Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 04:43 AM EDT

PDB ID	:	1IK3
Title	:	LIPOXYGENASE-3 (SOYBEAN) COMPLEX WITH 13(S)-HYDROPERO XY-9(Z),11(E)-OCTADECADIENOIC ACID
Authors	:	Skrzypczak-Jankun, E.; Funk Jr., M.O.
Deposited on	:	2001-05-01
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35
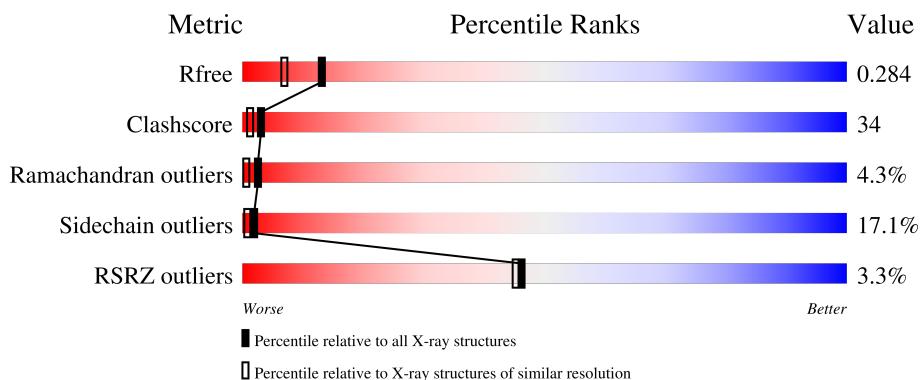
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
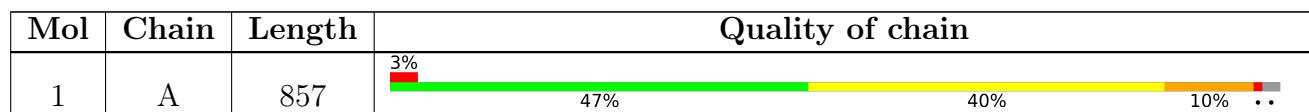
The reported resolution of this entry is 2.00 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.284
Clashscore		34
Ramachandran outliers		4.3%
Sidechain outliers		17.1%
RSRZ outliers		3.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	857	3% — 47% / 40% / 10% ··

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
3	13S	A	1859[A]	-	-	X	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 7314 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.
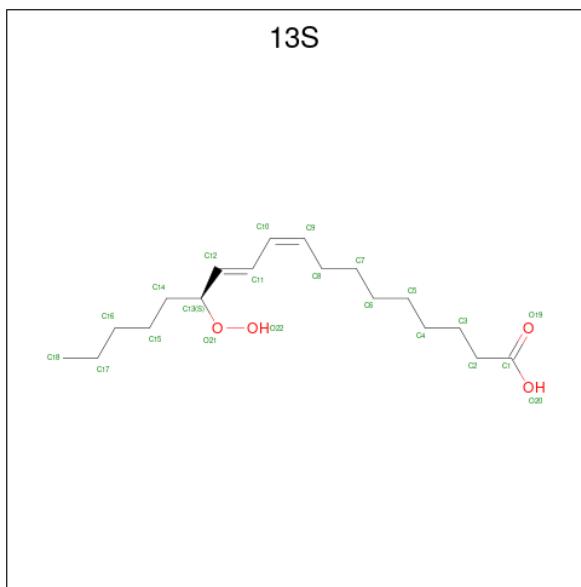
- Molecule 1 is a protein called LIPOXYGENASE-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total 6696	C 4278	N 1149	O 1251	S 18	0	0	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).
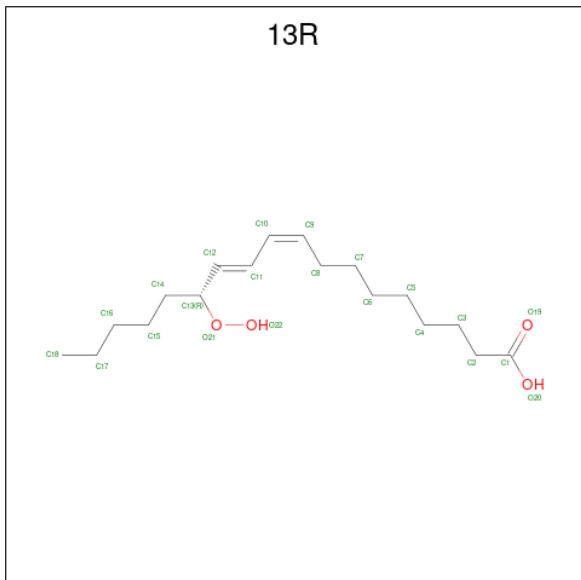
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Fe 1	0	0

- Molecule 3 is 13(S)-HYDROPEROXY-9(Z),11(E)-OCTADECADIENOIC ACID (three-letter code: 13S) (formula: $C_{18}H_{32}O_4$).
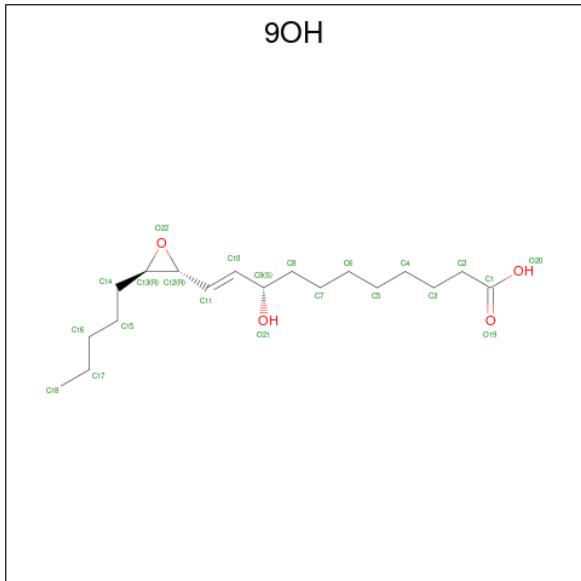
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 22	C 18	O 4	0	1

- Molecule 4 is 13(R)-HYDROPEROXY-9(Z),11(E)-OCTADECADIENOIC ACID (three-letter code: 13R) (formula: $C_{18}H_{32}O_4$).
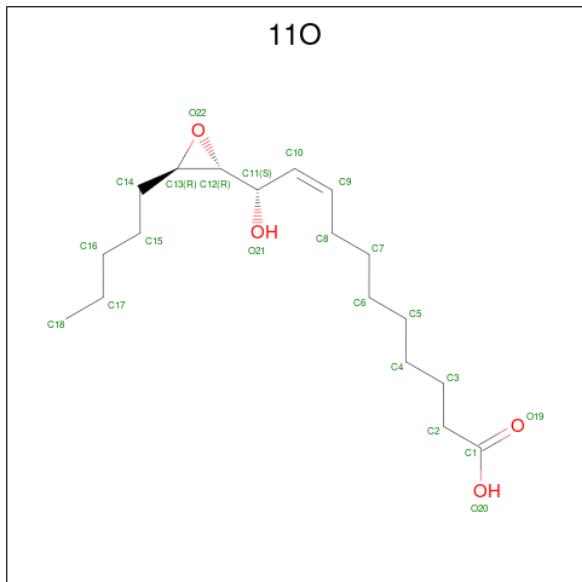
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	22	18	4	22	1

- Molecule 5 is (TRANS-12,13-EPOXY)-9-HYDROXY-10(E)-OCTADECENOIC ACID (three-letter code: 9OH) (formula: $C_{18}H_{32}O_4$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	22	18	4	22	1

- Molecule 6 is (TRANS-12,13-EPOXY)-11-HYDROXY-9(Z)-OCTADECENOIC ACID (three-letter code: 11O) (formula: $C_{18}H_{32}O_4$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	22	18	4	22	1
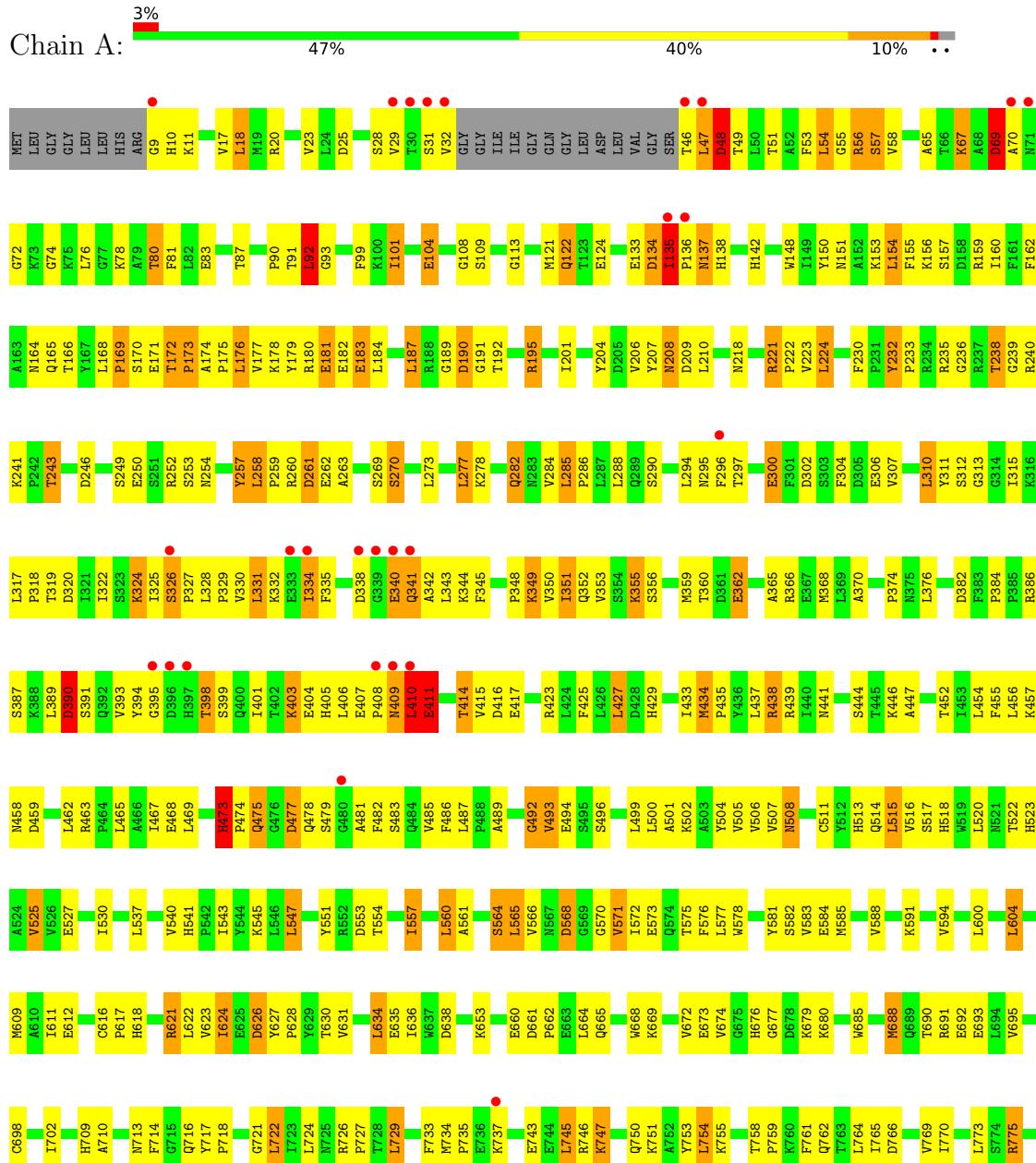
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	529	529	529	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: LIPOXYGENASE-3

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.65Å 137.28Å 61.89Å 90.00° 95.56° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 29.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	84.0 (40.00-2.00) 65.5 (29.98-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.92 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.196 , 0.296 0.192 , 0.284	Depositor DCC
R_{free} test set	4949 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 104.7	EDS
L-test for twinning [2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7314	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 13R, FE, 13S, 11O, 9OH

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	0.37	0/6867	0.66	1/9326 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	238	THR	N-CA-C	-5.70	95.62	111.00

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	6696	0	6615	456	0
2	A	1	0	0	0	0
3	A	22	0	30	20	0
4	A	22	0	30	0	0
5	A	22	0	29	0	0
6	A	22	0	31	0	0
7	A	529	0	0	63	0
All	All	7314	0	6735	456	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 34.

All (456) 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:A:394:TYR:HB3	1:A:481:ALA:HB2	1.23	1.15
1:A:788:ASN:HB2	1:A:789:PRO:HD3	1.26	1.09
1:A:389:LEU:HD13	1:A:394:TYR:HE2	1.16	1.03
1:A:243:THR:HG22	1:A:246:ASP:O	1.60	1.02
1:A:785:GLU:O	1:A:785:GLU:HG3	1.60	1.00
1:A:847:THR:HG22	1:A:849:ARG:HG2	1.49	0.95
1:A:315:ILE:HG23	1:A:343:LEU:HB3	1.48	0.93
1:A:514:GLN:HE22	1:A:515:LEU:HD23	1.34	0.93
1:A:604:LEU:HD21	1:A:630:THR:HG23	1.50	0.93
1:A:387:SER:HB3	1:A:395:GLY:HA2	1.47	0.93
1:A:518:HIS:HD1	3:A:1859[A]:13S:H81	1.31	0.92
1:A:169:PRO:HG3	1:A:661:ASP:OD1	1.70	0.92
1:A:389:LEU:HD13	1:A:394:TYR:CE2	2.06	0.90
1:A:584:GLU:HG3	7:A:971:HOH:O	1.71	0.89
1:A:514:GLN:NE2	1:A:515:LEU:HD23	1.90	0.87
1:A:611:ILE:HD11	1:A:621:ARG:HD2	1.57	0.86
1:A:135:ILE:HG23	1:A:136:PRO:HD3	1.57	0.85
1:A:514:GLN:HB2	3:A:1859[A]:13S:H61	1.59	0.84
1:A:690:THR:HG22	1:A:692:GLU:H	1.42	0.84
1:A:394:TYR:HB3	1:A:481:ALA:CB	2.06	0.83
1:A:734:MET:HE3	1:A:735:PRO:HD2	1.61	0.83
1:A:438:ARG:HG2	1:A:473:HIS:CE1	2.14	0.82
1:A:788:ASN:HB2	1:A:789:PRO:CD	2.07	0.82
1:A:775:ARG:HG3	1:A:775:ARG:HH11	1.43	0.82
1:A:169:PRO:HD3	1:A:541:HIS:CE1	2.14	0.81
1:A:238:THR:HG23	1:A:250:GLU:OE2	1.82	0.80
1:A:775:ARG:NH1	1:A:846:LEU:HD13	1.98	0.79
1:A:447:ALA:HB2	1:A:577:LEU:HD11	1.64	0.79
1:A:581:TYR:HB2	1:A:585:MET:HE2	1.65	0.79
1:A:502:LYS:HB2	7:A:1283:HOH:O	1.81	0.78
1:A:169:PRO:HG2	7:A:934:HOH:O	1.83	0.77
1:A:235:ARG:HH12	1:A:238:THR:HG22	1.50	0.77
1:A:408:PRO:O	1:A:409:ASN:HB3	1.84	0.77
1:A:511:CYS:O	1:A:514:GLN:HG3	1.84	0.76
1:A:522:THR:HG21	1:A:709:HIS:CD2	2.20	0.76
1:A:304:PHE:H	1:A:750:GLN:NE2	1.84	0.76
1:A:611:ILE:HD11	1:A:621:ARG:HH21	1.51	0.75
1:A:831:VAL:HG13	1:A:833:MET:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:HG12	1:A:136:PRO:N	2.02	0.74
1:A:819:ASN:HD22	1:A:827:ARG:HE	1.35	0.74
1:A:10:HIS:CD2	1:A:11:LYS:H	2.06	0.74
1:A:57:SER:HB2	7:A:1348:HOH:O	1.86	0.74
1:A:384:PRO:HD2	1:A:398:THR:HG21	1.68	0.74
1:A:169:PRO:HG3	1:A:661:ASP:CG	2.08	0.73
1:A:729:LEU:HD11	1:A:758:THR:HG23	1.70	0.73
1:A:438:ARG:HH22	1:A:439:ARG:NH2	1.86	0.72
1:A:224:LEU:HD12	1:A:230:PHE:HB3	1.70	0.72
1:A:260:ARG:O	1:A:261:ASP:HB2	1.89	0.72
1:A:819:ASN:ND2	1:A:827:ARG:HE	1.86	0.72
1:A:172:THR:HB	1:A:173:PRO:HD3	1.72	0.72
1:A:578:TRP:HB3	1:A:585:MET:CE	2.20	0.72
1:A:124:GLU:HB2	7:A:1385:HOH:O	1.89	0.72
1:A:169:PRO:O	1:A:171:GLU:HG2	1.89	0.72
1:A:522:THR:HG22	1:A:523:HIS:N	2.04	0.72
1:A:401:ILE:HD11	1:A:468:GLU:HB2	1.72	0.71
1:A:326:SER:H	1:A:327:PRO:HD2	1.56	0.71
1:A:438:ARG:HG3	7:A:939:HOH:O	1.89	0.71
1:A:525:VAL:HG23	7:A:1375:HOH:O	1.88	0.71
1:A:254:ASN:HB2	7:A:1181:HOH:O	1.90	0.71
1:A:836:THR:HG23	1:A:848:PHE:O	1.90	0.71
1:A:622:LEU:HD21	1:A:630:THR:HG21	1.70	0.70
1:A:284:VAL:O	1:A:288:LEU:HB2	1.91	0.70
1:A:25:ASP:O	1:A:29:VAL:HG23	1.90	0.70
1:A:492:GLY:HA3	7:A:1254:HOH:O	1.91	0.70
1:A:121:MET:O	1:A:122:GLN:HB2	1.89	0.69
1:A:151:ASN:OD1	1:A:153:LYS:HB2	1.92	0.69
1:A:518:HIS:ND1	3:A:1859[A]:13S:H81	2.06	0.69
1:A:160:ILE:CG2	1:A:183:GLU:HG3	2.22	0.69
1:A:277:LEU:HD23	3:A:1859[A]:13S:H182	1.75	0.69
1:A:403:LYS:HE2	1:A:404:GLU:HB3	1.74	0.69
1:A:847:THR:CG2	1:A:849:ARG:HG2	2.22	0.69
1:A:566:VAL:HG22	1:A:583:VAL:CG2	2.23	0.68
1:A:565:LEU:HD12	1:A:571:VAL:HG21	1.75	0.68
1:A:360:THR:HG22	1:A:362:GLU:H	1.58	0.68
1:A:690:THR:HG22	1:A:692:GLU:N	2.08	0.68
1:A:455:PHE:HB2	1:A:465:LEU:HD22	1.74	0.68
1:A:408:PRO:HD2	1:A:463:ARG:HH22	1.59	0.68
1:A:142:HIS:HB2	7:A:997:HOH:O	1.94	0.67
1:A:46:THR:C	1:A:48:ASP:H	1.97	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ASP:O	1:A:665:GLN:HG2	1.94	0.67
1:A:836:THR:OG1	1:A:839:LEU:HD22	1.95	0.67
1:A:317:LEU:O	1:A:341:GLN:HA	1.95	0.66
1:A:360:THR:CG2	1:A:362:GLU:HB2	2.25	0.66
1:A:315:ILE:HB	7:A:1114:HOH:O	1.95	0.66
1:A:438:ARG:HH22	1:A:439:ARG:HH21	1.43	0.66
1:A:783:LEU:O	1:A:785:GLU:N	2.29	0.66
1:A:522:THR:HG21	1:A:709:HIS:HD2	1.60	0.66
1:A:387:SER:OG	1:A:389:LEU:HD12	1.97	0.65
1:A:578:TRP:HB3	1:A:585:MET:HE3	1.77	0.65
1:A:764:LEU:HD22	7:A:1360:HOH:O	1.96	0.65
1:A:65:ALA:HB2	1:A:113:GLY:HA3	1.77	0.65
1:A:172:THR:HB	1:A:173:PRO:CD	2.27	0.65
1:A:734:MET:SD	7:A:1225:HOH:O	2.55	0.65
1:A:668:TRP:O	1:A:672:VAL:HG23	1.96	0.64
1:A:504:TYR:O	1:A:507:VAL:HG12	1.98	0.64
1:A:454:LEU:HB2	7:A:1248:HOH:O	1.97	0.64
1:A:166:THR:HB	1:A:545:LYS:HE3	1.80	0.64
1:A:446:LYS:HD2	1:A:733:PHE:CE2	2.33	0.63
1:A:441:ASN:HD21	1:A:447:ALA:H	1.47	0.63
1:A:51:THR:HA	1:A:54:LEU:HD22	1.81	0.62
1:A:547:LEU:HD21	7:A:1311:HOH:O	1.99	0.62
1:A:243:THR:HG23	1:A:246:ASP:H	1.65	0.61
1:A:604:LEU:HD21	1:A:630:THR:CG2	2.28	0.61
1:A:425:PHE:HB2	7:A:1248:HOH:O	1.99	0.61
1:A:18:LEU:HD21	1:A:99:PHE:HE2	1.65	0.61
1:A:394:TYR:CB	1:A:481:ALA:HB2	2.15	0.61
1:A:716:GLN:OE1	3:A:1859[A]:13S:H51	2.01	0.61
1:A:514:GLN:HE22	1:A:515:LEU:CD2	2.10	0.60
1:A:170:SER:C	1:A:172:THR:H	2.04	0.60
1:A:530:ILE:HB	7:A:1245:HOH:O	2.01	0.60
1:A:566:VAL:CG2	1:A:583:VAL:HG22	2.32	0.60
1:A:788:ASN:CB	1:A:789:PRO:HD3	2.17	0.60
1:A:583:VAL:HG23	7:A:1193:HOH:O	2.02	0.60
1:A:571:VAL:HB	7:A:935:HOH:O	2.01	0.60
1:A:300:GLU:HG2	7:A:1222:HOH:O	2.01	0.60
1:A:408:PRO:HD2	1:A:463:ARG:NH2	2.16	0.59
1:A:775:ARG:HG3	1:A:775:ARG:NH1	2.14	0.59
1:A:350:VAL:HG13	1:A:351:ILE:HG23	1.84	0.59
1:A:243:THR:CG2	1:A:246:ASP:H	2.16	0.59
1:A:565:LEU:HD21	3:A:1859[A]:13S:H152	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:HD13	1:A:857:ILE:HD13	1.83	0.58
1:A:360:THR:CG2	1:A:362:GLU:OE1	2.51	0.58
1:A:374:PRO:HD2	7:A:1210:HOH:O	2.02	0.58
1:A:857:ILE:O	3:A:1859[A]:13S:H162	2.02	0.58
1:A:360:THR:HG21	1:A:362:GLU:HB2	1.86	0.58
1:A:581:TYR:CB	1:A:585:MET:HE2	2.32	0.58
1:A:221:ARG:HG2	7:A:1191:HOH:O	2.03	0.58
1:A:734:MET:CE	1:A:735:PRO:HD2	2.31	0.58
1:A:576:PHE:HZ	3:A:1859[A]:13S:H41	1.68	0.58
1:A:588:VAL:O	1:A:591:LYS:HB2	2.04	0.58
1:A:410:LEU:HD21	1:A:457:LYS:HD2	1.86	0.57
1:A:766:ASP:O	1:A:770:ILE:HG12	2.05	0.57
1:A:104:GLU:HB2	7:A:1083:HOH:O	2.02	0.57
1:A:403:LYS:HB2	1:A:415:VAL:HG21	1.86	0.57
1:A:566:VAL:HG22	1:A:583:VAL:HG22	1.86	0.57
1:A:91:THR:O	1:A:92:LEU:O	2.23	0.57
1:A:530:ILE:HD12	7:A:1242:HOH:O	2.04	0.57
1:A:349:LYS:HA	1:A:352:GLN:HG3	1.86	0.57
1:A:578:TRP:HB3	1:A:585:MET:HE1	1.87	0.57
1:A:691:ARG:O	1:A:695:VAL:HG23	2.05	0.57
1:A:136:PRO:O	1:A:138:HIS:N	2.37	0.57
1:A:515:LEU:HD21	1:A:582:SER:HB3	1.87	0.57
1:A:561:ALA:HA	1:A:565:LEU:CD2	2.35	0.57
1:A:312:SER:O	1:A:344:LYS:HD3	2.05	0.57
1:A:514:GLN:HG2	1:A:576:PHE:CD1	2.39	0.56
1:A:843:LYS:O	1:A:844:GLU:CB	2.52	0.56
1:A:56:ARG:HG2	1:A:81:PHE:CE2	2.40	0.56
1:A:171:GLU:HA	1:A:180:ARG:HH11	1.71	0.56
1:A:9:GLY:O	1:A:10:HIS:HB2	2.03	0.56
1:A:441:ASN:HD22	1:A:446:LYS:HA	1.70	0.56
1:A:609:MET:O	1:A:623:VAL:HG22	2.05	0.56
1:A:221:ARG:HG3	1:A:222:PRO:HD2	1.87	0.56
1:A:326:SER:H	1:A:327:PRO:CD	2.18	0.56
1:A:729:LEU:O	1:A:729:LEU:HD22	2.05	0.56
1:A:611:ILE:HG13	1:A:621:ARG:HB3	1.87	0.56
1:A:190:ASP:OD1	1:A:191:GLY:N	2.39	0.56
1:A:338:ASP:HB3	1:A:342:ALA:HB3	1.86	0.55
1:A:87:THR:HG22	7:A:1022:HOH:O	2.06	0.55
1:A:290:SER:O	1:A:294:LEU:HB2	2.06	0.55
1:A:527:GLU:HG3	7:A:1245:HOH:O	2.05	0.55
1:A:302:ASP:HB2	1:A:306:GLU:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:SER:C	1:A:172:THR:N	2.59	0.55
1:A:239:GLY:N	7:A:1021:HOH:O	2.32	0.55
1:A:438:ARG:NH2	1:A:439:ARG:HE	2.05	0.55
1:A:514:GLN:NE2	1:A:515:LEU:CD2	2.67	0.55
1:A:566:VAL:HG22	1:A:583:VAL:HG21	1.87	0.55
1:A:572:ILE:HD11	3:A:1859[A]:13S:H71	1.87	0.55
1:A:729:LEU:HD21	1:A:758:THR:HA	1.89	0.55
1:A:496:SER:HB3	1:A:745:LEU:HD22	1.88	0.54
1:A:561:ALA:HA	1:A:565:LEU:HB2	1.88	0.54
1:A:173:PRO:HB2	1:A:176:LEU:HB2	1.89	0.54
1:A:348:PRO:HG2	1:A:351:ILE:HD12	1.88	0.54
1:A:137:ASN:HB3	7:A:1232:HOH:O	2.07	0.54
1:A:168:LEU:O	1:A:170:SER:N	2.40	0.54
1:A:172:THR:CB	1:A:173:PRO:HD3	2.38	0.54
1:A:330:VAL:C	1:A:332:LYS:H	2.10	0.54
1:A:171:GLU:HB2	1:A:177:VAL:HG22	1.88	0.54
1:A:844:GLU:HG2	1:A:845:GLY:N	2.23	0.54
1:A:151:ASN:OD1	1:A:153:LYS:HD2	2.08	0.54
1:A:313:GLY:O	1:A:344:LYS:HG2	2.08	0.54
1:A:319:THR:HG23	1:A:340:GLU:CD	2.27	0.54
1:A:160:ILE:HG21	1:A:183:GLU:HG3	1.91	0.53
1:A:387:SER:HG	1:A:389:LEU:HD12	1.72	0.53
1:A:328:LEU:N	1:A:328:LEU:HD23	2.24	0.53
1:A:410:LEU:HD23	1:A:463:ARG:NH1	2.23	0.53
1:A:57:SER:HB3	1:A:121:MET:HG2	1.90	0.53
1:A:514:GLN:HB2	3:A:1859[A]:13S:C6	2.37	0.53
1:A:169:PRO:HB2	1:A:662:PRO:HD2	1.91	0.53
1:A:423:ARG:NH1	1:A:456:LEU:O	2.42	0.53
1:A:827:ARG:O	1:A:834:PRO:HA	2.09	0.53
1:A:135:ILE:CG2	1:A:136:PRO:HD3	2.34	0.53
1:A:201:ILE:O	1:A:259:PRO:HG3	2.08	0.53
1:A:240:ARG:NH2	7:A:966:HOH:O	2.41	0.53
1:A:324:LYS:O	1:A:327:PRO:HD2	2.08	0.53
1:A:447:ALA:CB	1:A:577:LEU:HD11	2.36	0.53
1:A:10:HIS:CD2	1:A:11:LYS:N	2.77	0.53
1:A:565:LEU:HD12	1:A:571:VAL:CG2	2.38	0.53
1:A:785:GLU:HB2	1:A:805:GLY:HA3	1.90	0.53
1:A:441:ASN:ND2	1:A:446:LYS:HA	2.23	0.53
1:A:773:LEU:CD1	3:A:1859[A]:13S:H161	2.39	0.53
1:A:322:ILE:HG21	1:A:340:GLU:HG3	1.90	0.52
1:A:410:LEU:HD12	1:A:411:GLU:H	1.73	0.52

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:LEU:HD11	1:A:688:MET:HG3	1.91	0.52
1:A:743:GLU:O	1:A:747:LYS:HD3	2.09	0.52
1:A:775:ARG:HH11	1:A:846:LEU:HD13	1.71	0.52
1:A:133:GLU:HG2	7:A:1153:HOH:O	2.09	0.52
1:A:479:SER:HB2	7:A:1332:HOH:O	2.08	0.52
1:A:169:PRO:CG	1:A:662:PRO:HD2	2.40	0.52
1:A:58:VAL:HG23	7:A:1348:HOH:O	2.09	0.52
1:A:433:ILE:HD12	1:A:578:TRP:NE1	2.25	0.52
1:A:541:HIS:HD2	1:A:543:ILE:H	1.55	0.52
1:A:17:VAL:HG12	7:A:1011:HOH:O	2.09	0.52
1:A:750:GLN:O	1:A:754:LEU:HD22	2.09	0.52
1:A:169:PRO:C	1:A:171:GLU:N	2.62	0.52
1:A:235:ARG:NH1	1:A:238:THR:HG22	2.24	0.52
1:A:285:LEU:CB	1:A:286:PRO:HD3	2.39	0.52
1:A:29:VAL:O	1:A:269:SER:HB2	2.10	0.51
1:A:172:THR:O	1:A:173:PRO:C	2.48	0.51
1:A:353:VAL:HG11	1:A:832:GLN:OE1	2.10	0.51
1:A:307:VAL:O	1:A:310:LEU:HB2	2.11	0.51
1:A:46:THR:O	1:A:48:ASP:N	2.42	0.51
1:A:134:ASP:CG	1:A:135:ILE:H	2.14	0.51
1:A:159:ARG:NH1	7:A:1139:HOH:O	2.44	0.51
1:A:360:THR:HG22	1:A:362:GLU:HB2	1.91	0.51
1:A:502:LYS:CB	7:A:1283:HOH:O	2.49	0.51
1:A:90:PRO:HB2	7:A:1246:HOH:O	2.11	0.51
1:A:455:PHE:HB2	1:A:465:LEU:CD2	2.41	0.51
1:A:576:PHE:CZ	3:A:1859[A]:13S:H41	2.44	0.51
1:A:171:GLU:HA	1:A:180:ARG:NH1	2.26	0.51
1:A:769:VAL:O	1:A:773:LEU:HD13	2.11	0.51
1:A:393:VAL:HG12	1:A:393:VAL:O	2.11	0.51
1:A:514:GLN:OE1	1:A:515:LEU:HD22	2.10	0.51
1:A:238:THR:HG21	7:A:966:HOH:O	2.10	0.51
1:A:433:ILE:HD12	1:A:578:TRP:CD1	2.46	0.51
1:A:53:PHE:HA	7:A:1348:HOH:O	2.09	0.51
1:A:660:GLU:O	1:A:662:PRO:HD3	2.11	0.51
1:A:677:GLY:O	1:A:680:LYS:HG2	2.11	0.51
1:A:168:LEU:C	1:A:170:SER:H	2.14	0.50
1:A:499:LEU:HA	7:A:1283:HOH:O	2.10	0.50
1:A:523:HIS:HE1	1:A:557:ILE:HD12	1.77	0.50
1:A:581:TYR:HB2	1:A:585:MET:CE	2.38	0.50
1:A:393:VAL:H	1:A:479:SER:HA	1.76	0.50
1:A:399:SER:HB2	1:A:468:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD13	7:A:1054:HOH:O	2.12	0.50
1:A:516:VAL:HG13	1:A:520:LEU:HD23	1.94	0.50
1:A:393:VAL:HB	1:A:479:SER:HA	1.92	0.50
1:A:522:THR:HG23	1:A:855:ILE:CD1	2.42	0.50
1:A:568:ASP:O	1:A:573:GLU:OE1	2.30	0.50
1:A:729:LEU:CD2	1:A:758:THR:HA	2.42	0.50
1:A:278:LYS:O	1:A:282:GLN:HG3	2.11	0.50
1:A:300:GLU:HG3	7:A:1115:HOH:O	2.09	0.50
1:A:493:VAL:HG21	1:A:746:ARG:HH11	1.77	0.50
1:A:236:GLY:N	1:A:527:GLU:OE2	2.42	0.50
1:A:315:ILE:HG12	1:A:315:ILE:O	2.11	0.50
1:A:317:LEU:HG	1:A:318:PRO:HD2	1.93	0.50
1:A:438:ARG:NH2	1:A:439:ARG:NE	2.60	0.50
1:A:134:ASP:OD2	1:A:138:HIS:HB3	2.12	0.49
1:A:609:MET:HA	1:A:623:VAL:CG2	2.42	0.49
1:A:433:ILE:HG12	1:A:437:LEU:HD13	1.93	0.49
1:A:207:TYR:CD1	1:A:232:TYR:HD2	2.30	0.49
1:A:356:SER:O	1:A:359:MET:HG3	2.12	0.49
1:A:434:MET:HB3	1:A:435:PRO:CD	2.41	0.49
1:A:489:ALA:CB	1:A:494:GLU:HB3	2.42	0.49
1:A:505:VAL:O	1:A:508:ASN:HB2	2.13	0.49
1:A:710:ALA:HA	1:A:714:PHE:HD2	1.76	0.49
1:A:618:HIS:HE1	1:A:635:GLU:OE2	1.95	0.49
1:A:626:ASP:CB	7:A:1190:HOH:O	2.60	0.49
1:A:172:THR:CB	1:A:173:PRO:CD	2.90	0.49
1:A:273:LEU:HD13	1:A:857:ILE:CD1	2.42	0.49
1:A:315:ILE:HD11	1:A:317:LEU:HD13	1.94	0.49
1:A:360:THR:HG22	1:A:362:GLU:OE1	2.13	0.49
1:A:499:LEU:C	7:A:1283:HOH:O	2.51	0.49
1:A:729:LEU:CD1	1:A:758:THR:HG23	2.40	0.48
1:A:474:PRO:C	1:A:475:GLN:HG3	2.33	0.48
1:A:775:ARG:NH1	1:A:775:ARG:CG	2.77	0.48
1:A:631:VAL:HG12	1:A:818:ARG:CZ	2.42	0.48
1:A:169:PRO:HD3	1:A:541:HIS:HE1	1.76	0.48
1:A:522:THR:HG23	1:A:855:ILE:HG12	1.94	0.48
1:A:761:PHE:CE2	1:A:765:ILE:HD11	2.49	0.48
1:A:857:ILE:HG13	3:A:1859[A]:13S:H183	1.94	0.48
1:A:304:PHE:H	1:A:750:GLN:HE21	1.61	0.48
1:A:365:ALA:O	1:A:368:MET:HB2	2.14	0.48
1:A:791:TRP:CD1	1:A:791:TRP:N	2.81	0.48
1:A:148:TRP:HB3	7:A:1385:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:HG2	7:A:915:HOH:O	2.13	0.48
1:A:169:PRO:CB	1:A:662:PRO:HD2	2.44	0.47
1:A:206:VAL:CG1	1:A:207:TYR:N	2.76	0.47
1:A:623:VAL:O	1:A:624:ILE:HB	2.13	0.47
1:A:192:THR:O	1:A:195:ARG:NH2	2.47	0.47
1:A:208:ASN:HD22	1:A:208:ASN:H	1.61	0.47
1:A:174:ALA:HB3	1:A:175:PRO:HD3	1.96	0.47
1:A:208:ASN:ND2	1:A:235:ARG:HH21	2.12	0.47
1:A:260:ARG:O	1:A:261:ASP:CB	2.58	0.47
1:A:557:ILE:HB	7:A:1166:HOH:O	2.14	0.47
1:A:233:PRO:HB3	1:A:676:HIS:CE1	2.50	0.47
1:A:362:GLU:HB3	7:A:1202:HOH:O	2.15	0.47
1:A:516:VAL:HA	1:A:520:LEU:HB3	1.97	0.47
1:A:836:THR:OG1	1:A:849:ARG:HB3	2.15	0.47
1:A:560:LEU:HD23	1:A:565:LEU:CD2	2.44	0.47
1:A:273:LEU:HD12	7:A:1207:HOH:O	2.13	0.47
1:A:403:LYS:HD3	1:A:403:LYS:H	1.80	0.47
1:A:441:ASN:ND2	1:A:447:ALA:H	2.11	0.47
1:A:575:THR:HG21	1:A:766:ASP:HB2	1.97	0.47
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.78	0.47
1:A:473:HIS:HB3	1:A:477:ASP:HA	1.97	0.47
1:A:243:THR:HG22	1:A:246:ASP:C	2.32	0.46
1:A:206:VAL:HG11	1:A:223:VAL:CG2	2.45	0.46
1:A:751:LYS:HD2	1:A:755:LYS:HG3	1.97	0.46
1:A:410:LEU:CD1	1:A:411:GLU:H	2.27	0.46
1:A:729:LEU:HD22	1:A:729:LEU:C	2.36	0.46
1:A:831:VAL:CG1	1:A:833:MET:HB2	2.44	0.46
1:A:775:ARG:HG3	1:A:846:LEU:HD13	1.97	0.46
1:A:717:TYR:O	1:A:721:GLY:N	2.49	0.46
1:A:151:ASN:O	1:A:154:LEU:HD12	2.16	0.46
1:A:522:THR:HG22	1:A:523:HIS:H	1.77	0.46
1:A:631:VAL:HG12	1:A:818:ARG:NH1	2.31	0.46
1:A:348:PRO:O	1:A:351:ILE:HD13	2.16	0.46
1:A:351:ILE:HG21	1:A:722:LEU:HG	1.98	0.46
1:A:622:LEU:HD21	1:A:630:THR:CG2	2.42	0.46
1:A:857:ILE:O	3:A:1859[A]:13S:O22	2.33	0.46
1:A:496:SER:HB3	1:A:745:LEU:CD2	2.45	0.45
1:A:438:ARG:HG3	1:A:438:ARG:H	1.48	0.45
1:A:522:THR:CG2	1:A:523:HIS:N	2.76	0.45
1:A:609:MET:C	1:A:623:VAL:HG22	2.36	0.45
1:A:672:VAL:HG11	7:A:1026:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:VAL:O	1:A:332:LYS:N	2.49	0.45
1:A:427:LEU:HD13	1:A:429:HIS:CD2	2.51	0.45
1:A:612:GLU:HB2	7:A:1285:HOH:O	2.15	0.45
1:A:781:VAL:HG13	1:A:786:ARG:HG2	1.98	0.45
1:A:561:ALA:HA	1:A:565:LEU:HD23	1.98	0.45
1:A:76:LEU:N	1:A:76:LEU:HD12	2.32	0.45
1:A:150:TYR:HB2	1:A:155:PHE:HZ	1.82	0.45
1:A:133:GLU:O	1:A:134:ASP:O	2.35	0.45
1:A:296:PHE:HB3	1:A:318:PRO:HD3	1.98	0.45
1:A:390:ASP:HB3	1:A:391:SER:H	1.58	0.45
1:A:513:HIS:HA	1:A:517:SER:HB2	1.98	0.45
1:A:847:THR:C	1:A:849:ARG:H	2.21	0.45
1:A:168:LEU:C	1:A:170:SER:N	2.70	0.45
1:A:564:SER:O	1:A:571:VAL:HG22	2.17	0.45
1:A:46:THR:HG22	1:A:47:LEU:N	2.32	0.44
1:A:434:MET:HB3	1:A:435:PRO:HD3	1.98	0.44
1:A:500:LEU:HD12	1:A:753:TYR:HD1	1.81	0.44
1:A:20:ARG:O	1:A:23:VAL:HB	2.17	0.44
1:A:690:THR:HB	1:A:693:GLU:HG3	2.00	0.44
1:A:362:GLU:H	1:A:362:GLU:CD	2.21	0.44
1:A:457:LYS:HB2	1:A:459:ASP:OD1	2.18	0.44
1:A:506:VAL:CG1	1:A:727:PRO:HD2	2.47	0.44
1:A:781:VAL:HG12	1:A:853:ASN:ND2	2.32	0.44
1:A:781:VAL:HG12	1:A:786:ARG:HB3	1.99	0.44
1:A:258:LEU:HD12	1:A:262:GLU:HB2	1.99	0.44
1:A:438:ARG:NH2	1:A:439:ARG:HH21	2.12	0.44
1:A:277:LEU:CD2	3:A:1859[A]:13S:H182	2.43	0.44
1:A:360:THR:HG22	1:A:362:GLU:CD	2.38	0.44
1:A:530:ILE:HG12	1:A:551:TYR:CD1	2.53	0.44
1:A:600:LEU:HD23	1:A:634:LEU:HD13	1.99	0.44
1:A:168:LEU:HB3	1:A:169:PRO:HD2	1.99	0.44
1:A:208:ASN:HD21	1:A:235:ARG:NH2	2.16	0.44
1:A:788:ASN:CB	1:A:789:PRO:CD	2.87	0.44
1:A:67:LYS:HG2	1:A:108:GLY:O	2.18	0.44
1:A:29:VAL:HG13	1:A:32:VAL:HB	2.00	0.44
1:A:92:LEU:HB3	1:A:93:GLY:H	1.55	0.44
1:A:351:ILE:HB	1:A:355:LYS:HA	2.00	0.44
1:A:403:LYS:NZ	1:A:404:GLU:HG2	2.33	0.44
1:A:332:LYS:O	1:A:334:ILE:N	2.44	0.43
1:A:626:ASP:O	1:A:628:PRO:HD3	2.18	0.43
1:A:370:ALA:HB2	1:A:628:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:GLU:HB2	1:A:805:GLY:CA	2.47	0.43
1:A:561:ALA:HA	1:A:565:LEU:HD22	2.00	0.43
1:A:626:ASP:HB2	7:A:1190:HOH:O	2.17	0.43
1:A:664:LEU:HD22	7:A:1259:HOH:O	2.19	0.43
1:A:819:ASN:HD21	1:A:827:ARG:HH21	1.67	0.43
1:A:785:GLU:CB	1:A:805:GLY:HA3	2.47	0.43
1:A:581:TYR:O	1:A:585:MET:HG3	2.19	0.43
1:A:349:LYS:HB3	1:A:833:MET:CE	2.48	0.43
1:A:609:MET:HA	1:A:623:VAL:HG22	2.00	0.43
1:A:155:PHE:O	1:A:156:LYS:HB2	2.19	0.43
1:A:331:LEU:HD12	1:A:335:PHE:CZ	2.53	0.43
1:A:781:VAL:CG1	1:A:786:ARG:HB3	2.48	0.43
1:A:29:VAL:O	1:A:29:VAL:HG12	2.19	0.43
1:A:206:VAL:HG12	1:A:207:TYR:N	2.32	0.43
1:A:18:LEU:C	1:A:18:LEU:HD23	2.39	0.43
1:A:257:TYR:CD1	1:A:257:TYR:C	2.92	0.42
1:A:169:PRO:O	1:A:171:GLU:CG	2.63	0.42
1:A:178:LYS:O	1:A:182:GLU:HB2	2.19	0.42
1:A:232:TYR:CG	1:A:233:PRO:HD2	2.54	0.42
1:A:384:PRO:HD2	1:A:398:THR:CG2	2.43	0.42
1:A:717:TYR:HB3	1:A:718:PRO:HD3	2.01	0.42
1:A:171:GLU:CD	1:A:180:ARG:HD3	2.40	0.42
1:A:189:GLY:O	1:A:190:ASP:HB3	2.18	0.42
1:A:653:LYS:HG3	7:A:932:HOH:O	2.18	0.42
1:A:170:SER:HB2	7:A:992:HOH:O	2.18	0.42
1:A:178:LYS:HB2	7:A:1027:HOH:O	2.18	0.42
1:A:190:ASP:CG	1:A:191:GLY:N	2.73	0.42
1:A:669:LYS:HE2	1:A:673:GLU:OE2	2.19	0.42
1:A:773:LEU:HD11	3:A:1859[A]:13S:H161	2.02	0.42
1:A:785:GLU:OE1	1:A:802:LYS:HD3	2.19	0.42
1:A:360:THR:HG22	1:A:362:GLU:CB	2.49	0.42
1:A:501:ALA:N	7:A:1225:HOH:O	2.51	0.42
1:A:80:THR:HB	1:A:101:ILE:HD11	2.02	0.42
1:A:160:ILE:HD13	1:A:162:PHE:CZ	2.55	0.42
1:A:171:GLU:CB	1:A:180:ARG:HD3	2.49	0.42
1:A:243:THR:CG2	1:A:246:ASP:N	2.81	0.42
1:A:282:GLN:HG2	7:A:1182:HOH:O	2.19	0.42
1:A:729:LEU:CD2	1:A:729:LEU:C	2.88	0.42
1:A:761:PHE:HD2	1:A:762:GLN:OE1	2.02	0.42
1:A:438:ARG:HE	1:A:438:ARG:HB2	1.68	0.42
1:A:469:LEU:HD12	1:A:486:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:THR:HG22	7:A:1242:HOH:O	2.19	0.42
1:A:310:LEU:HD12	1:A:310:LEU:HA	1.87	0.42
1:A:618:HIS:HB2	7:A:1125:HOH:O	2.18	0.42
1:A:710:ALA:HA	1:A:714:PHE:CD2	2.54	0.42
1:A:857:ILE:CD1	3:A:1859[A]:13S:H183	2.50	0.42
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.86	0.42
1:A:160:ILE:HG22	1:A:183:GLU:HG3	1.98	0.42
1:A:174:ALA:N	1:A:175:PRO:CD	2.83	0.42
1:A:324:LYS:O	1:A:328:LEU:HD22	2.20	0.42
1:A:462:LEU:HD11	7:A:1248:HOH:O	2.20	0.42
1:A:204:TYR:CD1	1:A:674:VAL:HG11	2.55	0.41
1:A:240:ARG:HD3	1:A:253:SER:HB2	2.00	0.41
1:A:195:ARG:HD3	1:A:195:ARG:HA	1.79	0.41
1:A:467:ILE:HD11	1:A:502:LYS:HG2	2.02	0.41
1:A:46:THR:C	1:A:48:ASP:N	2.67	0.41
1:A:171:GLU:OE1	1:A:181:GLU:HG2	2.20	0.41
1:A:360:THR:HG22	1:A:362:GLU:N	2.31	0.41
1:A:636:ILE:HD12	1:A:838:LEU:HG	2.02	0.41
1:A:486:PHE:C	1:A:487:LEU:HD12	2.40	0.41
1:A:258:LEU:HD11	1:A:263:ALA:HB2	2.02	0.41
1:A:414:THR:OG1	1:A:417:GLU:HB2	2.20	0.41
1:A:775:ARG:HG3	1:A:846:LEU:CD1	2.50	0.41
1:A:499:LEU:CA	7:A:1283:HOH:O	2.66	0.41
1:A:685:TRP:HB2	7:A:1265:HOH:O	2.20	0.41
1:A:836:THR:HG1	1:A:839:LEU:HD22	1.85	0.41
1:A:69:ASP:CG	1:A:70:ALA:N	2.73	0.41
1:A:208:ASN:HD22	1:A:208:ASN:N	2.16	0.41
1:A:206:VAL:CG1	1:A:223:VAL:CG2	2.99	0.41
1:A:636:ILE:HD13	1:A:851:ILE:CD1	2.51	0.41
1:A:74:GLY:H	1:A:179:TYR:HE2	1.69	0.41
1:A:171:GLU:HB3	1:A:180:ARG:HD3	2.03	0.41
1:A:565:LEU:HD21	3:A:1859[A]:13S:C15	2.50	0.41
1:A:636:ILE:HD11	1:A:838:LEU:O	2.21	0.41
1:A:277:LEU:CG	3:A:1859[A]:13S:H182	2.51	0.41
1:A:433:ILE:HD12	1:A:578:TRP:HE1	1.86	0.41
1:A:698:CYS:O	1:A:702:ILE:HG13	2.21	0.41
1:A:759:PRO:HG2	1:A:762:GLN:NE2	2.36	0.40
1:A:340:GLU:HG3	1:A:341:GLN:H	1.86	0.40
1:A:425:PHE:HE1	1:A:456:LEU:HB2	1.85	0.40
1:A:717:TYR:N	1:A:718:PRO:CD	2.85	0.40
1:A:857:ILE:HD11	3:A:1859[A]:13S:H183	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:TRP:CB	1:A:585:MET:HE1	2.51	0.40
1:A:833:MET:C	7:A:1374:HOH:O	2.60	0.40
1:A:311:TYR:HA	1:A:345:PHE:O	2.21	0.40
1:A:522:THR:CG2	1:A:855:ILE:HG12	2.52	0.40
1:A:600:LEU:HG	1:A:604:LEU:HD22	2.03	0.40
1:A:616:CYS:HB3	1:A:617:PRO:HD2	2.03	0.40
1:A:788:ASN:OD1	1:A:788:ASN:N	2.54	0.40
1:A:329:PRO:O	1:A:330:VAL:HB	2.21	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	832/857 (97%)	730 (88%)	66 (8%)	36 (4%)	2	0

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	134	ASP
1	A	172	THR
1	A	270	SER
1	A	390	ASP
1	A	398	THR
1	A	409	ASN
1	A	410	LEU
1	A	473	HIS
1	A	737	LYS
1	A	784	GLY
1	A	789	PRO
1	A	844	GLU

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Mol	Chain	Res	Type
1	A	48	ASP
1	A	55	GLY
1	A	72	GLY
1	A	137	ASN
1	A	411	GLU
1	A	477	ASP
1	A	568	ASP
1	A	135	ILE
1	A	261	ASP
1	A	295	ASN
1	A	326	SER
1	A	331	LEU
1	A	341	GLN
1	A	788	ASN
1	A	69	ASP
1	A	169	PRO
1	A	101	ILE
1	A	624	ILE
1	A	492	GLY
1	A	325	ILE
1	A	570	GLY
1	A	407	GLU
1	A	173	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	735/749 (98%)	609 (83%)	126 (17%)	2	1

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	28	SER
1	A	31	SER

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Mol	Chain	Res	Type
1	A	47	LEU
1	A	48	ASP
1	A	49	THR
1	A	54	LEU
1	A	56	ARG
1	A	57	SER
1	A	67	LYS
1	A	69	ASP
1	A	78	LYS
1	A	80	THR
1	A	83	GLU
1	A	92	LEU
1	A	104	GLU
1	A	109	SER
1	A	122	GLN
1	A	135	ILE
1	A	154	LEU
1	A	157	SER
1	A	164	ASN
1	A	165	GLN
1	A	176	LEU
1	A	181	GLU
1	A	183	GLU
1	A	184	LEU
1	A	187	LEU
1	A	190	ASP
1	A	195	ARG
1	A	208	ASN
1	A	209	ASP
1	A	210	LEU
1	A	218	ASN
1	A	221	ARG
1	A	224	LEU
1	A	232	TYR
1	A	241	LYS
1	A	243	THR
1	A	249	SER
1	A	252	ARG
1	A	257	TYR
1	A	258	LEU
1	A	270	SER
1	A	277	LEU

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Mol	Chain	Res	Type
1	A	282	GLN
1	A	285	LEU
1	A	297	THR
1	A	300	GLU
1	A	310	LEU
1	A	320	ASP
1	A	324	LYS
1	A	334	ILE
1	A	340	GLU
1	A	349	LYS
1	A	351	ILE
1	A	355	LYS
1	A	362	GLU
1	A	366	ARG
1	A	376	LEU
1	A	382	ASP
1	A	386	ARG
1	A	390	ASP
1	A	403	LYS
1	A	405	HIS
1	A	406	LEU
1	A	410	LEU
1	A	411	GLU
1	A	414	THR
1	A	416	ASP
1	A	427	LEU
1	A	434	MET
1	A	438	ARG
1	A	444	SER
1	A	452	THR
1	A	458	ASN
1	A	473	HIS
1	A	475	GLN
1	A	478	GLN
1	A	482	PHE
1	A	483	SER
1	A	485	VAL
1	A	493	VAL
1	A	508	ASN
1	A	515	LEU
1	A	525	VAL
1	A	537	LEU

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Mol	Chain	Res	Type
1	A	540	VAL
1	A	547	LEU
1	A	553	ASP
1	A	557	ILE
1	A	560	LEU
1	A	564	SER
1	A	565	LEU
1	A	571	VAL
1	A	594	VAL
1	A	604	LEU
1	A	621	ARG
1	A	626	ASP
1	A	627	TYR
1	A	634	LEU
1	A	638	ASP
1	A	679	LYS
1	A	688	MET
1	A	713	ASN
1	A	722	LEU
1	A	724	LEU
1	A	726	ARG
1	A	729	LEU
1	A	745	LEU
1	A	747	LYS
1	A	754	LEU
1	A	775	ARG
1	A	785	GLU
1	A	786	ARG
1	A	787	ASP
1	A	788	ASN
1	A	795	THR
1	A	798	LEU
1	A	799	GLU
1	A	808	LEU
1	A	822	GLU
1	A	825	ARG
1	A	833	MET
1	A	837	LEU
1	A	838	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	96	GLN
1	A	164	ASN
1	A	208	ASN
1	A	218	ASN
1	A	219	HIS
1	A	289	GLN
1	A	441	ASN
1	A	458	ASN
1	A	473	HIS
1	A	484	GLN
1	A	521	ASN
1	A	534	ASN
1	A	541	HIS
1	A	556	ASN
1	A	618	HIS
1	A	645	HIS
1	A	665	GLN
1	A	681	ASN
1	A	725	ASN
1	A	750	GLN
1	A	806	ASN
1	A	813	ASN
1	A	819	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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
4	13R	A	1860[B]	2	20,21,21	3.21	3 (15%)	19,22,22	1.19	2 (10%)
5	9OH	A	1861[C]	2	21,22,22	0.91	1 (4%)	22,26,26	2.17	3 (13%)
3	13S	A	1859[A]	2	20,21,21	3.30	5 (25%)	19,22,22	1.09	1 (5%)
6	11O	A	1862[D]	1	22,22,22	0.97	1 (4%)	23,26,26	0.99	2 (8%)

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
4	13R	A	1860[B]	2	-	12/19/21/21	-
5	9OH	A	1861[C]	2	-	13/20/25/25	0/1/1/1
3	13S	A	1859[A]	2	-	12/19/21/21	-
6	11O	A	1862[D]	1	-	9/21/26/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1859[A]	13S	O22-O21	-13.48	1.22	1.46
4	A	1860[B]	13R	O22-O21	-13.48	1.22	1.46
3	A	1859[A]	13S	C14-C13	3.76	1.57	1.52
4	A	1860[B]	13R	C11-C10	-2.97	1.35	1.44
6	A	1862[D]	11O	C12-C13	2.82	1.50	1.46
3	A	1859[A]	13S	C10-C9	2.31	1.41	1.33
4	A	1860[B]	13R	O20-C1	-2.25	1.23	1.30
3	A	1859[A]	13S	C11-C10	-2.13	1.38	1.44
3	A	1859[A]	13S	O20-C1	-2.08	1.23	1.30
5	A	1861[C]	9OH	O22-C12	2.07	1.50	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1861[C]	9OH	O22-C13-C14	6.80	126.90	116.57
5	A	1861[C]	9OH	O22-C12-C11	5.52	129.06	115.37
5	A	1861[C]	9OH	O21-C9-C8	-4.50	100.08	109.22
3	A	1859[A]	13S	C15-C14-C13	-3.63	109.64	114.31
4	A	1860[B]	13R	C15-C14-C13	-3.07	110.36	114.31
6	A	1862[D]	11O	O22-C13-C14	-2.89	112.17	116.57
6	A	1862[D]	11O	C12-O22-C13	2.63	62.28	60.59
4	A	1860[B]	13R	O20-C1-C2	2.05	120.63	114.03

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1859[A]	13S	C12-C13-C14-C15
3	A	1859[A]	13S	O21-C13-C14-C15
4	A	1860[B]	13R	C11-C12-C13-O21
4	A	1860[B]	13R	C12-C13-C14-C15
4	A	1860[B]	13R	O21-C13-C14-C15
5	A	1861[C]	9OH	C7-C8-C9-C10
5	A	1861[C]	9OH	C7-C8-C9-O21
5	A	1861[C]	9OH	C11-C10-C9-C8
5	A	1861[C]	9OH	C11-C10-C9-O21
5	A	1861[C]	9OH	C10-C11-C12-O22
5	A	1861[C]	9OH	C1-C2-C3-C4
6	A	1862[D]	11O	C1-C2-C3-C4
3	A	1859[A]	13S	C1-C2-C3-C4
5	A	1861[C]	9OH	C5-C6-C7-C8
5	A	1861[C]	9OH	C14-C15-C16-C17
3	A	1859[A]	13S	C6-C7-C8-C9
3	A	1859[A]	13S	C2-C3-C4-C5
3	A	1859[A]	13S	C3-C4-C5-C6
4	A	1860[B]	13R	C2-C3-C4-C5
5	A	1861[C]	9OH	C2-C3-C4-C5
4	A	1860[B]	13R	C5-C6-C7-C8
6	A	1862[D]	11O	C2-C3-C4-C5
4	A	1860[B]	13R	C6-C7-C8-C9
6	A	1862[D]	11O	C5-C6-C7-C8
3	A	1859[A]	13S	C11-C12-C13-O21
4	A	1860[B]	13R	C15-C16-C17-C18
6	A	1862[D]	11O	O22-C13-C14-C15
3	A	1859[A]	13S	C11-C12-C13-C14
4	A	1860[B]	13R	C11-C12-C13-C14
4	A	1860[B]	13R	C13-C14-C15-C16

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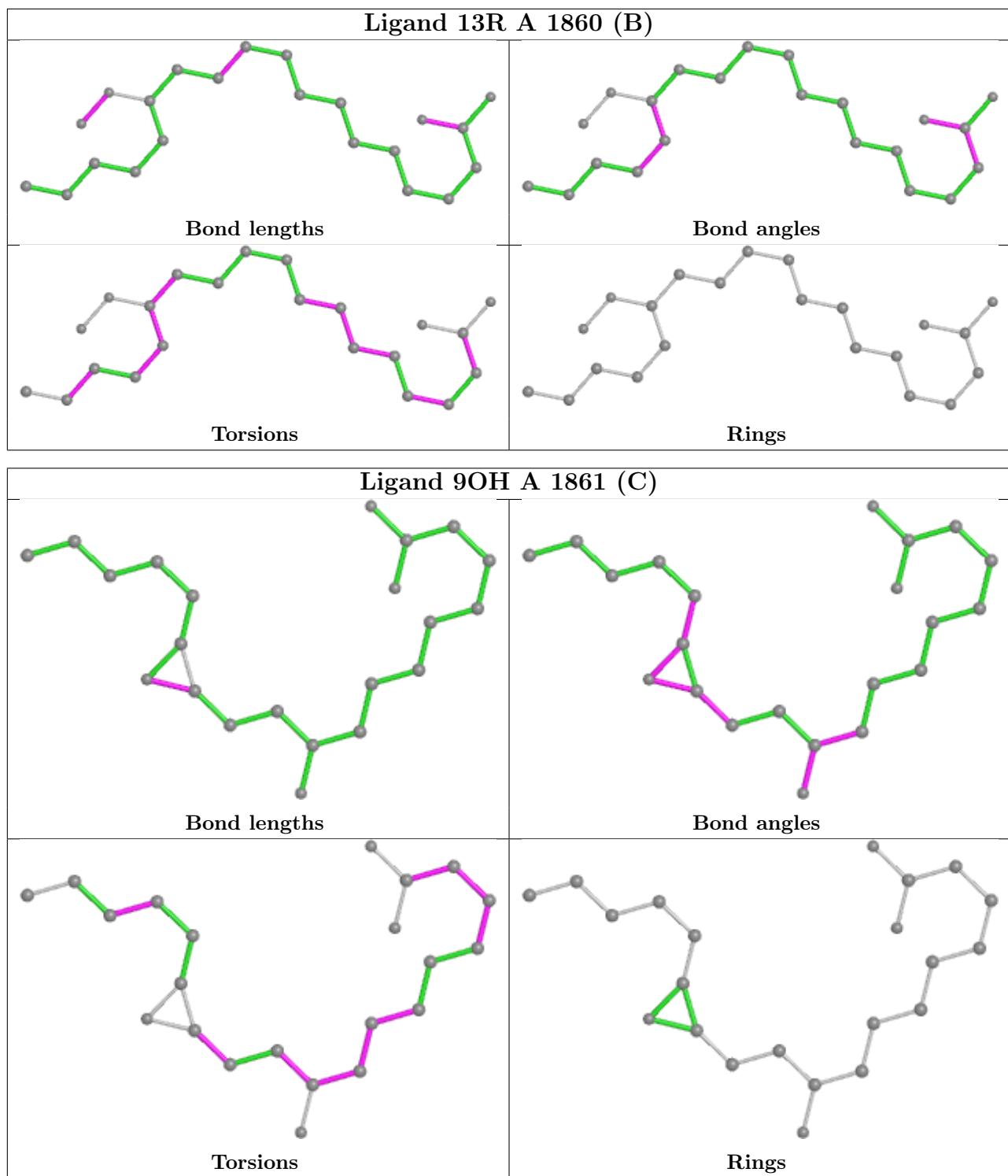
Mol	Chain	Res	Type	Atoms
3	A	1859[A]	13S	C13-C14-C15-C16
6	A	1862[D]	11O	C4-C5-C6-C7
3	A	1859[A]	13S	C15-C16-C17-C18
6	A	1862[D]	11O	C3-C4-C5-C6
5	A	1861[C]	9OH	C6-C7-C8-C9
6	A	1862[D]	11O	O19-C1-C2-C3
4	A	1860[B]	13R	C4-C5-C6-C7
6	A	1862[D]	11O	O20-C1-C2-C3
3	A	1859[A]	13S	O19-C1-C2-C3
6	A	1862[D]	11O	C7-C8-C9-C10
5	A	1861[C]	9OH	O20-C1-C2-C3
3	A	1859[A]	13S	O20-C1-C2-C3
4	A	1860[B]	13R	O19-C1-C2-C3
4	A	1860[B]	13R	O20-C1-C2-C3
5	A	1861[C]	9OH	O19-C1-C2-C3
5	A	1861[C]	9OH	C10-C11-C12-C13
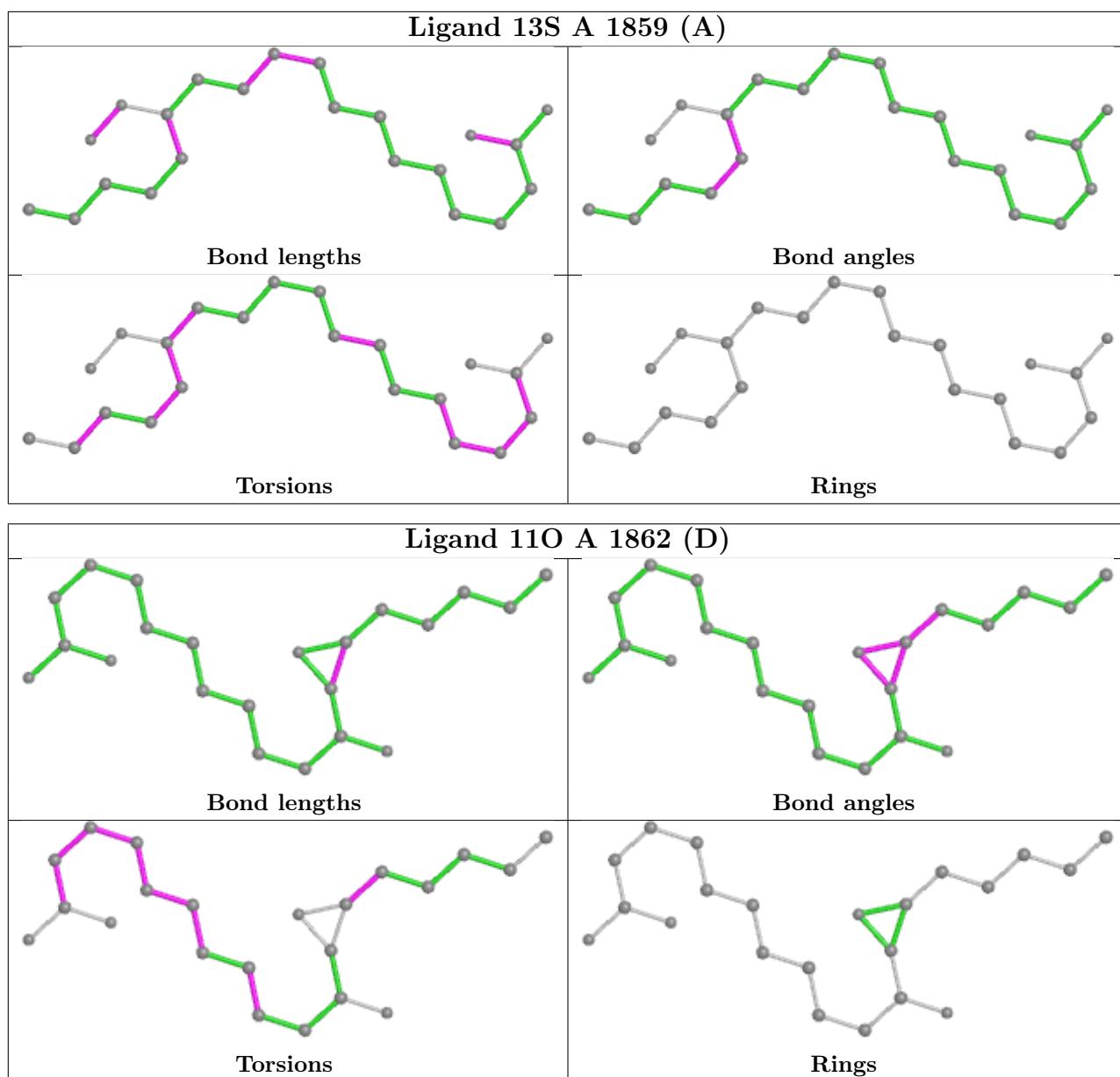
There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1859[A]	13S	20	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 then 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 13R A 1860 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 9OH A 1861 (C)

Bond lengths

Bond angles

Torsions

Rings

Ligand 13S A 1859 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand 11O A 1862 (D)

Bond lengths

Bond angles

Torsions

Rings

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	836/857 (97%)	-0.20	28 (3%)	46	45	11, 29, 74, 100	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	VAL	6.8
1	A	31	SER	4.8
1	A	46	THR	4.5
1	A	410	LEU	4.4
1	A	296	PHE	4.4
1	A	409	ASN	4.1
1	A	135	ILE	4.0
1	A	47	LEU	3.8
1	A	9	GLY	3.8
1	A	29	VAL	3.5
1	A	397	HIS	3.4
1	A	395	GLY	3.1
1	A	396	ASP	3.0
1	A	333	GLU	2.9
1	A	408	PRO	2.8
1	A	341	GLN	2.6
1	A	70	ALA	2.4
1	A	339	GLY	2.4
1	A	338	ASP	2.4
1	A	790	ASN	2.2
1	A	136	PRO	2.2
1	A	71	ASN	2.1
1	A	326	SER	2.1
1	A	334	ILE	2.1
1	A	737	LYS	2.0
1	A	340	GLU	2.0
1	A	480	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	30	THR	2.0

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

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

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

LIGAND-RSR INFOmissingINFO

6.5　Other polymers ⓘ

There are no such residues in this entry.