22	1.81	0.62
1:A:257:THR:HG22	1:A:268:SER:HB3	1.81	0.62
5:E:152:GLN:HB3	5:E:155:LYS:NZ	2.13	0.62
4:D:3:LEU:HD11	6:F:167:ASN:ND2	2.14	0.62
3:C:371:ILE:HG22	3:C:372:VAL:HG23	1.82	0.62
2:B:177:HIS:O	2:B:178:LEU:CB	2.47	0.62
3:C:358:ASP:OD1	3:C:360:ARG:HG2	2.00	0.62
2:B:345:GLU:HG3	2:B:346:ASP:H	1.65	0.61
2:B:175:LEU:CD1	2:B:178:LEU:HD12	2.26	0.61
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.65	0.61
2:B:198:LEU:HD23	2:B:202:TYR:O	1.99	0.61
1:A:176:HIS:HD2	1:A:192:HIS:CD2	2.18	0.61
2:B:326:LEU:HD23	2:B:326:LEU:C	2.25	0.61
5:E:97:THR:O	5:E:101:THR:HG23	2.00	0.61
4:D:53:THR:C	4:D:54:LYS:HD2	2.26	0.61
1:A:352:GLU:C	1:A:354:SER:H	2.07	0.60
1:A:116:PRO:O	1:A:117:LEU:HB2	2.01	0.60
3:C:185:TRP:CE3	3:C:235:MET:HE2	2.33	0.60
4:D:281:ARG:HH12	6:F:102:PHE:HZ	1.48	0.60
4:D:248:ARG:HD3	4:D:248:ARG:C	2.26	0.60
6:F:86:LEU:HB3	6:F:149:MET:HE2	1.84	0.60
5:E:75:ILE:HG23	5:E:144:LEU:HD11	1.83	0.60
6:F:130:LYS:HA	6:F:130:LYS:HE2	1.82	0.60
4:D:266:MET:HE3	6:F:93:PHE:CD1	2.36	0.60
2:B:235:LEU:HD23	6:F:107:LYS:HZ2	1.66	0.59
1:A:19:LEU:HG	1:A:29:PHE:HB2	1.83	0.59
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.32	0.59
6:F:4:THR:HG23	6:F:55:ARG:HH21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:LEU:HD23	6:F:107:LYS:NZ	2.16	0.59
3:C:365:ALA:C	3:C:366:LEU:HD12	2.28	0.59
5:E:87:SER:HA	5:E:153:ASN:OD1	2.02	0.58
3:C:370:LYS:O	3:C:371:ILE:HB	2.02	0.58
5:E:150:ASP:O	5:E:152:GLN:N	2.37	0.58
2:B:343:ARG:HG3	2:B:343:ARG:HH11	1.68	0.58
3:C:359:VAL:O	3:C:363:GLU:HG3	2.04	0.58
2:B:329:VAL:HG22	2:B:329:VAL:O	2.03	0.58
5:E:130:ARG:HG3	5:E:130:ARG:HH11	1.69	0.57
2:B:205:ASN:HD22	2:B:208:ALA:N	1.97	0.57
2:B:327:GLU:HA	2:B:332:GLY:H	1.69	0.57
6:F:79:ALA:HB3	6:F:83:GLU:OE2	2.03	0.57
2:B:166:ILE:O	2:B:168:PRO:HD3	2.03	0.57
3:C:200:SER:HB3	9:C:408:HOH:O	2.05	0.57
2:B:329:VAL:O	2:B:330:LEU:HD22	2.04	0.57
1:A:129:ILE:O	1:A:133:SER:HB2	2.05	0.57
3:C:126:GLU:HB2	3:C:131:TRP:CZ3	2.40	0.57
4:D:182:MET:HE2	4:D:223:ILE:HG13	1.87	0.57
4:D:233:ASN:OD1	4:D:235:SER:N	2.34	0.57
7:G:60:LYS:HG2	7:G:61:ASN:ND2	2.20	0.56
3:C:107:ASN:HD22	3:C:108:GLU:N	2.03	0.56
3:C:3:TYR:HB2	3:C:324:LEU:HG	1.85	0.56
3:C:221:SER:HB2	3:C:223:ASP:OD1	2.05	0.56
5:E:134:GLN:O	5:E:138:GLN:HG3	2.05	0.56
3:C:107:ASN:ND2	3:C:107:ASN:C	2.63	0.56
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.87	0.56
6:F:4:THR:CG2	6:F:55:ARG:HH21	2.19	0.56
1:A:289:ASN:HD22	1:A:289:ASN:C	2.14	0.55
2:B:163:VAL:HG21	2:B:181:ARG:NH2	2.21	0.55
2:B:163:VAL:HG21	2:B:181:ARG:HH22	1.71	0.55
2:B:306:GLY:HA2	2:B:309:MET:HE2	1.88	0.55
4:D:59:ILE:HB	4:D:116:LEU:HD13	1.87	0.55
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.88	0.55
3:C:26:CYS:SG	3:C:55:VAL:HB	2.47	0.55
3:C:156:LEU:HD11	3:C:183:THR:HG21	1.89	0.55
4:D:183:GLN:HB3	9:D:442:HOH:O	2.07	0.55
2:B:287:GLN:O	2:B:294:ARG:NH2	2.38	0.55
2:B:325:TYR:CD1	2:B:329:VAL:HG11	2.42	0.55
4:D:133:GLU:O	4:D:133:GLU:HG2	2.06	0.55
2:B:257:GLU:HA	2:B:260:GLU:HB2	1.89	0.54
3:C:363:GLU:OE2	3:C:371:ILE:HD12	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:182:MET:HG3	4:D:200:PHE:CD1	2.41	0.54
4:D:197:GLN:NE2	4:D:199:LEU:HD11	2.13	0.54
3:C:228:LEU:C	3:C:228:LEU:HD23	2.33	0.54
5:E:133:LEU:O	5:E:137:ARG:HG3	2.06	0.54
6:F:99:GLU:HG3	9:F:220:HOH:O	2.07	0.54
3:C:263:HIS:CD2	6:F:21:CYS:HB3	2.42	0.54
3:C:178:GLU:O	3:C:179:ARG:C	2.51	0.54
2:B:330:LEU:HG	2:B:336:LYS:CE	2.38	0.54
5:E:95:MET:HA	5:E:95:MET:CE	2.35	0.54
1:A:85:ASP:OD2	1:A:88:LEU:HD22	2.08	0.54
1:A:258:GLY:C	1:A:259:ILE:HD12	2.32	0.54
2:B:318:GLU:HG3	2:B:344:ILE:HD12	1.90	0.54
3:C:84:ARG:HG2	3:C:84:ARG:HH11	1.73	0.54
1:A:243:ASN:HD22	5:E:47:TYR:HE1	1.55	0.54
3:C:170:SER:HB2	3:C:195:MET:HE3	1.89	0.54
1:A:343:VAL:HG22	1:A:363:ILE:HD11	1.90	0.53
5:E:88:LYS:O	5:E:92:GLU:HG3	2.08	0.53
1:A:155:SER:HB2	1:A:370:HIS:HB3	1.90	0.53
1:A:191:LYS:CE	1:A:303:VAL:HG22	2.36	0.53
3:C:32:VAL:HG22	3:C:58:ILE:HD11	1.90	0.53
5:E:152:GLN:CB	5:E:155:LYS:HD2	2.39	0.53
2:B:225:TYR:CZ	2:B:319:ARG:HD2	2.44	0.53
4:D:158:LYS:HD3	4:D:158:LYS:C	2.33	0.53
6:F:86:LEU:HD22	6:F:149:MET:HE3	1.90	0.53
7:G:117:PRO:O	7:G:118:SER:HB3	2.09	0.53
1:A:343:VAL:HG13	1:A:363:ILE:HD11	1.91	0.53
7:G:20:ASP:C	7:G:22:ASN:H	2.17	0.53
7:G:87:LYS:N	7:G:87:LYS:CD	2.72	0.53
1:A:151:ALA:O	1:A:154:THR:HG22	2.09	0.53
3:C:90:LEU:HD23	3:C:91:VAL:H	1.73	0.53
7:G:71:VAL:HG13	7:G:72:LYS:N	2.24	0.53
5:E:56:LYS:HG3	5:E:170:ASN:HD21	1.74	0.53
3:C:102:VAL:HA	3:C:112:ALA:O	2.09	0.52
2:B:336:LYS:HE2	2:B:337:LEU:HA	1.91	0.52
5:E:105:ILE:HG12	5:E:108:GLU:OE1	2.10	0.52
6:F:80:ASP:OD1	6:F:82:ILE:HG22	2.10	0.52
1:A:243:ASN:ND2	5:E:47:TYR:CE1	2.71	0.52
1:A:263:SER:O	1:A:265:LYS:N	2.42	0.52
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.39	0.52
4:D:160:ARG:NH1	4:D:160:ARG:HB3	2.25	0.52
1:A:388:PRO:O	1:A:392:GLN:OE1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:GLU:CG	2:B:346:ASP:N	2.73	0.52
2:B:345:GLU:CG	2:B:346:ASP:H	2.23	0.52
1:A:237:ASP:OD2	1:A:240:LYS:HG3	2.09	0.51
3:C:144:THR:H	6:F:28:GLN:NE2	2.09	0.51
4:D:158:LYS:HG3	4:D:159:ASP:CG	2.34	0.51
7:G:60:LYS:HE2	7:G:61:ASN:HD21	1.76	0.51
6:F:4:THR:HG23	6:F:55:ARG:NE	2.22	0.51
7:G:87:LYS:N	7:G:87:LYS:CE	2.73	0.51
5:E:144:LEU:O	5:E:148:VAL:HG23	2.10	0.51
3:C:185:TRP:CZ2	3:C:231:ALA:HB2	2.45	0.51
1:A:153:TRP:HA	1:A:158:VAL:HG21	1.92	0.51
5:E:167:GLN:NE2	5:E:172:SER:HB2	2.26	0.51
3:C:107:ASN:HD22	3:C:109:LYS:H	1.54	0.51
4:D:233:ASN:OD1	4:D:235:SER:HB3	2.11	0.51
5:E:85:CYS:SG	5:E:149:PHE:HZ	2.34	0.51
1:A:116:PRO:HG2	1:A:178:ILE:HD13	1.93	0.50
2:B:336:LYS:HE2	2:B:337:LEU:CA	2.41	0.50
1:A:257:THR:HG22	1:A:268:SER:CB	2.42	0.50
3:C:254:THR:HA	3:C:340:ALA:O	2.11	0.50
5:E:78:CYS:O	5:E:82:LEU:HB2	2.11	0.50
1:A:38:LYS:HE2	1:A:72:TYR:CZ	2.46	0.50
1:A:392:GLN:OE1	1:A:392:GLN:N	2.45	0.50
1:A:393:VAL:HG21	1:A:414:PHE:CD2	2.47	0.50
2:B:334:VAL:HG21	7:G:19:TYR:CE1	2.46	0.50
1:A:143:VAL:HG12	9:A:516:HOH:O	2.12	0.50
4:D:199:LEU:HB2	4:D:224:THR:HB	1.93	0.50
5:E:60:ILE:HD11	5:E:116:ILE:HG21	1.93	0.50
3:C:185:TRP:CE2	3:C:231:ALA:HB2	2.47	0.49
2:B:170:TYR:O	2:B:171:GLU:C	2.54	0.49
4:D:84:LEU:C	4:D:84:LEU:HD23	2.37	0.49
5:E:145:CYS:C	5:E:147:LYS:H	2.19	0.49
2:B:160:GLY:O	2:B:185:ALA:HB1	2.12	0.49
2:B:330:LEU:HG	2:B:336:LYS:HD3	1.94	0.49
4:D:129:PHE:HD2	4:D:237:ARG:HG3	1.77	0.49
3:C:119:VAL:HG22	3:C:120:ILE:N	2.27	0.49
3:C:253:ILE:HB	3:C:342:CYS:HB3	1.93	0.49
4:D:188:GLY:HA3	6:F:165:LEU:CD2	2.42	0.49
7:G:39:GLU:HG2	7:G:78:ILE:HD11	1.94	0.49
2:B:334:VAL:HG22	2:B:334:VAL:O	2.12	0.49
3:C:92:ILE:HG22	3:C:94:ARG:HG3	1.94	0.49
3:C:142:ARG:NH2	7:G:25:VAL:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:74:GLU:OE1	4:D:74:GLU:N	2.43	0.49
4:D:134:GLU:OE2	4:D:136:LYS:HE2	2.12	0.49
5:E:95:MET:HG2	5:E:141:GLY:O	2.13	0.49
1:A:343:VAL:HG22	1:A:363:ILE:CD1	2.41	0.49
2:B:191:ARG:HG3	2:B:206:HIS:CE1	2.47	0.49
5:E:91:GLY:O	5:E:95:MET:HB2	2.12	0.49
4:D:212:THR:C	4:D:214:ALA:H	2.21	0.49
5:E:139:GLU:O	5:E:142:LEU:HD23	2.11	0.49
7:G:23:LYS:CG	7:G:24:PHE:H	2.09	0.49
1:A:120:PRO:HB3	1:A:409:ARG:HG2	1.95	0.49
1:A:183:GLY:HA3	1:A:413:VAL:HG21	1.95	0.49
1:A:340:LYS:HG2	1:A:365:VAL:HB	1.95	0.49
1:A:174:VAL:HG12	1:A:175:THR:N	2.28	0.48
2:B:163:VAL:CG2	2:B:164:THR:H	2.24	0.48
5:E:82:LEU:CD2	5:E:148:VAL:HG21	2.37	0.48
1:A:91:ARG:O	1:A:94:GLU:HB2	2.13	0.48
2:B:330:LEU:HG	2:B:336:LYS:HZ1	1.76	0.48
3:C:370:LYS:O	3:C:371:ILE:CB	2.61	0.48
4:D:75:LEU:HD23	4:D:75:LEU:C	2.38	0.48
5:E:32:ALA:CB	5:E:135:GLN:OE1	2.61	0.48
3:C:140:PRO:O	3:C:142:ARG:HG3	2.13	0.48
4:D:202:HIS:HD2	9:D:435:HOH:O	1.97	0.48
4:D:263:HIS:O	4:D:267:ARG:HG3	2.14	0.48
3:C:84:ARG:HG2	3:C:84:ARG:NH1	2.29	0.48
3:C:282:GLY:HA2	3:C:370:LYS:HE3	1.96	0.48
4:D:205:PRO:HB3	4:D:222:TYR:CZ	2.49	0.48
5:E:60:ILE:CD1	5:E:116:ILE:HD13	2.42	0.48
2:B:155:VAL:HG21	2:B:286:ILE:HD11	1.95	0.48
2:B:337:LEU:HD21	7:G:16:VAL:HG13	1.96	0.48
4:D:37:ASP:HB2	4:D:43:TYR:HE1	1.78	0.48
2:B:181:ARG:HB2	2:B:181:ARG:NH1	2.29	0.48
3:C:143:SER:OG	3:C:162:CYS:HB2	2.13	0.48
3:C:269:LEU:HD22	3:C:369:LEU:HD11	1.96	0.48
2:B:205:ASN:HB3	2:B:208:ALA:HB3	1.96	0.47
7:G:83:LEU:HD22	7:G:128:TRP:CD2	2.49	0.47
2:B:239:VAL:HG23	2:B:240:LEU:HD13	1.96	0.47
1:A:216:PRO:HB2	1:A:219:GLN:HB2	1.97	0.47
1:A:348:LYS:HE2	1:A:352:GLU:OE2	2.15	0.47
3:C:76:ALA:HB2	3:C:93:LEU:HD11	1.95	0.47
6:F:4:THR:CG2	6:F:55:ARG:HE	2.23	0.47
2:B:302:VAL:HG13	2:B:302:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:18:ASN:CG	5:E:118:ALA:H	2.22	0.47
1:A:289:ASN:HD22	1:A:290:PRO:N	2.12	0.47
2:B:175:LEU:O	2:B:177:HIS:N	2.48	0.47
2:B:194:ILE:HG13	2:B:213:VAL:HG11	1.96	0.47
5:E:153:ASN:OD1	5:E:154:ASP:N	2.46	0.47
2:B:180:ARG:HH12	2:B:285:THR:CA	2.25	0.47
3:C:10:PRO:HB3	3:C:350:MET:HA	1.96	0.47
5:E:74:TYR:CE1	5:E:137:ARG:HD2	2.50	0.47
6:F:43:SER:HB2	6:F:46:LEU:HD12	1.96	0.47
2:B:334:VAL:HG21	7:G:19:TYR:CZ	2.50	0.47
5:E:16:ILE:HG23	5:E:16:ILE:O	2.15	0.47
2:B:340:PHE:CD2	2:B:342:ILE:HD11	2.50	0.46
1:A:307:CYS:HB3	1:A:308:PRO:HD2	1.97	0.46
2:B:175:LEU:O	2:B:177:HIS:O	2.32	0.46
4:D:197:GLN:HB3	4:D:226:VAL:HB	1.98	0.46
6:F:4:THR:HG23	6:F:55:ARG:NH2	2.30	0.46
3:C:101:CYS:O	3:C:113:VAL:HA	2.15	0.46
5:E:22:LEU:HD23	5:E:41:ILE:HB	1.96	0.46
5:E:71:ILE:O	5:E:75:ILE:HG13	2.16	0.46
6:F:128:LYS:O	6:F:132:VAL:HG23	2.15	0.46
6:F:130:LYS:HA	6:F:130:LYS:CE	2.45	0.46
3:C:247:LEU:HA	3:C:262:GLY:HA3	1.97	0.46
5:E:9:MET:SD	5:E:63:GLU:HG2	2.55	0.46
5:E:86:ASN:O	5:E:87:SER:HB3	2.14	0.46
6:F:82:ILE:O	6:F:86:LEU:HG	2.15	0.46
1:A:143:VAL:HG13	1:A:146:VAL:HG23	1.96	0.46
4:D:228:PHE:H	4:D:231:HIS:CD2	2.21	0.46
1:A:239:VAL:HG23	1:A:240:LYS:N	2.30	0.46
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.50	0.46
4:D:182:MET:HE2	4:D:223:ILE:CG1	2.45	0.46
6:F:22:LEU:HD21	6:F:70:VAL:HG23	1.96	0.46
7:G:78:ILE:O	7:G:82:VAL:HG23	2.15	0.46
3:C:7:LEU:HD12	3:C:9:GLU:HB2	1.97	0.46
3:C:72:THR:HA	3:C:98:ALA:CB	2.45	0.46
5:E:23:PRO:HG3	5:E:33:PRO:HB2	1.98	0.46
1:A:90:GLU:HB3	9:A:509:HOH:O	2.16	0.45
4:D:160:ARG:HB3	4:D:160:ARG:HH11	1.81	0.45
2:B:278:VAL:HG13	2:B:279:ALA:N	2.31	0.45
3:C:69:THR:O	3:C:76:ALA:HA	2.17	0.45
4:D:274:LEU:O	4:D:278:ASN:ND2	2.46	0.45
1:A:52:MET:HE2	1:A:56:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:GLU:C	1:A:354:SER:N	2.74	0.45
2:B:163:VAL:CG2	2:B:164:THR:N	2.79	0.45
5:E:87:SER:N	5:E:154:ASP:HA	2.31	0.45
6:F:105:ARG:HG2	6:F:105:ARG:HH11	1.82	0.45
3:C:74:ARG:HD2	6:F:31:GLU:CG	2.47	0.45
2:B:325:TYR:O	2:B:326:LEU:C	2.60	0.45
1:A:349:LEU:O	1:A:353:LEU:HD23	2.17	0.45
1:A:359:LYS:N	1:A:360:PRO:HD3	2.32	0.45
6:F:86:LEU:HD13	6:F:149:MET:HB3	1.97	0.45
2:B:330:LEU:HG	2:B:336:LYS:CD	2.47	0.45
6:F:38:VAL:HG12	6:F:69:SER:OG	2.17	0.45
1:A:274:GLU:HA	1:A:277:LEU:HB2	1.98	0.44
2:B:239:VAL:HG23	2:B:240:LEU:CD1	2.47	0.44
2:B:246:LEU:HB3	2:B:247:PRO:HD2	1.99	0.44
2:B:299:LYS:NZ	2:B:300:HIS:HE1	2.15	0.44
1:A:158:VAL:HG23	1:A:158:VAL:O	2.18	0.44
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.53	0.44
5:E:18:ASN:ND2	5:E:118:ALA:N	2.57	0.44
7:G:87:LYS:N	7:G:87:LYS:HD3	2.33	0.44
1:A:111:LEU:HD23	1:A:111:LEU:C	2.42	0.44
1:A:284:HIS:N	1:A:285:PRO:HD3	2.33	0.44
2:B:166:ILE:HD13	2:B:282:LEU:HA	1.97	0.44
4:D:118:ARG:HD3	4:D:118:ARG:C	2.42	0.44
4:D:258:SER:O	4:D:262:ILE:HG12	2.17	0.44
4:D:263:HIS:CD2	4:D:266:MET:HE2	2.44	0.44
2:B:325:TYR:HA	2:B:329:VAL:HG12	1.99	0.44
5:E:82:LEU:HD13	5:E:95:MET:SD	2.57	0.44
1:A:205:GLN:NE2	1:A:220:SER:OG	2.48	0.44
1:A:311:VAL:C	1:A:314:PRO:HD2	2.42	0.44
2:B:257:GLU:H	2:B:257:GLU:CD	2.25	0.44
2:B:334:VAL:HG21	7:G:19:TYR:CD1	2.52	0.44
3:C:82:LYS:HD2	3:C:87:LYS:HG3	2.00	0.44
2:B:325:TYR:O	2:B:329:VAL:HG12	2.18	0.44
3:C:258:LEU:HB2	3:C:270:PHE:HB2	2.00	0.44
4:D:45:ILE:HA	4:D:56:MET:O	2.18	0.44
5:E:22:LEU:HA	5:E:23:PRO:HD3	1.82	0.44
3:C:14:HIS:H	3:C:331:GLN:HE22	1.66	0.44
5:E:75:ILE:O	5:E:79:LEU:HG	2.17	0.44
5:E:112:PRO:O	5:E:113:LEU:HB2	2.17	0.44
7:G:80:LEU:O	7:G:84:ILE:HD13	2.18	0.44
3:C:146:LEU:HD11	3:C:162:CYS:SG	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:263:HIS:HD2	4:D:266:MET:CE	2.27	0.43
7:G:133:LEU:HD13	7:G:141:ILE:HD11	1.99	0.43
4:D:182:MET:HG3	4:D:200:PHE:CE1	2.52	0.43
1:A:389:GLU:CA	1:A:392:GLN:OE1	2.65	0.43
5:E:74:TYR:CE1	5:E:98:LEU:HD12	2.54	0.43
7:G:124:VAL:O	7:G:127:GLN:HB2	2.18	0.43
3:C:131:TRP:HE3	3:C:131:TRP:C	2.26	0.43
4:D:67:LEU:HD13	4:D:120:CYS:O	2.18	0.43
3:C:129:ASN:HB2	3:C:131:TRP:CZ3	2.54	0.43
2:B:232:LYS:HB3	2:B:232:LYS:HE2	1.81	0.43
2:B:322:LYS:HD3	7:G:16:VAL:HG11	2.01	0.43
2:B:323:GLN:HB3	7:G:11:PHE:O	2.18	0.43
2:B:164:THR:HB	2:B:182:LEU:HB3	2.00	0.43
2:B:198:LEU:C	2:B:200:ARG:H	2.26	0.43
2:B:247:PRO:HG2	8:B:401:CKH:H6	2.01	0.43
3:C:225:THR:HG22	3:C:241:ALA:HA	2.01	0.43
4:D:75:LEU:HD13	4:D:123:SER:N	2.33	0.43
6:F:60:LYS:HE3	6:F:112:TYR:CE2	2.54	0.43
7:G:104:ASP:OD2	7:G:143:ARG:NE	2.39	0.43
2:B:295:SER:O	2:B:299:LYS:HG2	2.19	0.42
3:C:30:HIS:HB2	9:C:402:HOH:O	2.19	0.42
4:D:248:ARG:C	4:D:248:ARG:CD	2.92	0.42
7:G:87:LYS:O	7:G:88:ALA:C	2.62	0.42
1:A:313:ARG:CZ	1:A:363:ILE:HG22	2.50	0.42
4:D:158:LYS:HD3	4:D:158:LYS:O	2.18	0.42
2:B:158:ASP:CG	2:B:304:SER:HB3	2.40	0.42
3:C:12:SER:HB2	3:C:26:CYS:HB3	2.01	0.42
3:C:107:ASN:ND2	3:C:109:LYS:HB2	2.34	0.42
1:A:300:VAL:O	1:A:304:ILE:HG13	2.19	0.42
5:E:102:ASN:HD21	5:E:130:ARG:NE	2.17	0.42
6:F:102:PHE:HE1	6:F:126:MET:HE1	1.85	0.42
7:G:10:ARG:O	7:G:11:PHE:CB	2.60	0.42
1:A:30:ILE:HD13	1:A:375:TYR:CZ	2.55	0.42
1:A:143:VAL:CG1	1:A:146:VAL:HG23	2.49	0.42
2:B:183:ASP:C	2:B:184:ILE:HG13	2.45	0.42
7:G:149:LYS:HE3	7:G:149:LYS:HB2	1.89	0.42
3:C:74:ARG:HH11	6:F:31:GLU:CD	2.28	0.42
1:A:39:GLU:O	1:A:39:GLU:CG	2.62	0.42
1:A:259:ILE:HD12	1:A:259:ILE:N	2.34	0.42
1:A:369:THR:HA	1:A:373:GLN:OE1	2.20	0.42
1:A:38:LYS:NZ	1:A:71:THR:CG2	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ILE:HG23	1:A:265:LYS:O	2.20	0.41
5:E:120:PRO:HG3	5:E:126:ASP:OD1	2.19	0.41
5:E:121:ALA:HB3	5:E:125:GLU:OE2	2.20	0.41
3:C:347:THR:OG1	3:C:355:SER:HB2	2.20	0.41
5:E:150:ASP:C	5:E:152:GLN:N	2.78	0.41
3:C:321:LEU:HD11	6:F:129:HIS:CE1	2.56	0.41
3:C:47:GLU:OE1	3:C:49:LYS:NZ	2.50	0.41
2:B:303:LEU:HD21	2:B:344:ILE:HG21	2.02	0.41
3:C:151:HIS:CE1	3:C:152:PRO:HG2	2.56	0.41
4:D:137:GLU:OE2	4:D:158:LYS:HE2	2.21	0.41
6:F:138:PHE:O	6:F:142:ILE:HG23	2.20	0.41
1:A:19:LEU:HD23	1:A:19:LEU:N	2.35	0.41
1:A:228:LYS:O	1:A:232:SER:HB2	2.19	0.41
3:C:119:VAL:HG22	3:C:120:ILE:H	1.86	0.41
1:A:91:ARG:HD2	9:A:501:HOH:O	2.21	0.41
2:B:194:ILE:CG1	2:B:213:VAL:HG21	2.44	0.41
4:D:45:ILE:HG12	4:D:57:VAL:HG22	2.03	0.41
4:D:282:PRO:HD3	6:F:125:GLN:O	2.21	0.41
1:A:263:SER:C	1:A:265:LYS:N	2.79	0.41
1:A:339:LEU:HD23	1:A:365:VAL:HG13	2.03	0.41
1:A:343:VAL:O	1:A:347:LEU:HD13	2.20	0.41
2:B:325:TYR:O	2:B:327:GLU:N	2.54	0.41
5:E:44:GLU:HG2	5:E:48:TYR:CE2	2.55	0.41
6:F:31:GLU:OE2	6:F:32:ARG:CG	2.63	0.41
1:A:348:LYS:HG2	1:A:352:GLU:OE2	2.21	0.41
7:G:118:SER:O	7:G:119:ASP:C	2.64	0.41
3:C:370:LYS:HE2	3:C:370:LYS:HB2	1.97	0.40
7:G:99:ASP:O	7:G:100:LYS:C	2.64	0.40
1:A:240:LYS:O	1:A:244:LYS:HG3	2.21	0.40
1:A:307:CYS:HB3	1:A:308:PRO:CD	2.52	0.40
2:B:212:THR:O	2:B:216:ILE:HG13	2.21	0.40
3:C:207:GLY:O	3:C:219:TRP:HA	2.21	0.40
3:C:219:TRP:CE2	3:C:227:CYS:HB2	2.57	0.40
3:C:266:PHE:CD1	3:C:284:ARG:HG3	2.57	0.40
5:E:132:TYR:CE2	5:E:136:LEU:HD11	2.57	0.40
2:B:175:LEU:O	2:B:176:PRO:C	2.63	0.40
7:G:71:VAL:CG1	7:G:72:LYS:N	2.84	0.40
1:A:53:LYS:O	1:A:56:ASP:OD2	2.39	0.40
6:F:85:ILE:HD12	6:F:85:ILE:C	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/418 (94%)	373 (94%)	19 (5%)	3 (1%)	16	28
2	B	191/394 (48%)	168 (88%)	16 (8%)	7 (4%)	2	3
3	C	343/372 (92%)	321 (94%)	20 (6%)	2 (1%)	21	35
4	D	280/300 (93%)	268 (96%)	10 (4%)	2 (1%)	18	32
5	E	171/178 (96%)	156 (91%)	12 (7%)	3 (2%)	6	11
6	F	165/168 (98%)	160 (97%)	4 (2%)	1 (1%)	21	35
7	G	132/151 (87%)	123 (93%)	6 (4%)	3 (2%)	5	7
All	All	1677/1981 (85%)	1569 (94%)	87 (5%)	21 (1%)	9	16

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	SER
1	A	264	LYS
2	B	329	VAL
7	G	11	PHE
2	B	171	GLU
2	B	290	ASP
2	B	326	LEU
3	C	371	ILE
4	D	237	ARG
6	F	102	PHE
2	B	178	LEU
3	C	50	GLU
5	E	151	PRO
5	E	153	ASN
1	A	353	LEU
2	B	328	ARG
5	E	87	SER
2	B	176	PRO

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Mol	Chain	Res	Type
4	D	213	ASP
7	G	21	GLU
7	G	118	SER

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	344/363 (95%)	334 (97%)	10 (3%)	37	62
2	B	165/345 (48%)	153 (93%)	12 (7%)	13	25
3	C	296/313 (95%)	285 (96%)	11 (4%)	30	54
4	D	248/264 (94%)	244 (98%)	4 (2%)	55	77
5	E	153/159 (96%)	143 (94%)	10 (6%)	15	30
6	F	152/155 (98%)	150 (99%)	2 (1%)	61	80
7	G	109/123 (89%)	103 (94%)	6 (6%)	19	37
All	All	1467/1722 (85%)	1412 (96%)	55 (4%)	30	54

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	19	LEU
1	A	82	ILE
1	A	88	LEU
1	A	230	ARG
1	A	309	ILE
1	A	335	LEU
1	A	343	VAL
1	A	363	ILE
1	A	394	CYS
2	B	158	ASP
2	B	161	ASP
2	B	175	LEU
2	B	176	PRO

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Mol	Chain	Res	Type
2	B	182	LEU
2	B	200	ARG
2	B	220	LEU
2	B	235	LEU
2	B	240	LEU
2	B	257	GLU
2	B	336	LYS
2	B	341	LYS
3	C	8	VAL
3	C	21	THR
3	C	54	GLN
3	C	90	LEU
3	C	107	ASN
3	C	128	GLU
3	C	131	TRP
3	C	140	PRO
3	C	179	ARG
3	C	183	THR
3	C	297	THR
4	D	29	GLU
4	D	116	LEU
4	D	229	PRO
4	D	277	LEU
5	E	22	LEU
5	E	25	ARG
5	E	63	GLU
5	E	82	LEU
5	E	98	LEU
5	E	130	ARG
5	E	133	LEU
5	E	142	LEU
5	E	144	LEU
5	E	151	PRO
6	F	101	PHE
6	F	165	LEU
7	G	21	GLU
7	G	27	GLU
7	G	39	GLU
7	G	69	GLN
7	G	87	LYS
7	G	93	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	157	GLN
1	A	176	HIS
1	A	192	HIS
1	A	205	GLN
1	A	255	GLN
1	A	289	ASN
1	A	318	ASN
1	A	371	HIS
1	A	395	HIS
1	A	410	HIS
2	B	205	ASN
2	B	206	HIS
2	B	231	GLN
2	B	267	GLN
2	B	284	ASN
2	B	287	GLN
2	B	323	GLN
3	C	46	HIS
3	C	54	GLN
3	C	107	ASN
3	C	303	GLN
3	C	304	ASN
3	C	331	GLN
4	D	140	ASN
4	D	197	GLN
4	D	231	HIS
4	D	263	HIS
5	E	18	ASN
5	E	102	ASN
5	E	167	GLN
6	F	28	GLN
6	F	49	GLN
6	F	125	GLN
6	F	167	ASN
7	G	61	ASN
7	G	96	GLN

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](#)

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	$\# Z > 2$
8	CKH	B	401	-	24,24,24	1.33	4 (16%)	33,33,33	1.90	6 (18%)

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
8	CKH	B	401	-	-	0/10/10/10	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	401	CKH	CAP-NAO	-3.19	1.33	1.37
8	B	401	CKH	CAN-NAO	-2.76	1.33	1.38
8	B	401	CKH	CAC-CAD	-2.58	1.39	1.44
8	B	401	CKH	CAQ-CAP	2.15	1.53	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	401	CKH	CAQ-CAP-CAD	-6.94	125.01	130.58
8	B	401	CKH	CAQ-CAP-NAO	4.29	124.73	120.00
8	B	401	CKH	CAC-CAD-CAP	-4.15	105.27	106.98
8	B	401	CKH	CAM-CAN-CAC	-2.77	119.51	122.19
8	B	401	CKH	CAT-CAS-CAI	-2.68	120.19	123.07
8	B	401	CKH	CAJ-CAI-CAS	2.23	119.17	116.70

There are no chirality outliers.

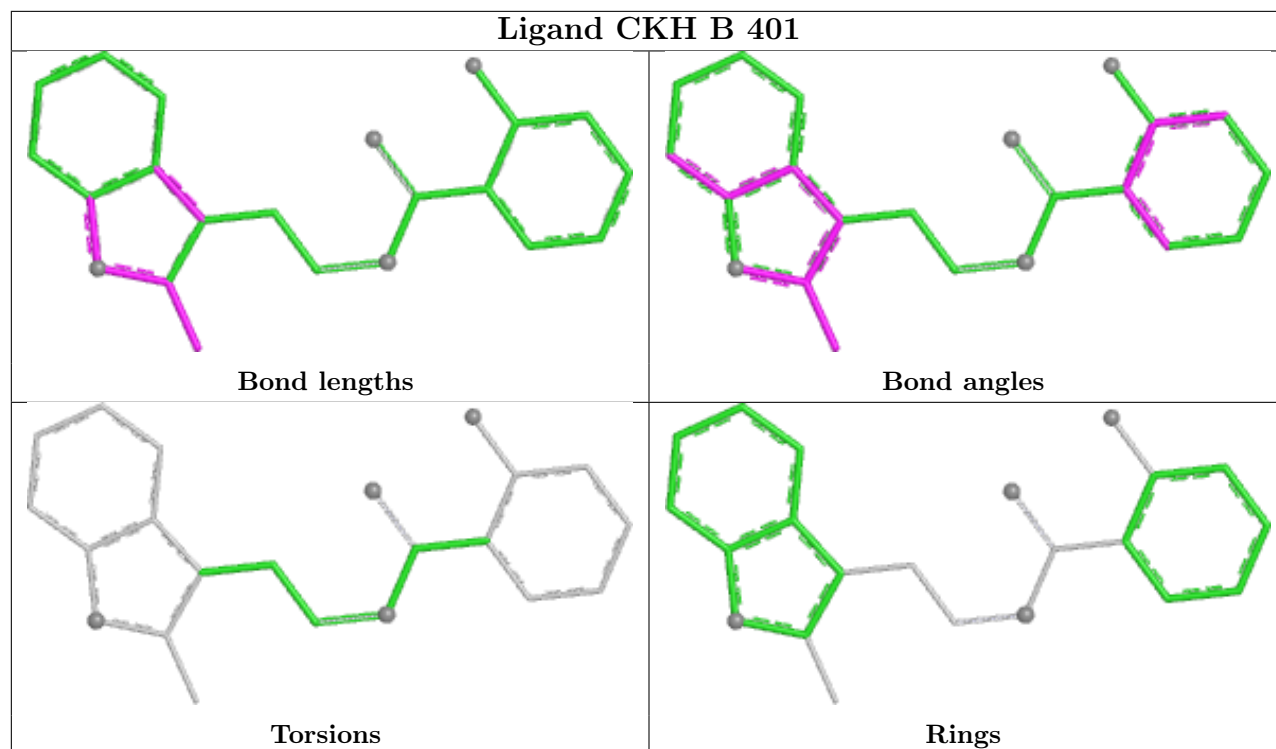
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	401	CKH	1	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	401/418 (95%)	0.16	20 (4%) 34 30	17, 40, 77, 89	0
2	B	193/394 (48%)	0.79	26 (13%) 7 5	22, 54, 98, 105	0
3	C	349/372 (93%)	-0.01	14 (4%) 42 38	21, 36, 74, 94	0
4	D	282/300 (94%)	0.05	6 (2%) 63 60	18, 38, 57, 75	0
5	E	173/178 (97%)	0.71	15 (8%) 16 14	36, 55, 88, 96	0
6	F	167/168 (99%)	-0.28	3 (1%) 67 65	17, 30, 45, 73	0
7	G	136/151 (90%)	0.70	15 (11%) 10 8	26, 55, 82, 87	0
All	All	1701/1981 (85%)	0.23	99 (5%) 29 25	17, 41, 82, 105	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	178	LEU	6.8
2	B	346	ASP	6.6
7	G	9	ALA	6.0
2	B	173	PHE	5.5
1	A	40	SER	4.9
5	E	85	CYS	4.9
7	G	35	ALA	4.8
5	E	151	PRO	4.5
4	D	211	ASP	4.1
7	G	120	ASN	4.0
1	A	354	SER	3.9
3	C	297	THR	3.8
2	B	332	GLY	3.7
1	A	359	LYS	3.6
1	A	158	VAL	3.6
1	A	417	MET	3.5
3	C	127	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
6	F	31	GLU	3.4
3	C	304	ASN	3.4
1	A	262	ILE	3.3
2	B	341	LYS	3.3
2	B	187	ARG	3.3
2	B	170	TYR	3.3
1	A	265	LYS	3.2
3	C	302	PHE	3.2
2	B	337	LEU	3.2
1	A	353	LEU	3.1
2	B	329	VAL	3.1
2	B	336	LYS	3.1
5	E	146	GLU	3.0
6	F	2	THR	3.0
2	B	289	ALA	3.0
1	A	264	LYS	3.0
3	C	201	SER	3.0
7	G	64	ILE	2.9
3	C	301	ARG	2.9
7	G	50	ASN	2.9
7	G	37	PRO	2.9
1	A	52	MET	2.9
5	E	93	LYS	2.8
3	C	298	ALA	2.7
6	F	92	ARG	2.7
1	A	349	LEU	2.7
2	B	169	VAL	2.6
2	B	291	ILE	2.6
1	A	51	VAL	2.6
3	C	372	VAL	2.6
2	B	342	ILE	2.5
3	C	320	GLY	2.5
5	E	152	GLN	2.5
7	G	93	LYS	2.5
5	E	96	TYR	2.5
3	C	371	ILE	2.5
2	B	177	HIS	2.5
2	B	206	HIS	2.5
7	G	122	SER	2.5
5	E	154	ASP	2.4
4	D	130	GLN	2.4
1	A	71	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	175	GLU	2.4
2	B	292	ASP	2.4
4	D	107	ASP	2.4
7	G	74	ARG	2.4
2	B	334	VAL	2.4
7	G	151	VAL	2.3
1	A	218	GLU	2.3
2	B	297	PHE	2.3
1	A	350	SER	2.3
7	G	23	LYS	2.3
1	A	157	GLN	2.2
5	E	107	GLY	2.2
5	E	174	SER	2.2
2	B	293	THR	2.2
2	B	172	GLY	2.2
2	B	296	GLU	2.2
7	G	13	LYS	2.2
4	D	212	THR	2.2
1	A	250	SER	2.2
3	C	368	ASP	2.2
5	E	38	ASP	2.2
7	G	66	THR	2.1
5	E	89	SER	2.1
5	E	121	ALA	2.1
1	A	267	PHE	2.1
1	A	213	VAL	2.1
3	C	366	LEU	2.1
2	B	294	ARG	2.1
4	D	189	ARG	2.1
7	G	21	GLU	2.1
3	C	178	GLU	2.1
5	E	110	GLY	2.0
2	B	174	SER	2.0
2	B	156	VAL	2.0
5	E	148	VAL	2.0
4	D	236	ALA	2.0
1	A	214	GLY	2.0
7	G	36	GLY	2.0
2	B	344	ILE	2.0
5	E	39	THR	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](#)

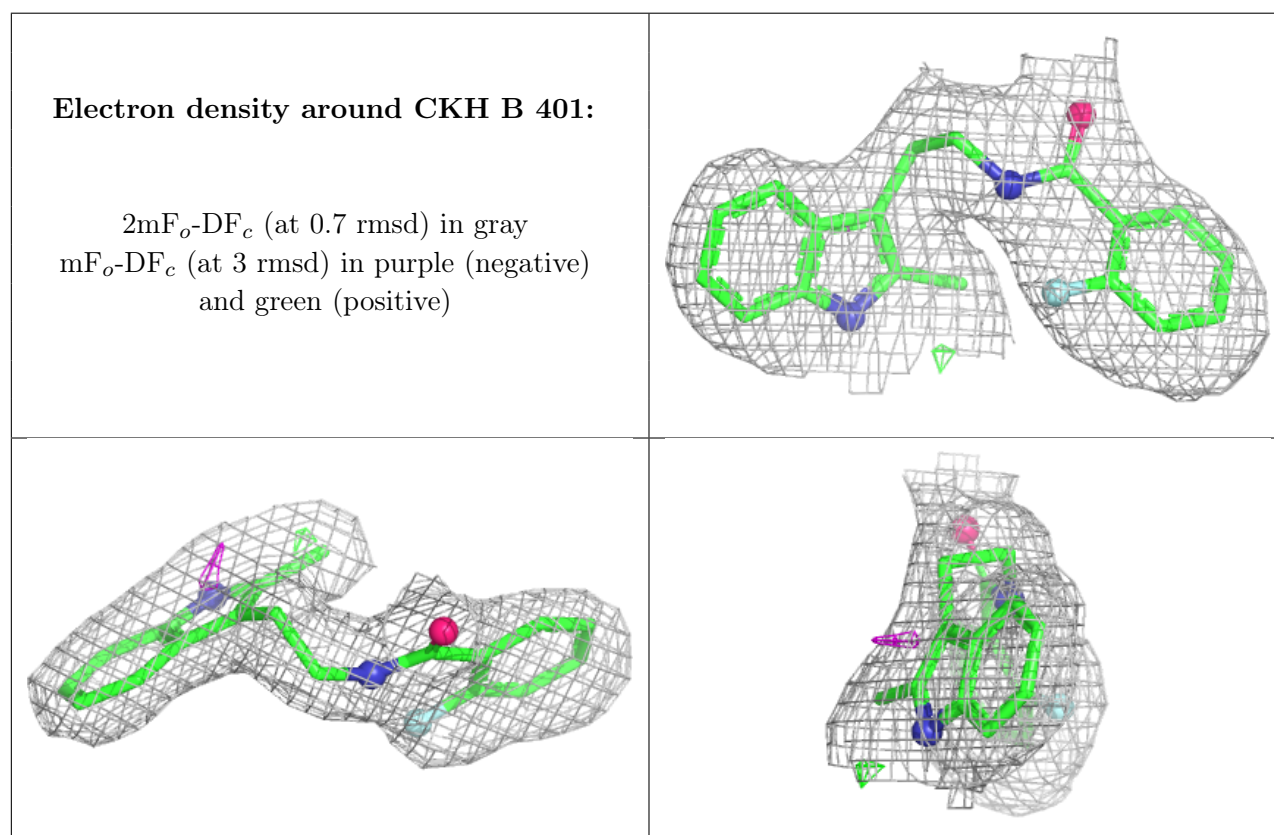
There are no oligosaccharides in this entry.

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
8	CKH	B	401	22/22	0.92	0.09	36,39,47,48	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.