



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:09 PM UTC

PDB ID : 4Y6K / pdb_00004y6k
Title : Complex structure of presenilin homologue PSH bound to an inhibitor
Authors : Dang, S.; Wu, S.; Wang, J.; Shi, Y.
Deposited on : 2015-02-13
Resolution : 3.85 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

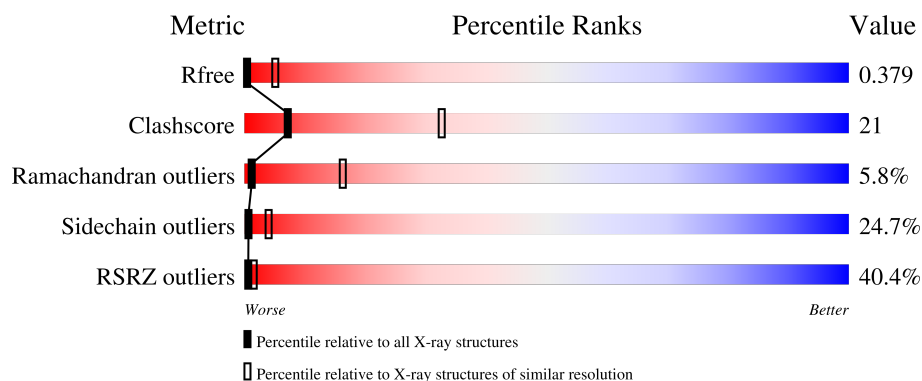
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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	1165 (4.02-3.70)
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
Sidechain outliers	187428	1142 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)

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	301	29% 37% 34% 11% 18%
1	B	301	33% 38% 32% 10% 19%
1	C	301	33% 40% 29% 9% 21%
1	D	301	34% 36% 31% 10% 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7200 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.

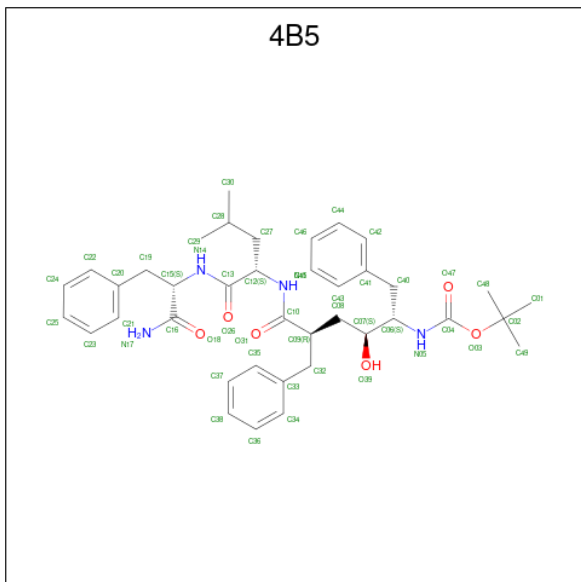
- Molecule 1 is a protein called Uncharacterized protein PSH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	B	245	Total	C	N	O	S	0	0	0
			1797	1217	275	294	11			
1	C	238	Total	C	N	O	S	0	0	0
			1763	1197	267	288	11			
1	D	237	Total	C	N	O	S	0	0	0
			1740	1180	264	285	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ASN	ASP	engineered mutation	UNP A3CWV0
A	42	SER	GLU	engineered mutation	UNP A3CWV0
A	147	GLU	ALA	engineered mutation	UNP A3CWV0
A	148	PRO	VAL	engineered mutation	UNP A3CWV0
A	229	VAL	ALA	engineered mutation	UNP A3CWV0
B	40	ASN	ASP	engineered mutation	UNP A3CWV0
B	42	SER	GLU	engineered mutation	UNP A3CWV0
B	147	GLU	ALA	engineered mutation	UNP A3CWV0
B	148	PRO	VAL	engineered mutation	UNP A3CWV0
B	229	VAL	ALA	engineered mutation	UNP A3CWV0
C	40	ASN	ASP	engineered mutation	UNP A3CWV0
C	42	SER	GLU	engineered mutation	UNP A3CWV0
C	147	GLU	ALA	engineered mutation	UNP A3CWV0
C	148	PRO	VAL	engineered mutation	UNP A3CWV0
C	229	VAL	ALA	engineered mutation	UNP A3CWV0
D	40	ASN	ASP	engineered mutation	UNP A3CWV0
D	42	SER	GLU	engineered mutation	UNP A3CWV0
D	147	GLU	ALA	engineered mutation	UNP A3CWV0
D	148	PRO	VAL	engineered mutation	UNP A3CWV0
D	229	VAL	ALA	engineered mutation	UNP A3CWV0

- Molecule 2 is N-{(2R,4S,5S)-2-benzyl-5-[(tert-butoxycarbonyl)amino]-4-hydroxy-6-phenylhexanoyl}-L-leucyl-L-phenylalaninamide (CCD ID: 4B5) (formula: C₃₉H₅₂N₄O₆).

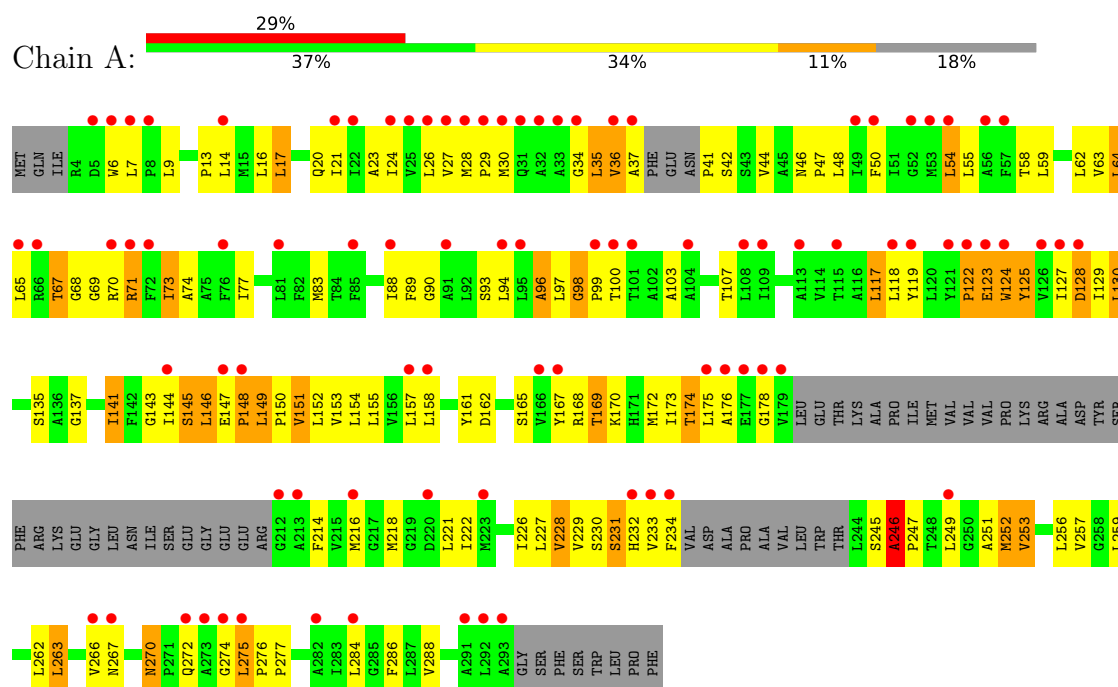


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			49	39	4	6		
2	D	1	Total	C	N	O	0	0
			49	39	4	6		

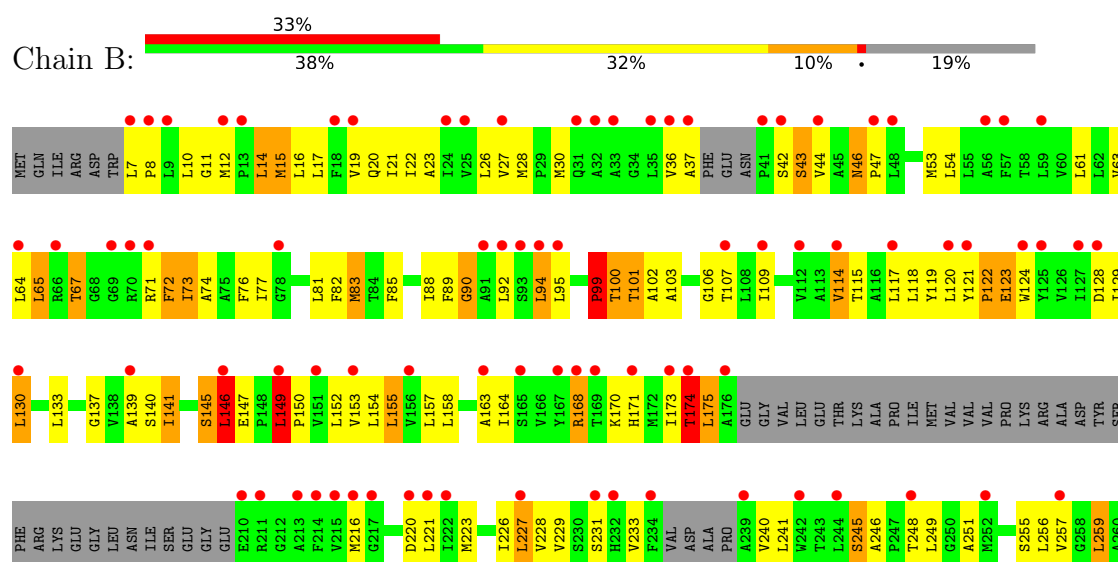
3 Residue-property plots [i](#)

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: Uncharacterized protein PSH

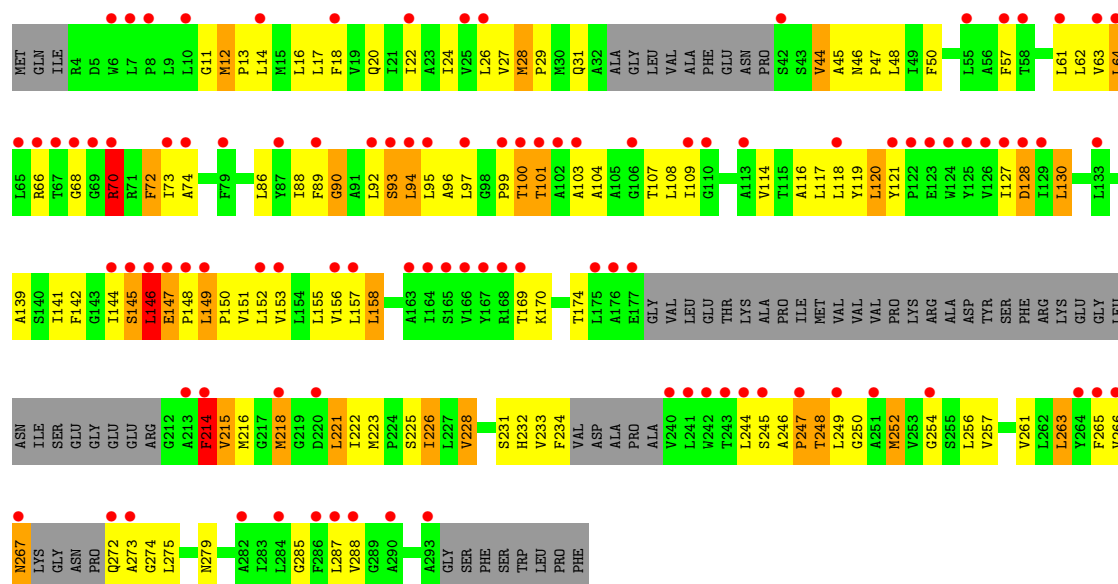


• Molecule 1: Uncharacterized protein PSH

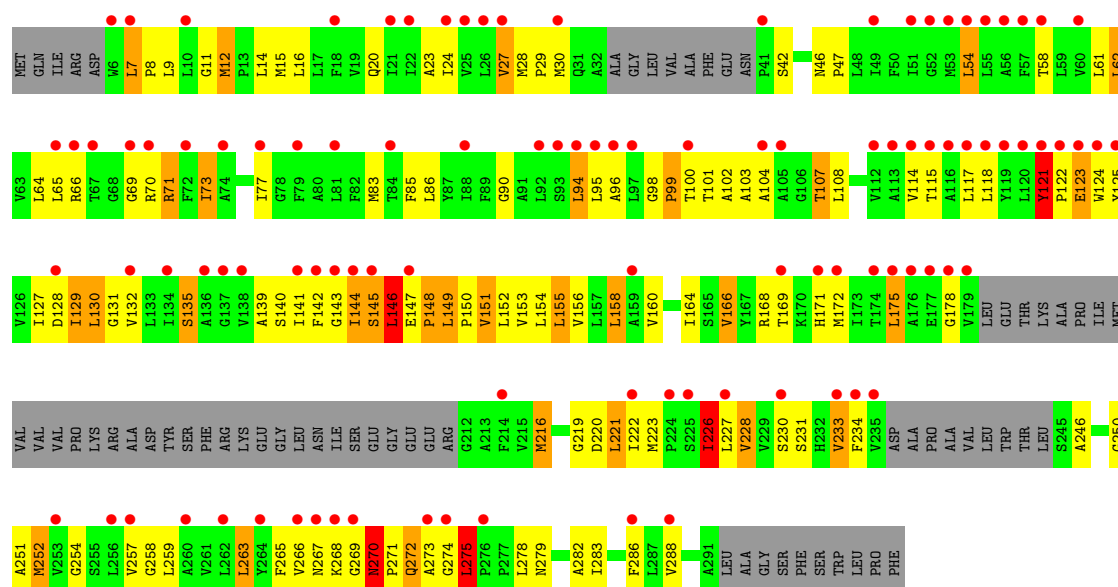




• Molecule 1: Uncharacterized protein PSH



• Molecule 1: Uncharacterized protein PSH



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	168.62Å 201.69Å 117.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.20 – 3.85 48.20 – 3.85	Depositor EDS
% Data completeness (in resolution range)	40.0 (48.20-3.85) 40.0 (48.20-3.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.320 , 0.367 0.334 , 0.379	Depositor DCC
R_{free} test set	361 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	-6.1	Xtriage
Anisotropy	3.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 144.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	7200	wwPDB-VP
Average B, all atoms (Å ²)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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: 4B5

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	0.43	0/1839	1.04	12/2511 (0.5%)
1	B	0.46	0/1834	1.08	9/2505 (0.4%)
1	C	0.47	0/1799	1.07	9/2457 (0.4%)
1	D	0.50	0/1777	1.17	13/2427 (0.5%)
All	All	0.47	0/7249	1.09	43/9900 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
1	C	0	2
1	D	0	1
All	All	0	11

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	121	TYR	CA-C-N	10.24	132.64	119.84
1	D	121	TYR	C-N-CA	10.24	132.64	119.84
1	D	275	LEU	CA-C-N	-9.44	110.66	120.38
1	D	275	LEU	C-N-CA	-9.44	110.66	120.38
1	D	228	VAL	N-CA-C	-9.02	104.06	111.81
1	B	121	TYR	CA-C-N	7.96	129.78	119.84
1	B	121	TYR	C-N-CA	7.96	129.78	119.84
1	D	269	GLY	CA-C-N	7.70	129.33	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	269	GLY	C-N-CA	7.70	129.33	119.78
1	A	270	ASN	CA-C-N	6.95	128.53	119.84
1	A	270	ASN	C-N-CA	6.95	128.53	119.84
1	C	147	GLU	CA-C-N	6.91	127.48	119.47
1	C	147	GLU	C-N-CA	6.91	127.48	119.47
1	C	121	TYR	CA-C-N	6.72	128.25	119.84
1	C	121	TYR	C-N-CA	6.72	128.25	119.84
1	A	98	GLY	CA-C-N	6.71	128.22	119.84
1	A	98	GLY	C-N-CA	6.71	128.22	119.84
1	A	7	LEU	CA-C-N	-6.60	113.16	119.76
1	A	7	LEU	C-N-CA	-6.60	113.16	119.76
1	C	68	GLY	N-CA-C	-6.29	102.97	112.41
1	A	125	TYR	N-CA-C	-6.22	104.39	112.23
1	B	223	MET	N-CA-C	6.00	121.05	113.25
1	D	270	ASN	N-CA-C	5.71	120.00	112.35
1	C	214	PHE	N-CA-C	5.71	118.44	111.82
1	B	276	PRO	N-CA-C	5.68	117.63	110.70
1	B	7	LEU	CA-C-N	-5.60	114.04	119.87
1	B	7	LEU	C-N-CA	-5.60	114.04	119.87
1	D	146	LEU	N-CA-C	5.57	116.42	108.74
1	C	215	VAL	N-CA-C	-5.45	104.64	110.36
1	B	275	LEU	N-CA-C	5.45	120.89	113.16
1	B	231	SER	N-CA-C	-5.40	107.05	113.97
1	A	275	LEU	CA-C-N	-5.31	114.91	120.38
1	A	275	LEU	C-N-CA	-5.31	114.91	120.38
1	D	226	ILE	CB-CA-C	-5.30	104.98	112.14
1	A	173	ILE	N-CA-C	-5.29	105.69	110.82
1	C	28	MET	CA-C-N	-5.29	114.22	119.56
1	C	28	MET	C-N-CA	-5.29	114.22	119.56
1	B	100	THR	N-CA-C	5.25	117.64	109.60
1	D	98	GLY	CA-C-N	-5.21	113.33	119.84
1	D	98	GLY	C-N-CA	-5.21	113.33	119.84
1	A	73	ILE	N-CA-C	-5.17	105.50	110.72
1	A	276	PRO	N-CA-C	5.09	116.91	110.70
1	D	94	LEU	N-CA-C	-5.07	105.93	111.82

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	TRP	Peptide
1	A	145	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	146	LEU	Peptide
1	A	246	ALA	Peptide
1	A	272	GLN	Peptide
1	B	145	SER	Peptide
1	B	146	LEU	Peptide
1	B	99	PRO	Peptide
1	C	145	SER	Peptide
1	C	146	LEU	Peptide
1	D	146	LEU	Peptide

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	1802	0	1949	71	0
1	B	1797	0	1949	73	0
1	C	1763	0	1903	76	0
1	D	1740	0	1881	97	0
2	C	49	0	52	14	0
2	D	49	0	52	10	0
All	All	7200	0	7786	312	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 21.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:PHE:HB3	1:D:271:PRO:HG2	1.47	0.94
1:D:216:MET:HE3	2:D:501:4B5:H34	1.51	0.92
1:D:139:ALA:HA	1:D:226:ILE:HG12	1.55	0.89
1:B:246:ALA:HA	1:B:249:LEU:HD12	1.55	0.88
1:D:151:VAL:HG13	1:D:227:LEU:HD13	1.56	0.85
1:D:251:ALA:HB2	1:D:286:PHE:HB2	1.59	0.84
1:C:100:THR:OG1	1:C:101:THR:N	2.04	0.83
1:D:263:LEU:O	1:D:267:ASN:ND2	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:HA	1:B:64:LEU:HD12	1.65	0.78
1:A:36:VAL:HG12	1:A:37:ALA:H	1.47	0.78
1:A:253:VAL:HA	1:A:256:LEU:HD12	1.66	0.76
1:D:270:ASN:H	1:D:270:ASN:ND2	1.83	0.76
1:C:216:MET:HE1	2:C:501:4B5:H26	1.49	0.75
1:C:170:LYS:NZ	1:C:272:GLN:OE1	2.19	0.75
1:C:263:LEU:O	1:C:267:ASN:ND2	2.21	0.74
1:A:118:LEU:HD12	1:A:130:LEU:HD12	1.69	0.73
1:D:29:PRO:HB3	1:D:95:LEU:HG	1.69	0.73
1:D:129:ILE:HD13	1:D:130:LEU:HD23	1.70	0.73
1:B:100:THR:OG1	1:B:101:THR:N	2.21	0.73
1:D:147:GLU:HB3	1:D:148:PRO:HD2	1.72	0.72
1:A:30:MET:HE1	1:A:141:ILE:HA	1.71	0.72
1:B:36:VAL:HG12	1:B:37:ALA:H	1.55	0.71
1:C:26:LEU:HD22	1:C:92:LEU:HD13	1.72	0.71
1:C:169:THR:HG22	1:D:71:ARG:HH12	1.56	0.70
1:C:61:LEU:HD22	2:C:501:4B5:C45	2.22	0.70
1:D:155:LEU:HG	1:D:227:LEU:HD12	1.74	0.69
1:B:259:LEU:HB2	1:B:278:LEU:HD11	1.73	0.69
1:D:220:ASP:HB2	1:D:275:LEU:HD22	1.75	0.68
1:C:273:ALA:HB3	1:C:274:GLY:HA2	1.76	0.68
1:D:131:GLY:O	1:D:135:SER:OG	2.10	0.68
1:C:90:GLY:O	1:C:94:LEU:N	2.20	0.68
1:A:65:LEU:HD23	1:A:73:ILE:HD13	1.77	0.67
1:C:16:LEU:HA	1:C:221:LEU:HD11	1.77	0.67
1:B:30:MET:HE1	1:B:141:ILE:HA	1.75	0.66
1:B:65:LEU:HG	1:B:73:ILE:HD13	1.78	0.66
1:A:30:MET:HE2	1:A:144:ILE:HD12	1.78	0.65
1:C:90:GLY:HA2	1:C:107:THR:HG21	1.79	0.65
1:B:262:LEU:HD23	1:B:263:LEU:HD23	1.77	0.65
1:D:143:GLY:HA2	1:D:230:SER:HB2	1.79	0.65
1:D:148:PRO:O	1:D:151:VAL:N	2.30	0.65
1:A:148:PRO:O	1:A:151:VAL:N	2.30	0.64
1:C:279:ASN:OD1	2:C:501:4B5:H29	1.97	0.64
1:C:216:MET:HE1	2:C:501:4B5:N14	2.13	0.63
1:A:63:VAL:O	1:A:67:THR:OG1	2.11	0.63
1:C:74:ALA:O	1:C:119:TYR:OH	2.09	0.63
1:B:73:ILE:HA	1:B:76:PHE:HB3	1.81	0.63
1:D:151:VAL:HG22	1:D:227:LEU:HD22	1.81	0.62
1:C:88:ILE:O	1:C:92:LEU:HB2	1.99	0.62
1:B:63:VAL:O	1:B:67:THR:OG1	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ALA:O	1:C:107:THR:HG23	1.98	0.62
1:A:74:ALA:O	1:A:119:TYR:OH	2.17	0.61
1:B:280:GLY:O	1:B:284:LEU:HG	2.00	0.61
1:D:24:ILE:O	1:D:27:VAL:HB	2.00	0.61
1:D:65:LEU:O	1:D:69:GLY:N	2.34	0.61
1:D:216:MET:HE1	2:D:501:4B5:N14	2.16	0.61
1:C:88:ILE:HA	1:C:92:LEU:HD12	1.83	0.61
1:D:61:LEU:HA	1:D:64:LEU:HD12	1.84	0.60
1:B:82:PHE:HA	1:B:115:THR:HG21	1.83	0.60
1:C:139:ALA:HA	1:C:226:ILE:HG13	1.84	0.60
1:D:275:LEU:HB3	1:D:278:LEU:HB2	1.84	0.60
1:B:171:HIS:HA	1:B:174:THR:HG23	1.85	0.59
1:B:85:PHE:HE1	1:B:133:LEU:HD23	1.66	0.59
1:B:146:LEU:HD12	1:B:147:GLU:HG2	1.83	0.59
1:B:251:ALA:HB2	1:B:286:PHE:HB2	1.83	0.59
1:C:158:LEU:HD12	2:C:501:4B5:H22	1.85	0.59
1:A:36:VAL:HG13	1:A:145:SER:HA	1.85	0.58
1:A:98:GLY:O	1:A:100:THR:N	2.36	0.58
1:D:145:SER:O	1:D:146:LEU:HD13	2.04	0.58
1:C:275:LEU:HD13	2:C:501:4B5:C22	2.33	0.58
1:D:254:GLY:HA2	1:D:257:VAL:HG12	1.84	0.58
1:D:258:GLY:HA3	1:D:278:LEU:HD13	1.85	0.58
1:D:275:LEU:HA	1:D:278:LEU:HD23	1.85	0.58
1:C:247:PRO:O	1:C:250:GLY:N	2.35	0.57
1:A:41:PRO:C	1:A:146:LEU:HG	2.29	0.57
1:A:263:LEU:O	1:A:267:ASN:ND2	2.33	0.57
1:D:148:PRO:HD3	1:D:230:SER:O	2.05	0.57
1:D:54:LEU:O	1:D:58:THR:HG23	2.04	0.57
1:D:100:THR:HG21	1:D:104:ALA:HB2	1.87	0.57
1:D:216:MET:CE	2:D:501:4B5:H34	2.32	0.57
1:B:74:ALA:O	1:B:119:TYR:OH	2.23	0.57
1:A:147:GLU:HB3	1:A:148:PRO:HD2	1.86	0.56
1:C:118:LEU:HD12	1:C:130:LEU:HD12	1.87	0.56
1:B:88:ILE:HD11	1:B:137:GLY:HA3	1.88	0.56
1:A:262:LEU:HD23	1:A:277:PRO:HG2	1.88	0.56
1:D:216:MET:HE2	2:D:501:4B5:H25	1.71	0.56
1:B:155:LEU:HD12	1:B:227:LEU:HD12	1.86	0.56
1:A:17:LEU:HD21	1:A:256:LEU:HD11	1.88	0.56
1:A:165:SER:O	1:A:169:THR:HG23	2.07	0.55
1:D:155:LEU:HD22	1:D:279:ASN:ND2	2.22	0.55
1:B:22:ILE:O	1:B:26:LEU:HG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:TYR:HD2	1:B:120:LEU:HD22	1.70	0.55
1:C:222:ILE:O	1:C:225:SER:OG	2.19	0.55
1:C:45:ALA:HA	1:C:48:LEU:HD12	1.88	0.54
1:D:160:VAL:O	1:D:164:ILE:HG12	2.08	0.54
1:C:57:PHE:HE2	2:C:501:4B5:H44	1.73	0.54
1:A:246:ALA:HB1	1:A:247:PRO:HD2	1.90	0.54
1:D:70:ARG:O	1:D:71:ARG:HB2	2.08	0.54
1:C:11:GLY:O	1:C:14:LEU:HB3	2.08	0.54
1:C:257:VAL:O	1:C:261:VAL:HG23	2.08	0.53
1:D:146:LEU:O	1:D:230:SER:OG	2.17	0.53
1:D:155:LEU:HD12	1:D:283:ILE:HG13	1.90	0.53
1:D:151:VAL:HG13	1:D:227:LEU:HB3	1.91	0.53
1:D:16:LEU:O	1:D:20:GLN:HG3	2.07	0.53
1:D:250:GLY:O	1:D:254:GLY:N	2.38	0.53
1:A:218:MET:O	1:A:221:LEU:HB3	2.08	0.53
1:A:229:VAL:O	1:A:231:SER:N	2.42	0.52
1:A:228:VAL:HG21	1:A:252:MET:HG3	1.91	0.52
1:B:173:ILE:O	1:B:175:LEU:N	2.42	0.52
1:C:158:LEU:HD12	2:C:501:4B5:C19	2.39	0.52
1:A:90:GLY:HA2	1:A:107:THR:HG21	1.90	0.52
1:D:219:GLY:O	1:D:222:ILE:HB	2.09	0.52
1:A:24:ILE:HA	1:A:27:VAL:HG23	1.91	0.52
1:B:16:LEU:O	1:B:20:GLN:HG3	2.10	0.52
1:B:90:GLY:O	1:B:94:LEU:HB3	2.09	0.52
1:B:94:LEU:HD11	1:B:100:THR:HA	1.91	0.52
1:B:241:LEU:HA	1:B:245:SER:H	1.75	0.52
1:C:275:LEU:HD13	2:C:501:4B5:C24	2.40	0.52
1:D:7:LEU:HB2	1:D:8:PRO:HD3	1.91	0.52
1:D:272:GLN:HE22	1:D:275:LEU:H	1.57	0.52
1:A:54:LEU:O	1:A:58:THR:HG23	2.08	0.52
1:D:139:ALA:HA	1:D:226:ILE:CG1	2.35	0.52
1:C:222:ILE:HG22	1:C:226:ILE:HD12	1.92	0.51
1:D:125:TYR:O	1:D:129:ILE:HG22	2.11	0.51
1:A:170:LYS:O	1:A:174:THR:HG23	2.11	0.51
1:C:44:VAL:HA	1:C:150:PRO:HG3	1.91	0.51
1:D:227:LEU:HA	1:D:230:SER:HB3	1.93	0.51
1:A:42:SER:HB2	1:A:146:LEU:HD12	1.92	0.51
1:D:16:LEU:HA	1:D:221:LEU:HD11	1.93	0.51
1:D:142:PHE:HB2	1:D:226:ILE:HD13	1.91	0.51
1:D:154:LEU:HD23	1:D:227:LEU:HD11	1.92	0.51
1:B:47:PRO:HB3	1:B:154:LEU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:GLY:O	1:D:14:LEU:HB3	2.12	0.50
1:B:26:LEU:HD22	1:B:92:LEU:HB3	1.93	0.50
1:B:19:VAL:HG21	1:B:221:LEU:HG	1.94	0.50
1:A:59:LEU:HD23	1:B:72:PHE:CZ	2.46	0.50
1:A:251:ALA:HB2	1:A:286:PHE:HB2	1.93	0.50
1:B:43:SER:O	1:B:46:ASN:HB2	2.11	0.50
1:C:247:PRO:O	1:C:249:LEU:N	2.45	0.49
1:C:16:LEU:O	1:C:20:GLN:HG3	2.11	0.49
1:C:94:LEU:HD11	1:C:104:ALA:HA	1.93	0.49
1:D:118:LEU:HD12	1:D:130:LEU:HD12	1.95	0.49
1:D:149:LEU:HB3	1:D:150:PRO:HD3	1.94	0.49
1:C:20:GLN:NE2	1:C:252:MET:HG2	2.27	0.49
1:A:24:ILE:O	1:A:27:VAL:N	2.45	0.49
1:B:102:ALA:O	1:B:106:GLY:N	2.41	0.49
1:A:23:ALA:O	1:A:27:VAL:HG23	2.12	0.49
1:C:216:MET:SD	2:C:501:4B5:H34	2.53	0.49
1:C:12:MET:SD	1:C:13:PRO:HD3	2.52	0.49
1:C:223:MET:HG3	2:C:501:4B5:C24	2.43	0.49
1:D:28:MET:HB3	1:D:29:PRO:HD3	1.94	0.49
1:D:83:MET:O	1:D:86:LEU:HB2	2.12	0.49
1:B:100:THR:HG1	1:B:101:THR:H	1.58	0.49
1:D:62:LEU:HD12	1:D:65:LEU:HD12	1.95	0.49
1:C:12:MET:N	1:C:13:PRO:HD2	2.27	0.49
1:C:29:PRO:HG2	1:C:92:LEU:HD22	1.94	0.49
1:B:30:MET:HG2	1:B:92:LEU:HD21	1.94	0.48
1:C:47:PRO:O	1:C:50:PHE:HB3	2.13	0.48
1:A:16:LEU:HA	1:A:221:LEU:HD11	1.94	0.48
1:B:173:ILE:C	1:B:175:LEU:H	2.21	0.48
1:D:65:LEU:HG	1:D:73:ILE:HD12	1.94	0.48
1:B:94:LEU:O	1:B:99:PRO:HA	2.12	0.48
1:D:42:SER:H	1:D:146:LEU:HD11	1.78	0.48
2:D:501:4B5:H34	2:D:501:4B5:H16	1.94	0.48
1:B:89:PHE:HB3	1:B:107:THR:HB	1.95	0.48
1:D:270:ASN:ND2	1:D:270:ASN:N	2.59	0.48
1:C:169:THR:HG22	1:D:71:ARG:NH1	2.27	0.47
1:C:16:LEU:HD23	1:C:256:LEU:HD23	1.96	0.47
1:A:13:PRO:HD3	1:A:259:LEU:HD21	1.96	0.47
1:A:20:GLN:CD	1:A:252:MET:HG2	2.40	0.47
1:D:228:VAL:HG22	1:D:251:ALA:HB1	1.97	0.47
1:C:231:SER:HB3	1:C:248:THR:HG22	1.96	0.47
1:D:216:MET:HE1	2:D:501:4B5:H26	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HD23	1:B:256:LEU:HD23	1.95	0.47
1:B:23:ALA:O	1:B:27:VAL:HG23	2.15	0.47
1:B:103:ALA:O	1:B:107:THR:HG23	2.14	0.47
1:B:255:SER:HB2	1:B:282:ALA:HB2	1.97	0.47
1:C:254:GLY:HA3	1:C:285:GLY:HA3	1.96	0.47
1:A:124:TRP:HA	1:A:127:ILE:HG12	1.97	0.46
1:C:72:PHE:HD1	1:C:72:PHE:H	1.62	0.46
1:C:146:LEU:HD12	1:C:147:GLU:CD	2.40	0.46
2:D:501:4B5:H41	2:D:501:4B5:H15	1.69	0.46
1:A:149:LEU:HB3	1:A:150:PRO:HD3	1.97	0.46
1:C:149:LEU:HB3	1:C:150:PRO:HD3	1.98	0.46
1:C:275:LEU:HB3	2:C:501:4B5:C23	2.46	0.46
1:A:262:LEU:HD21	1:A:274:GLY:HA2	1.97	0.46
1:B:149:LEU:HB3	1:B:150:PRO:HD3	1.96	0.46
1:D:158:LEU:HD23	1:D:158:LEU:HA	1.72	0.46
1:A:249:LEU:HA	1:A:252:MET:HE3	1.98	0.46
1:B:15:MET:HE3	1:B:128:ASP:HB3	1.98	0.46
1:A:28:MET:HB3	1:A:29:PRO:HD3	1.97	0.46
1:B:140:SER:HA	1:B:229:VAL:HG21	1.98	0.46
1:C:116:ALA:O	1:C:120:LEU:HG	2.16	0.46
1:D:90:GLY:HA2	1:D:107:THR:HG21	1.97	0.46
1:D:100:THR:HB	1:D:103:ALA:HB3	1.98	0.46
1:D:273:ALA:HA	1:D:274:GLY:HA2	1.57	0.46
1:A:58:THR:O	1:A:62:LEU:HG	2.16	0.46
1:D:158:LEU:HD13	2:D:501:4B5:H23	1.97	0.45
1:C:214:PHE:O	1:C:218:MET:HG3	2.16	0.45
1:D:103:ALA:O	1:D:107:THR:HG23	2.17	0.45
1:D:166:VAL:HG21	1:D:273:ALA:N	2.32	0.45
1:A:135:SER:HA	1:A:222:ILE:HD11	1.98	0.45
1:A:93:SER:HA	1:A:96:ALA:HB3	1.98	0.45
1:A:98:GLY:C	1:A:100:THR:H	2.23	0.45
1:B:118:LEU:HD12	1:B:130:LEU:HD12	1.98	0.45
1:C:24:ILE:O	1:C:27:VAL:HG12	2.17	0.45
1:D:227:LEU:N	1:D:227:LEU:HD23	2.31	0.45
1:A:94:LEU:O	1:A:98:GLY:HA2	2.16	0.45
1:B:17:LEU:HG	1:B:256:LEU:HD21	1.99	0.45
1:C:24:ILE:HD11	1:C:228:VAL:HG12	1.98	0.45
1:B:163:ALA:HB2	1:B:276:PRO:CG	2.46	0.45
2:D:501:4B5:H16	2:D:501:4B5:C34	2.47	0.45
1:A:68:GLY:HA2	1:A:69:GLY:HA3	1.62	0.45
1:D:47:PRO:HB3	1:D:154:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:THR:OG1	1:D:102:ALA:N	2.50	0.45
1:B:129:ILE:HG22	1:B:130:LEU:HD23	1.98	0.44
1:A:27:VAL:HA	1:A:144:ILE:HD11	2.00	0.44
1:C:93:SER:HA	1:C:96:ALA:HB3	1.98	0.44
1:A:103:ALA:O	1:A:107:THR:HG23	2.17	0.44
1:D:254:GLY:HA3	1:D:282:ALA:HA	1.99	0.44
1:D:27:VAL:O	1:D:144:ILE:HD11	2.16	0.44
1:D:171:HIS:CE1	1:D:175:LEU:HD13	2.52	0.44
1:A:50:PHE:CD1	1:A:50:PHE:C	2.95	0.44
1:A:88:ILE:HD11	1:A:137:GLY:HA3	1.99	0.44
1:B:61:LEU:O	1:B:64:LEU:HB2	2.18	0.44
1:B:88:ILE:O	1:B:92:LEU:HB2	2.18	0.44
1:C:275:LEU:HD12	2:C:501:4B5:H12	2.00	0.44
1:D:12:MET:HG2	1:D:15:MET:HE3	1.98	0.44
1:C:275:LEU:HD23	1:C:275:LEU:HA	1.68	0.44
1:D:272:GLN:NE2	1:D:275:LEU:H	2.16	0.44
1:A:47:PRO:HB3	1:A:154:LEU:HB2	1.98	0.44
1:A:128:ASP:OD1	1:A:128:ASP:N	2.51	0.44
1:B:85:PHE:CE1	1:B:133:LEU:HD23	2.49	0.44
1:C:99:PRO:HB2	1:C:100:THR:HG22	1.99	0.44
1:A:36:VAL:HG12	1:A:37:ALA:N	2.24	0.44
1:A:161:TYR:HE2	1:B:71:ARG:HH21	1.66	0.44
1:D:155:LEU:CG	1:D:227:LEU:HD12	2.45	0.44
1:B:149:LEU:HD22	1:B:149:LEU:HA	1.87	0.43
1:C:86:LEU:HD23	1:C:86:LEU:HA	1.88	0.43
1:B:47:PRO:HG3	1:B:150:PRO:O	2.17	0.43
1:B:146:LEU:HD13	1:B:146:LEU:HA	1.76	0.43
1:C:28:MET:HB3	1:C:29:PRO:HD3	1.99	0.43
1:B:122:PRO:HB2	1:B:123:GLU:H	1.52	0.43
1:B:164:ILE:O	1:B:168:ARG:HB2	2.19	0.43
1:D:20:GLN:OE1	1:D:252:MET:HG2	2.17	0.43
1:D:23:ALA:O	1:D:27:VAL:HG23	2.18	0.43
1:A:123:GLU:HB3	1:A:125:TYR:CE2	2.53	0.43
1:A:127:ILE:HG22	1:A:214:PHE:HE2	1.83	0.43
1:D:99:PRO:HA	1:D:100:THR:HA	1.77	0.43
1:D:275:LEU:CB	1:D:278:LEU:HB2	2.47	0.43
1:D:24:ILE:O	1:D:27:VAL:N	2.50	0.43
1:D:155:LEU:HD22	1:D:279:ASN:CG	2.43	0.43
1:A:26:LEU:C	1:A:29:PRO:HD2	2.43	0.43
1:B:30:MET:HB3	1:B:30:MET:HE2	1.52	0.43
1:D:128:ASP:O	1:D:132:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLN:OE1	1:A:252:MET:HG2	2.17	0.43
1:A:30:MET:CE	1:A:144:ILE:HD12	2.46	0.43
1:B:11:GLY:O	1:B:14:LEU:HB3	2.19	0.43
1:B:92:LEU:HA	1:B:92:LEU:HD23	1.83	0.43
1:D:123:GLU:O	1:D:125:TYR:N	2.51	0.43
1:D:272:GLN:H	1:D:273:ALA:HA	1.84	0.43
1:C:29:PRO:HG2	1:C:92:LEU:CD2	2.49	0.42
1:C:64:LEU:HD21	1:C:73:ILE:HA	2.01	0.42
1:C:215:VAL:HG11	2:C:501:4B5:C45	2.49	0.42
1:C:27:VAL:O	1:C:144:ILE:HD11	2.20	0.42
1:C:86:LEU:O	1:C:90:GLY:N	2.52	0.42
1:C:148:PRO:HG2	1:C:234:PHE:HD2	1.84	0.42
1:C:214:PHE:O	1:C:215:VAL:C	2.62	0.42
1:C:218:MET:O	1:C:222:ILE:HG13	2.19	0.42
1:D:151:VAL:CG2	1:D:227:LEU:HD22	2.47	0.42
1:A:143:GLY:HA3	1:A:229:VAL:HB	2.01	0.42
1:D:226:ILE:HG22	1:D:227:LEU:HD23	2.02	0.42
1:A:117:LEU:HD22	1:A:122:PRO:HB3	2.02	0.42
1:C:72:PHE:N	1:C:72:PHE:CD1	2.88	0.42
1:D:223:MET:HG3	2:D:501:4B5:C22	2.49	0.42
1:A:97:LEU:HB2	1:A:103:ALA:HB2	2.01	0.42
1:B:139:ALA:HA	1:B:226:ILE:CD1	2.49	0.42
1:C:28:MET:O	1:C:31:GLN:HG2	2.19	0.42
1:B:26:LEU:HD22	1:B:92:LEU:HD13	2.02	0.42
1:B:119:TYR:O	1:B:120:LEU:HB2	2.19	0.42
1:A:162:ASP:HB2	1:A:275:LEU:HD12	2.02	0.42
1:C:70:ARG:HA	1:C:70:ARG:HD3	1.62	0.42
1:A:64:LEU:HD11	1:A:73:ILE:HG23	2.02	0.41
1:D:274:GLY:O	1:D:275:LEU:HB2	2.19	0.41
1:B:145:SER:O	1:B:146:LEU:HB2	2.20	0.41
1:D:151:VAL:CG1	1:D:227:LEU:HB3	2.50	0.41
1:B:173:ILE:C	1:B:175:LEU:N	2.78	0.41
1:B:233:VAL:O	1:B:233:VAL:HG12	2.20	0.41
1:D:227:LEU:O	1:D:231:SER:HB3	2.21	0.41
1:A:48:LEU:HD23	1:B:83:MET:HE1	2.02	0.41
1:A:59:LEU:HB2	1:B:72:PHE:CE1	2.56	0.41
1:B:8:PRO:O	1:B:11:GLY:N	2.54	0.41
1:D:30:MET:HE3	1:D:30:MET:O	2.21	0.41
1:D:271:PRO:HA	1:D:272:GLN:HA	1.77	0.41
1:A:36:VAL:CG1	1:A:37:ALA:H	2.26	0.41
1:A:71:ARG:HB2	1:A:71:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ALA:HA	1:C:247:PRO:C	2.45	0.41
1:D:140:SER:O	1:D:144:ILE:HB	2.20	0.41
1:A:34:GLY:O	1:A:35:LEU:HB2	2.20	0.41
1:B:276:PRO:N	1:B:277:PRO:HD2	2.35	0.41
1:C:128:ASP:N	1:C:128:ASP:OD1	2.54	0.41
1:A:146:LEU:HA	1:A:146:LEU:HD13	1.84	0.41
1:B:114:VAL:HG13	1:B:130:LEU:HD13	2.03	0.41
1:C:18:PHE:O	1:C:22:ILE:HG13	2.21	0.41
1:B:100:THR:O	1:B:101:THR:OG1	2.34	0.40
1:C:157:LEU:HD11	1:D:108:LEU:HD21	2.03	0.40
1:D:121:TYR:HA	1:D:122:PRO:HD2	1.80	0.40
1:A:50:PHE:C	1:A:50:PHE:HD1	2.29	0.40
1:A:89:PHE:HB3	1:A:107:THR:HB	2.03	0.40
1:C:142:PHE:HA	1:C:145:SER:HB3	2.03	0.40
1:D:151:VAL:HG13	1:D:227:LEU:CD1	2.38	0.40
1:B:21:ILE:HG22	1:B:22:ILE:HD13	2.04	0.40
1:C:86:LEU:HD21	1:C:108:LEU:HA	2.03	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	238/301 (79%)	198 (83%)	27 (11%)	13 (6%)	1	17
1	B	237/301 (79%)	198 (84%)	23 (10%)	16 (7%)	1	14
1	C	228/301 (76%)	192 (84%)	25 (11%)	11 (5%)	2	19
1	D	229/301 (76%)	192 (84%)	23 (10%)	14 (6%)	1	15
All	All	932/1204 (77%)	780 (84%)	98 (10%)	54 (6%)	1	16

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	99	PRO
1	A	122	PRO
1	A	246	ALA
1	B	42	SER
1	B	43	SER
1	B	72	PHE
1	B	99	PRO
1	B	149	LEU
1	C	120	LEU
1	C	248	THR
1	D	71	ARG
1	D	124	TRP
1	D	148	PRO
1	D	275	LEU
1	A	35	LEU
1	A	96	ALA
1	A	230	SER
1	A	231	SER
1	B	101	THR
1	B	122	PRO
1	B	123	GLU
1	B	124	TRP
1	B	146	LEU
1	B	174	THR
1	B	274	GLY
1	C	89	PHE
1	C	93	SER
1	C	146	LEU
1	C	245	SER
1	D	96	ALA
1	D	178	GLY
1	D	268	LYS
1	A	148	PRO
1	A	178	GLY
1	B	277	PRO
1	D	7	LEU
1	D	99	PRO
1	D	123	GLU
1	A	6	TRP
1	B	90	GLY
1	B	240	VAL
1	C	70	ARG

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Mol	Chain	Res	Type
1	C	101	THR
1	C	244	LEU
1	D	121	TYR
1	D	234	PHE
1	B	273	ALA
1	A	176	ALA
1	C	90	GLY
1	D	246	ALA
1	D	233	VAL
1	A	270	ASN
1	C	247	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/236 (80%)	141 (75%)	47 (25%)	0	4
1	B	188/236 (80%)	141 (75%)	47 (25%)	0	4
1	C	185/236 (78%)	141 (76%)	44 (24%)	1	5
1	D	183/236 (78%)	137 (75%)	46 (25%)	0	4
All	All	744/944 (79%)	560 (75%)	184 (25%)	1	4

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	14	LEU
1	A	17	LEU
1	A	21	ILE
1	A	44	VAL
1	A	46	ASN
1	A	54	LEU
1	A	55	LEU
1	A	64	LEU
1	A	67	THR

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Mol	Chain	Res	Type
1	A	70	ARG
1	A	71	ARG
1	A	77	ILE
1	A	83	MET
1	A	117	LEU
1	A	123	GLU
1	A	128	ASP
1	A	129	ILE
1	A	130	LEU
1	A	141	ILE
1	A	149	LEU
1	A	151	VAL
1	A	152	LEU
1	A	153	VAL
1	A	155	LEU
1	A	157	LEU
1	A	158	LEU
1	A	168	ARG
1	A	169	THR
1	A	172	MET
1	A	174	THR
1	A	175	LEU
1	A	216	MET
1	A	226	ILE
1	A	227	LEU
1	A	228	VAL
1	A	232	HIS
1	A	233	VAL
1	A	234	PHE
1	A	245	SER
1	A	252	MET
1	A	253	VAL
1	A	257	VAL
1	A	263	LEU
1	A	266	VAL
1	A	284	LEU
1	A	288	VAL
1	B	10	LEU
1	B	12	MET
1	B	14	LEU
1	B	15	MET
1	B	28	MET

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Mol	Chain	Res	Type
1	B	44	VAL
1	B	46	ASN
1	B	53	MET
1	B	54	LEU
1	B	65	LEU
1	B	67	THR
1	B	73	ILE
1	B	77	ILE
1	B	81	LEU
1	B	83	MET
1	B	94	LEU
1	B	95	LEU
1	B	109	ILE
1	B	114	VAL
1	B	117	LEU
1	B	130	LEU
1	B	141	ILE
1	B	146	LEU
1	B	149	LEU
1	B	152	LEU
1	B	153	VAL
1	B	155	LEU
1	B	157	LEU
1	B	158	LEU
1	B	168	ARG
1	B	170	LYS
1	B	174	THR
1	B	175	LEU
1	B	216	MET
1	B	220	ASP
1	B	227	LEU
1	B	228	VAL
1	B	245	SER
1	B	248	THR
1	B	257	VAL
1	B	259	LEU
1	B	261	VAL
1	B	262	LEU
1	B	263	LEU
1	B	266	VAL
1	B	272	GLN
1	B	288	VAL

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Mol	Chain	Res	Type
1	C	12	MET
1	C	17	LEU
1	C	44	VAL
1	C	46	ASN
1	C	62	LEU
1	C	63	VAL
1	C	64	LEU
1	C	66	ARG
1	C	70	ARG
1	C	72	PHE
1	C	94	LEU
1	C	95	LEU
1	C	97	LEU
1	C	100	THR
1	C	109	ILE
1	C	114	VAL
1	C	117	LEU
1	C	127	ILE
1	C	128	ASP
1	C	130	LEU
1	C	141	ILE
1	C	146	LEU
1	C	149	LEU
1	C	151	VAL
1	C	152	LEU
1	C	153	VAL
1	C	155	LEU
1	C	156	VAL
1	C	158	LEU
1	C	174	THR
1	C	214	PHE
1	C	218	MET
1	C	221	LEU
1	C	226	ILE
1	C	228	VAL
1	C	232	HIS
1	C	233	VAL
1	C	252	MET
1	C	263	LEU
1	C	265	PHE
1	C	266	VAL
1	C	267	ASN

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Mol	Chain	Res	Type
1	C	287	LEU
1	C	288	VAL
1	D	9	LEU
1	D	12	MET
1	D	27	VAL
1	D	46	ASN
1	D	54	LEU
1	D	62	LEU
1	D	66	ARG
1	D	73	ILE
1	D	77	ILE
1	D	85	PHE
1	D	94	LEU
1	D	107	THR
1	D	114	VAL
1	D	115	THR
1	D	117	LEU
1	D	127	ILE
1	D	129	ILE
1	D	130	LEU
1	D	135	SER
1	D	141	ILE
1	D	144	ILE
1	D	145	SER
1	D	146	LEU
1	D	149	LEU
1	D	151	VAL
1	D	152	LEU
1	D	153	VAL
1	D	155	LEU
1	D	156	VAL
1	D	158	LEU
1	D	166	VAL
1	D	168	ARG
1	D	169	THR
1	D	172	MET
1	D	175	LEU
1	D	216	MET
1	D	221	LEU
1	D	226	ILE
1	D	233	VAL
1	D	252	MET

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Mol	Chain	Res	Type
1	D	259	LEU
1	D	263	LEU
1	D	266	VAL
1	D	270	ASN
1	D	272	GLN
1	D	288	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	20	GLN
1	C	20	GLN
1	C	46	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	4B5	D	501	-	51,51,51	2.07	8 (15%)	65,69,69	1.65	9 (13%)
2	4B5	C	501	-	51,51,51	2.01	8 (15%)	65,69,69	1.44	9 (13%)

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	4B5	D	501	-	-	14/53/53/53	0/3/3/3
2	4B5	C	501	-	-	16/53/53/53	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	4B5	C13-N14	6.71	1.48	1.34
2	C	501	4B5	C13-N14	6.55	1.48	1.34
2	C	501	4B5	C10-N11	6.46	1.47	1.34
2	D	501	4B5	C10-N11	6.43	1.47	1.34
2	D	501	4B5	O03-C04	5.53	1.45	1.34
2	C	501	4B5	O03-C04	5.34	1.45	1.34
2	D	501	4B5	C04-N05	4.97	1.47	1.34
2	C	501	4B5	C04-N05	4.93	1.47	1.34
2	D	501	4B5	C16-N17	4.14	1.42	1.32
2	C	501	4B5	C16-N17	3.93	1.42	1.32
2	D	501	4B5	C32-C33	2.92	1.58	1.51
2	C	501	4B5	C32-C33	2.45	1.57	1.51
2	D	501	4B5	C40-C41	2.37	1.56	1.51
2	C	501	4B5	C40-C41	2.26	1.56	1.51
2	C	501	4B5	O39-C07	-2.14	1.38	1.43
2	D	501	4B5	O39-C07	-2.11	1.38	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	4B5	O03-C04-N05	6.35	120.43	110.03
2	C	501	4B5	O03-C04-N05	6.04	119.92	110.03
2	D	501	4B5	C33-C32-C09	4.95	123.16	113.74
2	D	501	4B5	C08-C09-C32	3.92	117.00	111.61
2	D	501	4B5	O47-C04-N05	-3.43	119.24	124.86
2	C	501	4B5	C28-C27-C12	-3.36	106.39	115.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	4B5	C02-O03-C04	-3.31	115.95	120.97
2	D	501	4B5	C12-N11-C10	3.13	128.38	121.65
2	C	501	4B5	O47-C04-N05	-3.12	119.74	124.86
2	D	501	4B5	C28-C27-C12	-3.03	107.27	115.40
2	D	501	4B5	O03-C04-O47	-2.99	120.33	125.64
2	C	501	4B5	O03-C04-O47	-2.99	120.33	125.64
2	D	501	4B5	C02-O03-C04	-2.82	116.69	120.97
2	C	501	4B5	C33-C32-C09	2.39	118.29	113.74
2	D	501	4B5	C15-C16-N17	2.35	120.77	116.76
2	C	501	4B5	C15-C16-N17	2.03	120.22	116.76
2	C	501	4B5	C13-C12-N11	-2.02	105.65	111.11
2	C	501	4B5	C21-C20-C22	2.02	121.23	118.23

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	4B5	N05-C04-O03-C02
2	C	501	4B5	C08-C09-C10-O31
2	C	501	4B5	C08-C09-C10-N11
2	D	501	4B5	C08-C09-C10-O31
2	D	501	4B5	C08-C09-C10-N11
2	D	501	4B5	C08-C09-C32-C33
2	D	501	4B5	C10-C09-C32-C33
2	C	501	4B5	O47-C04-O03-C02
2	D	501	4B5	O47-C04-O03-C02
2	D	501	4B5	C27-C12-N11-C10
2	D	501	4B5	N14-C15-C19-C20
2	D	501	4B5	N05-C04-O03-C02
2	D	501	4B5	C16-C15-C19-C20
2	C	501	4B5	N11-C12-C27-C28
2	D	501	4B5	N11-C12-C27-C28
2	C	501	4B5	C13-C12-C27-C28
2	D	501	4B5	C13-C12-C27-C28
2	C	501	4B5	N14-C15-C19-C20
2	C	501	4B5	C27-C12-N11-C10
2	D	501	4B5	C19-C15-N14-C13
2	C	501	4B5	C16-C15-C19-C20
2	C	501	4B5	C08-C09-C32-C33
2	C	501	4B5	C19-C15-N14-C13
2	C	501	4B5	C32-C09-C10-O31
2	D	501	4B5	N11-C12-C13-O26

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Mol	Chain	Res	Type	Atoms
2	D	501	4B5	N11-C12-C13-N14
2	C	501	4B5	N11-C12-C13-O26
2	C	501	4B5	N11-C12-C13-N14
2	C	501	4B5	C48-C02-O03-C04
2	C	501	4B5	C32-C09-C10-N11

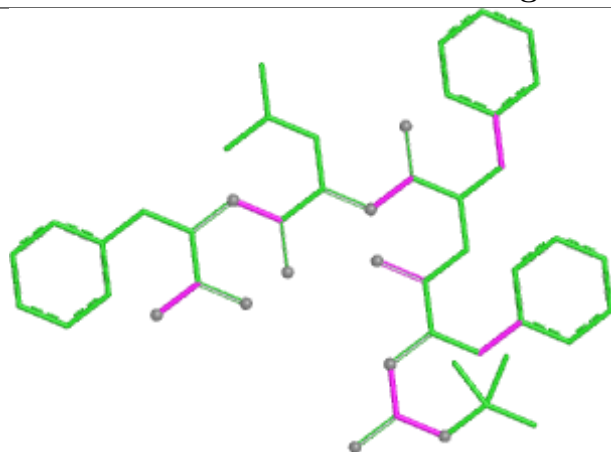
There are no ring outliers.

2 monomers are involved in 24 short contacts:

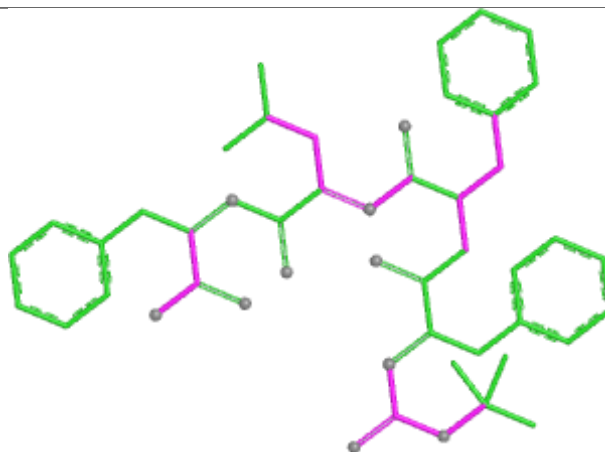
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	4B5	10	0
2	C	501	4B5	14	0

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.

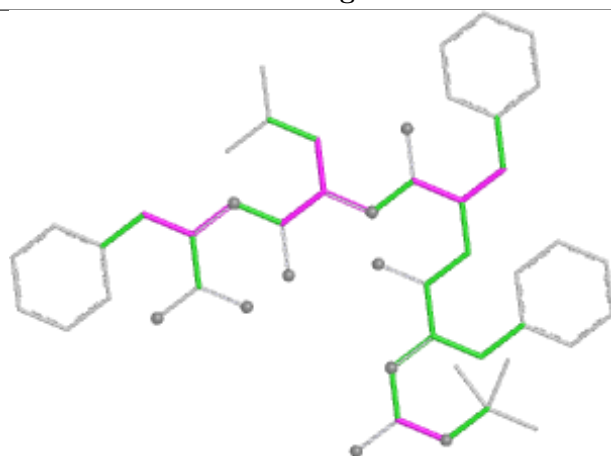
Ligand 4B5 D 501



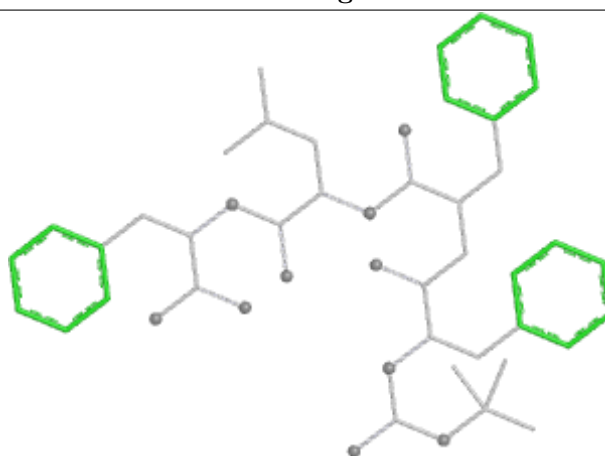
Bond lengths



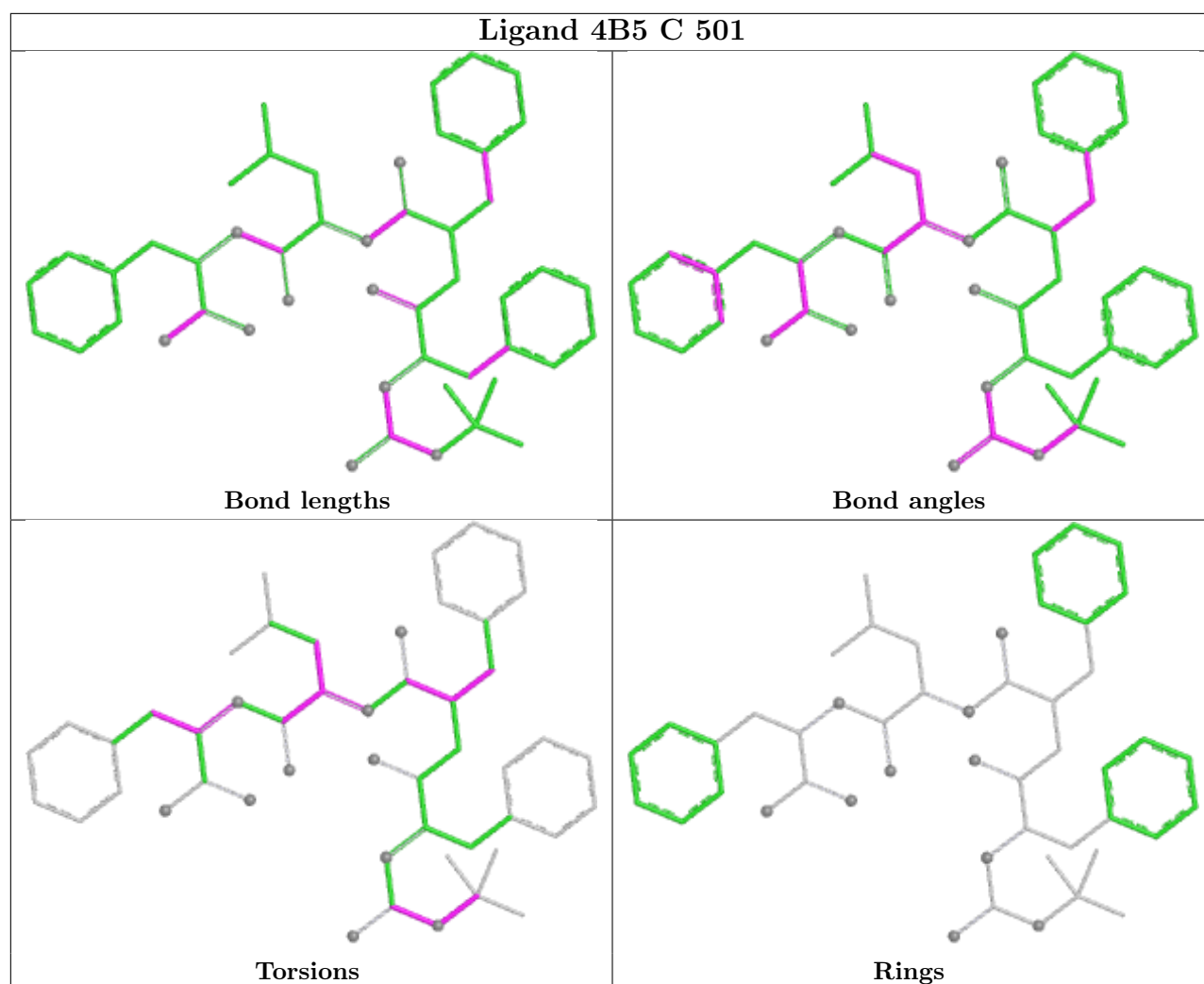
Bond angles



Torsions



Rings



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	246/301 (81%)	1.70	88 (35%) 1 2	56, 135, 215, 283	0
1	B	245/301 (81%)	1.87	100 (40%) 0 1	72, 161, 226, 290	0
1	C	238/301 (79%)	2.04	99 (41%) 0 1	66, 150, 247, 304	0
1	D	237/301 (78%)	2.05	103 (43%) 0 1	64, 168, 248, 290	0
All	All	966/1204 (80%)	1.91	390 (40%) 0 1	56, 152, 239, 304	0

All (390) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	242	TRP	22.4
1	C	102	ALA	10.6
1	C	68	GLY	10.5
1	A	25	VAL	9.4
1	D	141	ILE	9.2
1	B	44	VAL	8.8
1	B	37	ALA	7.8
1	A	34	GLY	7.1
1	B	9	LEU	7.1
1	A	124	TRP	7.0
1	B	69	GLY	6.9
1	A	6	TRP	6.9
1	C	241	LEU	6.7
1	D	171	HIS	6.6
1	D	142	PHE	6.5
1	D	172	MET	6.2
1	B	284	LEU	6.2
1	D	57	PHE	6.2
1	C	106	GLY	6.0
1	D	96	ALA	5.9
1	C	156	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
1	D	116	ALA	5.8
1	C	284	LEU	5.7
1	B	220	ASP	5.7
1	B	41	PRO	5.6
1	B	261	VAL	5.6
1	D	268	LYS	5.5
1	C	66	ARG	5.4
1	C	167	TYR	5.4
1	D	175	LEU	5.4
1	C	127	ILE	5.4
1	C	25	VAL	5.3
1	D	117	LEU	5.3
1	A	37	ALA	5.3
1	C	99	PRO	5.3
1	C	166	VAL	5.3
1	C	7	LEU	5.3
1	B	276	PRO	5.2
1	C	243	THR	5.1
1	C	92	LEU	5.1
1	D	52	GLY	5.0
1	C	121	TYR	5.0
1	D	93	SER	5.0
1	C	287	LEU	4.9
1	A	54	LEU	4.8
1	B	35	LEU	4.8
1	A	178	GLY	4.8
1	B	262	LEU	4.8
1	B	263	LEU	4.8
1	C	245	SER	4.8
1	D	81	LEU	4.8
1	C	122	PRO	4.7
1	D	7	LEU	4.7
1	B	265	PHE	4.7
1	D	21	ILE	4.6
1	A	52	GLY	4.5
1	A	177	GLU	4.5
1	C	67	THR	4.5
1	A	57	PHE	4.5
1	C	73	ILE	4.4
1	A	99	PRO	4.4
1	A	232	HIS	4.4
1	D	114	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	115	THR	4.4
1	A	7	LEU	4.4
1	C	129	ILE	4.3
1	B	165	SER	4.3
1	B	280	GLY	4.3
1	B	288	VAL	4.3
1	A	273	ALA	4.3
1	A	65	LEU	4.3
1	B	7	LEU	4.3
1	B	234	PHE	4.2
1	B	214	PHE	4.2
1	C	101	THR	4.2
1	D	92	LEU	4.2
1	B	272	GLN	4.2
1	C	146	LEU	4.1
1	B	36	VAL	4.1
1	A	33	ALA	4.1
1	D	66	ARG	4.1
1	C	164	ILE	4.1
1	D	134	ILE	4.1
1	D	6	TRP	4.0
1	A	28	MET	4.0
1	A	101	THR	4.0
1	B	176	ALA	4.0
1	D	56	ALA	4.0
1	D	138	VAL	4.0
1	D	113	ALA	4.0
1	A	233	VAL	3.9
1	C	288	VAL	3.9
1	A	29	PRO	3.9
1	D	22	ILE	3.9
1	C	113	ALA	3.9
1	C	247	PRO	3.9
1	A	5	ASP	3.9
1	C	244	LEU	3.8
1	A	234	PHE	3.8
1	B	109	ILE	3.8
1	D	177	GLU	3.8
1	B	71	ARG	3.8
1	B	273	ALA	3.8
1	B	27	VAL	3.8
1	D	235	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	53	MET	3.8
1	A	267	ASN	3.7
1	C	176	ALA	3.7
1	D	65	LEU	3.7
1	B	31	GLN	3.7
1	B	124	TRP	3.7
1	B	167	TYR	3.7
1	B	94	LEU	3.7
1	D	54	LEU	3.7
1	C	109	ILE	3.7
1	C	94	LEU	3.7
1	A	91	ALA	3.7
1	D	233	VAL	3.7
1	B	231	SER	3.7
1	B	277	PRO	3.7
1	A	266	VAL	3.6
1	C	95	LEU	3.6
1	B	24	ILE	3.6
1	B	171	HIS	3.6
1	D	144	ILE	3.6
1	D	69	GLY	3.6
1	B	270	ASN	3.6
1	C	26	LEU	3.6
1	C	293	ALA	3.6
1	C	55	LEU	3.6
1	D	179	VAL	3.6
1	B	232	HIS	3.6
1	B	210	GLU	3.5
1	C	177	GLU	3.5
1	D	273	ALA	3.5
1	D	174	THR	3.5
1	A	113	ALA	3.5
1	D	115	THR	3.5
1	A	31	GLN	3.5
1	B	92	LEU	3.5
1	C	147	GLU	3.5
1	C	282	ALA	3.5
1	B	153	VAL	3.5
1	A	30	MET	3.5
1	D	53	MET	3.5
1	A	121	TYR	3.5
1	D	100	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	264	TYR	3.4
1	C	70	ARG	3.4
1	D	118	LEU	3.4
1	D	288	VAL	3.4
1	A	104	ALA	3.4
1	B	149	LEU	3.4
1	C	123	GLU	3.4
1	A	275	LEU	3.4
1	A	95	LEU	3.4
1	B	274	GLY	3.4
1	B	291	ALA	3.4
1	D	257	VAL	3.4
1	C	42	SER	3.4
1	C	18	PHE	3.4
1	A	274	GLY	3.3
1	C	249	LEU	3.3
1	A	123	GLU	3.3
1	A	122	PRO	3.3
1	D	122	PRO	3.3
1	A	126	VAL	3.3
1	B	66	ARG	3.3
1	D	256	LEU	3.3
1	D	269	GLY	3.3
1	B	12	MET	3.3
1	C	58	THR	3.3
1	C	124	TRP	3.3
1	A	179	VAL	3.3
1	B	64	LEU	3.3
1	B	287	LEU	3.3
1	C	103	ALA	3.3
1	D	88	ILE	3.2
1	C	148	PRO	3.2
1	C	128	ASP	3.2
1	C	165	SER	3.2
1	C	220	ASP	3.2
1	D	67	THR	3.2
1	A	118	LEU	3.2
1	B	211	ARG	3.2
1	C	251	ALA	3.2
1	B	173	ILE	3.2
1	D	119	TYR	3.2
1	D	27	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	176	ALA	3.2
1	C	125	TYR	3.1
1	A	293	ALA	3.1
1	B	227	LEU	3.1
1	B	271	PRO	3.1
1	C	149	LEU	3.1
1	D	124	TRP	3.1
1	D	225	SER	3.1
1	A	72	PHE	3.1
1	A	148	PRO	3.1
1	A	292	LEU	3.1
1	C	213	ALA	3.1
1	D	49	ILE	3.1
1	B	216	MET	3.0
1	D	214	PHE	3.0
1	A	88	ILE	3.0
1	D	24	ILE	3.0
1	D	169	THR	3.0
1	A	70	ARG	3.0
1	D	95	LEU	3.0
1	B	117	LEU	3.0
1	A	158	LEU	3.0
1	B	13	PRO	2.9
1	A	94	LEU	2.9
1	D	25	VAL	2.9
1	D	222	ILE	2.9
1	A	216	MET	2.9
1	A	128	ASP	2.9
1	C	118	LEU	2.9
1	A	76	PHE	2.9
1	A	56	ALA	2.9
1	A	175	LEU	2.9
1	D	55	LEU	2.9
1	D	178	GLY	2.9
1	D	121	TYR	2.9
1	C	267	ASN	2.9
1	A	32	ALA	2.9
1	B	239	ALA	2.9
1	C	69	GLY	2.8
1	D	125	TYR	2.8
1	A	147	GLU	2.8
1	C	100	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	105	ALA	2.8
1	B	213	ALA	2.8
1	C	6	TRP	2.8
1	B	25	VAL	2.8
1	A	85	PHE	2.8
1	B	242	TRP	2.8
1	C	10	LEU	2.8
1	D	41	PRO	2.8
1	B	78	GLY	2.8
1	D	224	PRO	2.7
1	D	84	THR	2.7
1	C	64	LEU	2.7
1	A	71	ARG	2.7
1	B	130	LEU	2.7
1	C	133	LEU	2.7
1	D	10	LEU	2.7
1	A	157	LEU	2.7
1	A	167	TYR	2.7
1	B	252	MET	2.7
1	C	153	VAL	2.7
1	C	8	PRO	2.7
1	D	77	ILE	2.7
1	A	21	ILE	2.7
1	D	18	PHE	2.7
1	C	175	LEU	2.6
1	A	144	ILE	2.6
1	B	168	ARG	2.6
1	C	144	ILE	2.6
1	A	8	PRO	2.6
1	D	74	ALA	2.6
1	C	152	LEU	2.6
1	B	215	VAL	2.6
1	D	266	VAL	2.6
1	C	273	ALA	2.6
1	A	284	LEU	2.6
1	D	120	LEU	2.6
1	A	22	ILE	2.6
1	C	240	VAL	2.6
1	A	212	GLY	2.6
1	C	61	LEU	2.6
1	D	123	GLU	2.6
1	A	176	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	112	VAL	2.6
1	B	163	ALA	2.6
1	D	145	SER	2.5
1	C	266	VAL	2.5
1	D	128	ASP	2.5
1	B	48	LEU	2.5
1	C	74	ALA	2.5
1	D	26	LEU	2.5
1	D	234	PHE	2.5
1	B	47	PRO	2.5
1	D	276	PRO	2.5
1	A	291	ALA	2.5
1	A	127	ILE	2.5
1	A	249	LEU	2.5
1	B	91	ALA	2.5
1	B	120	LEU	2.5
1	C	97	LEU	2.5
1	D	97	LEU	2.5
1	A	213	ALA	2.4
1	D	104	ALA	2.4
1	B	42	SER	2.4
1	B	151	VAL	2.4
1	C	126	VAL	2.4
1	A	223	MET	2.4
1	D	30	MET	2.4
1	D	112	VAL	2.4
1	D	72	PHE	2.4
1	C	286	PHE	2.4
1	D	51	ILE	2.4
1	C	157	LEU	2.4
1	B	156	VAL	2.4
1	B	95	LEU	2.4
1	B	275	LEU	2.4
1	C	254	GLY	2.4
1	A	50	PHE	2.4
1	B	128	ASP	2.4
1	C	218	MET	2.4
1	A	49	ILE	2.3
1	D	230	SER	2.3
1	C	14	LEU	2.3
1	B	56	ALA	2.3
1	D	132	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	19	VAL	2.3
1	D	253	VAL	2.3
1	B	121	TYR	2.3
1	D	227	LEU	2.3
1	A	27	VAL	2.3
1	B	248	THR	2.3
1	B	70	ARG	2.3
1	C	272	GLN	2.3
1	C	145	SER	2.3
1	A	220	ASP	2.3
1	B	114	VAL	2.3
1	C	168	ARG	2.3
1	D	267	ASN	2.3
1	A	108	LEU	2.3
1	C	22	ILE	2.3
1	D	79	PHE	2.3
1	D	260	ALA	2.3
1	D	137	GLY	2.3
1	A	26	LEU	2.2
1	B	146	LEU	2.2
1	B	18	PHE	2.2
1	D	147	GLU	2.2
1	D	60	VAL	2.2
1	B	59	LEU	2.2
1	B	57	PHE	2.2
1	B	222	ILE	2.2
1	C	89	PHE	2.2
1	B	93	SER	2.2
1	D	70	ARG	2.2
1	D	143	GLY	2.2
1	D	159	ALA	2.2
1	D	94	LEU	2.2
1	B	125	TYR	2.2
1	C	264	TYR	2.2
1	D	286	PHE	2.2
1	B	268	LYS	2.2
1	C	65	LEU	2.2
1	D	262	LEU	2.2
1	B	127	ILE	2.2
1	C	163	ALA	2.1
1	A	119	TYR	2.1
1	B	8	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	244	LEU	2.1
1	B	32	ALA	2.1
1	C	214	PHE	2.1
1	B	107	THR	2.1
1	A	81	LEU	2.1
1	A	282	ALA	2.1
1	B	33	ALA	2.1
1	B	217	GLY	2.1
1	A	14	LEU	2.1
1	B	221	LEU	2.1
1	A	109	ILE	2.1
1	C	79	PHE	2.1
1	A	166	VAL	2.1
1	C	87	TYR	2.1
1	C	265	PHE	2.1
1	A	36	VAL	2.1
1	C	110	GLY	2.0
1	B	169	THR	2.0
1	C	169	THR	2.0
1	D	58	THR	2.0
1	A	24	ILE	2.0
1	D	136	ALA	2.0
1	A	272	GLN	2.0
1	A	100	THR	2.0
1	A	66	ARG	2.0
1	D	274	GLY	2.0
1	B	174	THR	2.0
1	C	57	PHE	2.0
1	B	139	ALA	2.0
1	C	93	SER	2.0
1	C	290	ALA	2.0
1	B	257	VAL	2.0
1	C	63	VAL	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 ⓘ

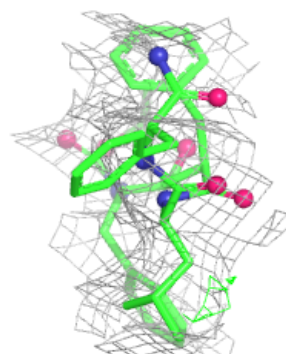
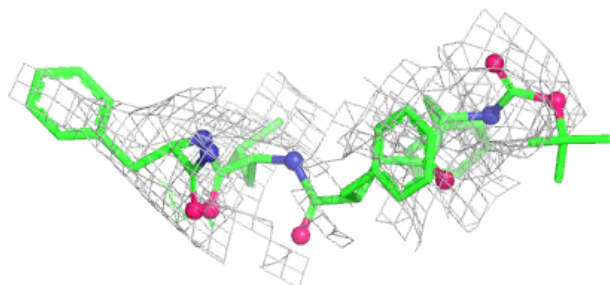
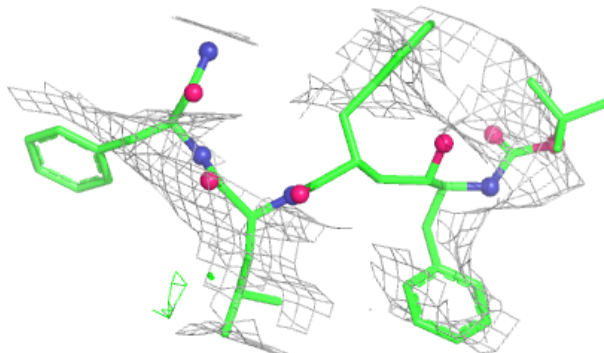
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	4B5	C	501	49/49	0.72	0.22	0,105,124,124	0
2	4B5	D	501	49/49	0.73	0.23	32,60,73,74	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.

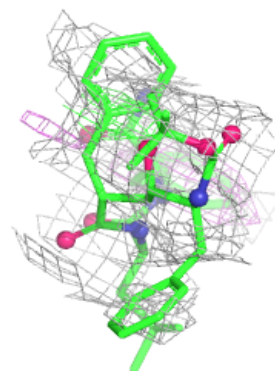
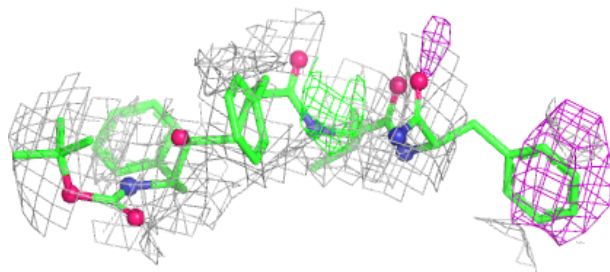
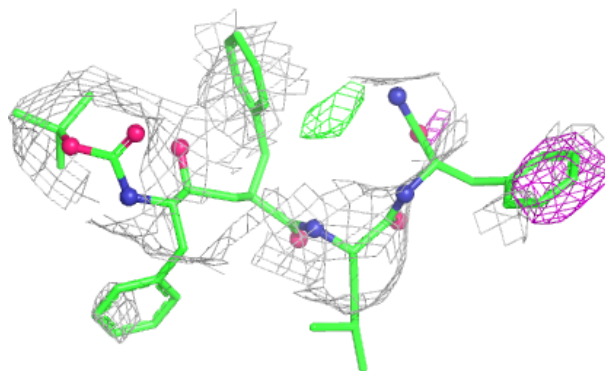
Electron density around 4B5 C 501:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 4B5 D 501:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.