



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 01:25 am BST

PDB ID : 3V99
Title : S663D Stable-5-LOX in complex with Arachidonic Acid
Authors : Gilbert, N.C.; Rui, Z.; Neau, D.B.; Waight, M.; Bartlett, S.G.; Boeglin, W.E.;
Brash, A.R.; Newcomer, M.E.
Deposited on : 2011-12-23
Resolution : 2.25 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

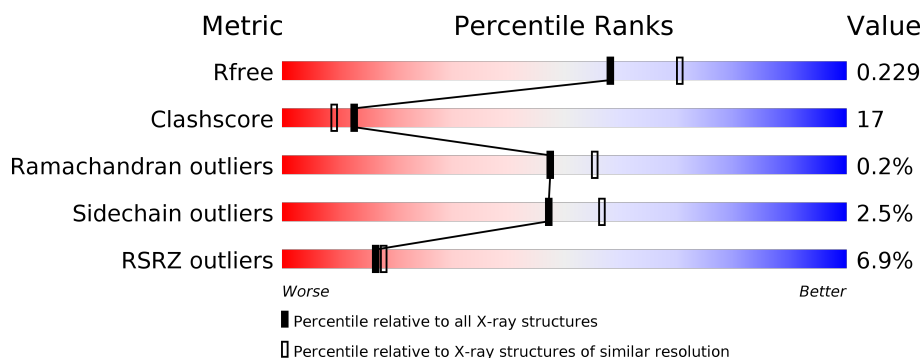
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 on 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	691	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>• 9%</div> </div> </div>
1	B	691	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>• 8%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10799 atoms, of which 31 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 Arachidonate 5-lipoxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	630	Total	C	N	O	S	0	2	0
			5147	3305	867	953	22			
1	B	639	Total	C	N	O	S	0	0	0
			5205	3336	889	958	22			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	EXPRESSION TAG	UNP P09917
A	-16	GLY	-	EXPRESSION TAG	UNP P09917
A	-15	SER	-	EXPRESSION TAG	UNP P09917
A	-14	SER	-	EXPRESSION TAG	UNP P09917
A	-13	HIS	-	EXPRESSION TAG	UNP P09917
A	-12	HIS	-	EXPRESSION TAG	UNP P09917
A	-11	HIS	-	EXPRESSION TAG	UNP P09917
A	-10	HIS	-	EXPRESSION TAG	UNP P09917
A	-9	HIS	-	EXPRESSION TAG	UNP P09917
A	-8	HIS	-	EXPRESSION TAG	UNP P09917
A	-7	SER	-	EXPRESSION TAG	UNP P09917
A	-6	SER	-	EXPRESSION TAG	UNP P09917
A	-5	GLY	-	EXPRESSION TAG	UNP P09917
A	-4	LEU	-	EXPRESSION TAG	UNP P09917
A	-3	VAL	-	EXPRESSION TAG	UNP P09917
A	-2	PRO	-	EXPRESSION TAG	UNP P09917
A	-1	ARG	-	EXPRESSION TAG	UNP P09917
A	0	GLY	-	EXPRESSION TAG	UNP P09917
A	1	SER	-	EXPRESSION TAG	UNP P09917
A	2	HIS	-	EXPRESSION TAG	UNP P09917
A	16	GLU	TRP	ENGINEERED MUTATION	UNP P09917
A	17	HIS	PHE	ENGINEERED MUTATION	UNP P09917
A	43	GLY	ASN	SEE REMARK 999	UNP P09917
A	44	SER	ASP	SEE REMARK 999	UNP P09917
A	75	GLY	TRP	ENGINEERED MUTATION	UNP P09917

Continued on next page...

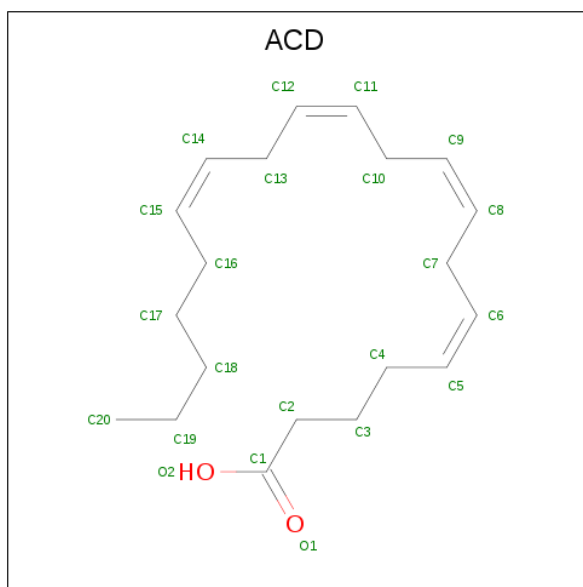
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	SER	LEU	ENGINEERED MUTATION	UNP P09917
A	240	ALA	CYS	ENGINEERED MUTATION	UNP P09917
A	561	ALA	CYS	ENGINEERED MUTATION	UNP P09917
A	653	GLU	LYS	ENGINEERED MUTATION	UNP P09917
A	654	ASN	LYS	ENGINEERED MUTATION	UNP P09917
A	655	LEU	LYS	ENGINEERED MUTATION	UNP P09917
A	663	ASP	SER	ENGINEERED MUTATION	UNP P09917
B	-12	MET	-	EXPRESSION TAG	UNP P09917
B	-11	GLY	-	EXPRESSION TAG	UNP P09917
B	-10	SER	-	EXPRESSION TAG	UNP P09917
B	-9	SER	-	EXPRESSION TAG	UNP P09917
B	-8	HIS	-	EXPRESSION TAG	UNP P09917
B	-7	HIS	-	EXPRESSION TAG	UNP P09917
B	-6	HIS	-	EXPRESSION TAG	UNP P09917
B	-5	HIS	-	EXPRESSION TAG	UNP P09917
B	-4	HIS	-	EXPRESSION TAG	UNP P09917
B	-3	HIS	-	EXPRESSION TAG	UNP P09917
B	-3A	SER	-	EXPRESSION TAG	UNP P09917
B	-3B	SER	-	EXPRESSION TAG	UNP P09917
B	-3C	GLY	-	EXPRESSION TAG	UNP P09917
B	-3D	LEU	-	EXPRESSION TAG	UNP P09917
B	-3E	VAL	-	EXPRESSION TAG	UNP P09917
B	-3F	PRO	-	EXPRESSION TAG	UNP P09917
B	-3G	ARG	-	EXPRESSION TAG	UNP P09917
B	-3H	GLY	-	EXPRESSION TAG	UNP P09917
B	-3I	SER	-	EXPRESSION TAG	UNP P09917
B	-3J	HIS	-	EXPRESSION TAG	UNP P09917
B	16	GLU	TRP	ENGINEERED MUTATION	UNP P09917
B	17	HIS	PHE	ENGINEERED MUTATION	UNP P09917
B	43	GLY	ASN	SEE REMARK 999	UNP P09917
B	44	SER	ASP	SEE REMARK 999	UNP P09917
B	75	GLY	TRP	ENGINEERED MUTATION	UNP P09917
B	76	SER	LEU	ENGINEERED MUTATION	UNP P09917
B	240	ALA	CYS	ENGINEERED MUTATION	UNP P09917
B	561	ALA	CYS	ENGINEERED MUTATION	UNP P09917
B	653	GLU	LYS	ENGINEERED MUTATION	UNP P09917
B	654	ASN	LYS	ENGINEERED MUTATION	UNP P09917
B	655	LEU	LYS	ENGINEERED MUTATION	UNP P09917
B	663	ASP	SER	ENGINEERED MUTATION	UNP P09917

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

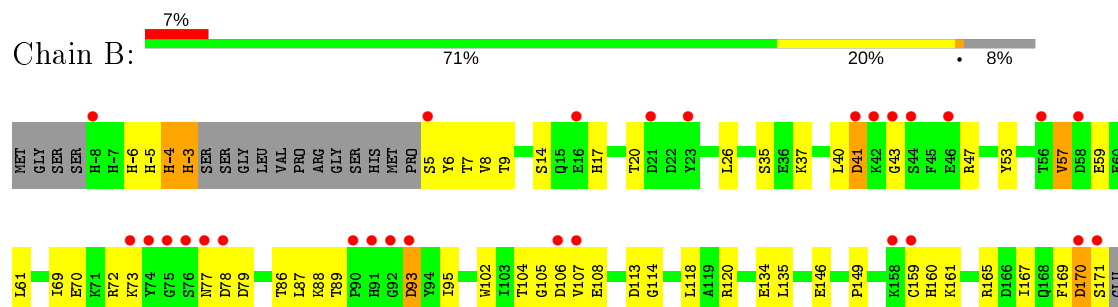
- Molecule 3 is ARACHIDONIC ACID (three-letter code: ACD) (formula: $C_{20}H_{32}O_2$).

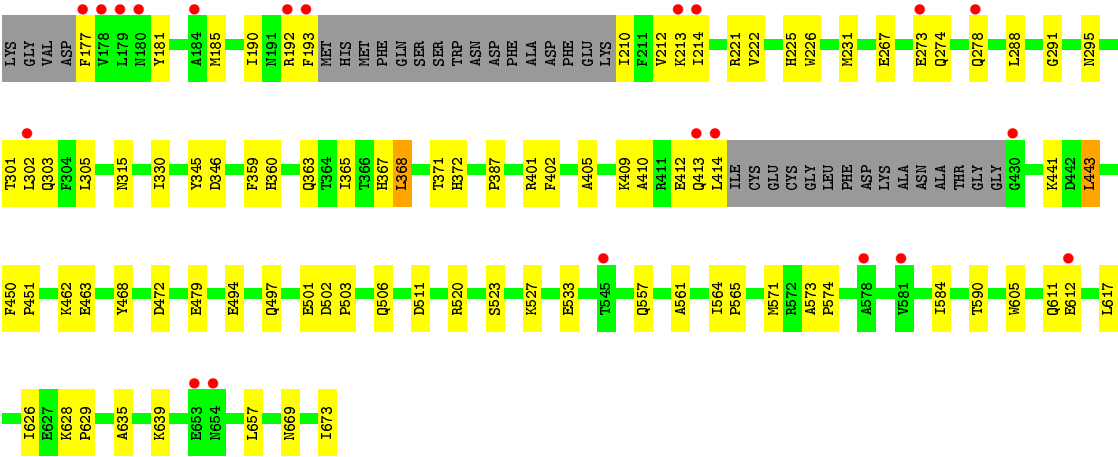


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			53	20	31	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	188	Total	O	0	0
			188	188		
4	B	204	Total	O	0	0
			204	204		





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.76 Å 200.84 Å 72.18 Å 90.00° 105.65° 90.00°	Depositor
Resolution (Å)	35.57 – 2.25 35.57 – 2.25	Depositor EDS
% Data completeness (in resolution range)	93.8 (35.57-2.25) 93.9 (35.57-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.30 (at 2.24 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.186 , 0.233 0.184 , 0.229	Depositor DCC
R_{free} test set	2000 reflections (3.19%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10799	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: FE2, ACD

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	0.24	0/5278	0.40	0/7160
1	B	0.23	0/5336	0.40	0/7240
All	All	0.23	0/10614	0.40	0/14400

There are no bond length outliers.

There are no bond angle outliers.

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	5147	0	5035	192	0
1	B	5205	0	5101	149	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	31	31	5	0
4	A	188	0	0	18	0
4	B	204	0	0	12	0
All	All	10768	31	10167	340	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 17.

All (340) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LYS:NZ	1:B:77:ASN:HA	1.45	1.32
1:A:367:HIS:O	1:A:371:THR:HG22	1.61	0.99
1:B:210:ILE:N	4:B:985:HOH:O	1.95	0.98
1:A:22:ASP:OD1	4:A:968:HOH:O	1.85	0.95
1:B:302:LEU:HG	1:B:305:LEU:HD12	1.47	0.95
1:B:73:LYS:HZ1	1:B:77:ASN:HA	1.07	0.95
1:A:180:ASN:OD1	1:A:181:TYR:N	2.01	0.94
1:A:179:LEU:N	1:A:179:LEU:HD23	1.81	0.94
1:B:134:GLU:OE2	4:B:980:HOH:O	1.85	0.94
1:B:73:LYS:HZ3	1:B:77:ASN:HA	1.35	0.91
1:A:302:LEU:CD1	1:A:305:LEU:HD12	2.01	0.91
1:A:170:ASP:O	1:A:171:SER:HB3	1.72	0.87
1:A:558:TYR:HD1	1:A:604:VAL:HG12	1.39	0.86
1:A:403:THR:HG22	1:A:671:VAL:HG22	1.54	0.85
1:A:179:LEU:HB3	1:A:183:LYS:HE2	1.58	0.85
1:A:635:ALA:O	1:A:639:LYS:HD3	1.76	0.85
1:B:413:GLN:C	1:B:414:LEU:HD12	2.00	0.82
1:A:25:TYR:CE2	1:A:72:ARG:HG3	2.15	0.81
1:A:187:ASN:OD1	1:A:188:LEU:N	2.14	0.81
1:A:185:MET:HE1	1:A:201:TRP:HZ3	1.45	0.81
1:B:214:ILE:HG21	1:B:605:TRP:CZ3	2.14	0.81
1:A:302:LEU:HD12	1:A:302:LEU:O	1.80	0.81
1:A:76:SER:O	4:A:968:HOH:O	1.99	0.81
1:A:146:GLU:OE2	1:A:149:PRO:HA	1.82	0.80
1:B:-4:HIS:ND1	1:B:-4:HIS:N	2.30	0.80
1:B:73:LYS:HZ1	1:B:77:ASN:CA	1.92	0.80
1:A:494:GLU:HG2	1:A:498:VAL:HG21	1.63	0.79
1:A:558:TYR:CD1	1:A:604:VAL:HG12	2.18	0.79
1:B:295:ASN:N	1:B:301:THR:OG1	2.15	0.79
1:A:178:VAL:HG13	1:A:179:LEU:HD23	1.65	0.78
1:A:189:PHE:O	4:A:949:HOH:O	1.99	0.78
1:B:274:GLN:O	1:B:278:GLN:HG2	1.82	0.78
1:A:568:PRO:O	4:A:802:HOH:O	2.02	0.78
1:A:558:TYR:HA	1:A:604:VAL:CG1	2.15	0.77
1:B:213:LYS:NZ	4:B:953:HOH:O	2.18	0.77
1:B:443:LEU:O	1:B:520:ARG:NH2	2.17	0.77
1:B:165:ARG:HH22	1:B:170:ASP:HA	1.50	0.76
1:A:586:GLN:HB2	4:A:986:HOH:O	1.86	0.76
1:B:302:LEU:HD23	1:B:302:LEU:O	1.87	0.74
1:A:199:SER:HB3	1:A:203:ASP:OD2	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HD21	1:A:573:ALA:C	2.08	0.74
1:B:410:ALA:O	1:B:413:GLN:HB2	1.88	0.74
3:A:702:ACD:O1	4:A:977:HOH:O	2.05	0.74
1:A:19:GLY:O	4:A:981:HOH:O	2.05	0.73
1:A:22:ASP:HA	1:A:74:TYR:HB3	1.68	0.73
1:B:502:ASP:O	1:B:506:GLN:HG2	1.89	0.73
1:B:79:ASP:OD1	1:B:104:THR:HG22	1.89	0.73
1:A:177:PHE:HB2	1:A:180:ASN:ND2	2.03	0.72
1:A:300:CYS:O	1:A:301:THR:HB	1.89	0.72
1:B:412:GLU:HB3	1:B:414:LEU:CD1	2.19	0.72
1:B:302:LEU:HG	1:B:305:LEU:CD1	2.19	0.72
1:A:614:GLU:N	4:A:985:HOH:O	2.21	0.71
1:A:188:LEU:HD11	1:A:210:ILE:HG23	1.72	0.71
1:A:344:LYS:O	4:A:943:HOH:O	2.09	0.71
1:A:114:GLY:HA3	1:A:626:ILE:HD13	1.71	0.71
1:B:102:TRP:HZ2	1:B:170:ASP:HB2	1.55	0.71
1:A:214:ILE:HG13	1:A:214:ILE:O	1.91	0.70
1:B:114:GLY:HA3	1:B:626:ILE:HD13	1.73	0.70
1:B:102:TRP:CZ2	1:B:170:ASP:HB2	2.26	0.70
1:A:500:GLU:HG3	1:A:530:LYS:CD	2.21	0.70
1:B:450:PHE:HB3	1:B:451:PRO:HD3	1.74	0.70
1:A:107:VAL:HG22	1:A:108:GLU:N	2.07	0.69
1:B:107:VAL:HG22	1:B:108:GLU:N	2.07	0.69
1:B:413:GLN:HG3	1:B:414:LEU:N	2.07	0.69
1:B:527:LYS:NZ	4:B:846:HOH:O	2.24	0.69
1:B:5:SER:N	4:B:932:HOH:O	2.26	0.69
1:A:302:LEU:HD11	1:A:305:LEU:HD12	1.72	0.69
1:B:441:LYS:HD2	1:B:441:LYS:N	2.06	0.69
1:A:7:THR:HB	1:A:88:LYS:HB3	1.74	0.69
1:B:73:LYS:NZ	1:B:77:ASN:OD1	2.24	0.68
1:A:107:VAL:HG22	1:A:108:GLU:H	1.56	0.68
1:A:73:LYS:HE2	1:A:77:ASN:CG	2.13	0.68
1:A:603:ALA:O	1:A:607:LEU:HG	1.93	0.68
1:A:206:ASP:HB3	1:A:209:LYS:CD	2.24	0.68
1:A:302:LEU:HB3	1:A:571:MET:O	1.93	0.68
1:A:73:LYS:HE2	1:A:77:ASN:ND2	2.08	0.68
1:B:107:VAL:HG22	1:B:108:GLU:H	1.59	0.67
1:B:346:ASP:OD2	4:B:902:HOH:O	2.11	0.67
1:A:71:LYS:HE3	1:A:104:THR:C	2.15	0.66
1:A:558:TYR:HA	1:A:604:VAL:HG11	1.76	0.66
1:A:9:THR:HB	1:A:86:THR:OG1	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ASP:O	1:A:506:GLN:HG2	1.95	0.66
1:A:79:ASP:O	4:A:981:HOH:O	2.13	0.66
1:A:302:LEU:HD13	1:A:305:LEU:HD12	1.77	0.66
1:A:42:LYS:HD2	1:A:42:LYS:H	1.61	0.66
1:B:639:LYS:N	1:B:639:LYS:HD3	2.10	0.66
1:B:302:LEU:CG	1:B:305:LEU:HD12	2.21	0.65
1:A:180:ASN:HD22	1:A:607:LEU:HD21	1.62	0.65
1:B:-3:HIS:N	1:B:-3:HIS:CD2	2.65	0.65
1:A:178:VAL:HG13	1:A:179:LEU:CD2	2.27	0.65
1:B:160:HIS:CG	1:B:409:LYS:HE2	2.31	0.64
1:A:181:TYR:HD2	1:A:181:TYR:C	2.00	0.64
1:A:300:CYS:N	1:A:570:THR:HG1	1.96	0.64
1:A:605:TRP:O	1:A:608:SER:HB3	1.97	0.64
1:A:628:LYS:HB3	1:A:629:PRO:HD3	1.80	0.64
1:B:120:ARG:NH2	1:B:494:GLU:OE2	2.31	0.64
1:A:462:LYS:NZ	1:A:466:PRO:O	2.29	0.63
1:A:181:TYR:CD2	1:A:181:TYR:C	2.72	0.63
1:B:169:PHE:C	1:B:171:SER:H	2.02	0.63
1:B:359:PHE:O	1:B:363:GLN:HG2	2.00	0.62
1:A:180:ASN:HA	1:A:183:LYS:HG2	1.82	0.62
1:A:450:PHE:HB3	1:A:451:PRO:HD3	1.81	0.62
1:A:23:TYR:CD2	1:A:74:TYR:HB2	2.35	0.62
1:A:169:PHE:HB3	1:A:409:LYS:HZ2	1.65	0.62
1:A:221:ARG:HD3	1:A:225:HIS:CD2	2.34	0.62
1:B:225:HIS:HB2	1:B:231:MET:HE3	1.81	0.62
1:B:118:LEU:HD12	1:B:120:ARG:NH1	2.15	0.61
1:A:558:TYR:CE1	1:A:605:TRP:HB2	2.35	0.61
1:A:610:PHE:O	1:A:610:PHE:HD1	1.83	0.61
1:B:221:ARG:NH1	1:B:657:LEU:HD13	2.15	0.61
1:A:406:ILE:HD13	1:A:672:ALA:C	2.20	0.61
1:A:557:GLN:O	1:A:561:ALA:HB3	2.00	0.61
1:A:207:PHE:HA	1:A:598:CYS:SG	2.41	0.61
1:B:190:ILE:HB	1:B:193:PHE:CD1	2.36	0.60
1:A:170:ASP:O	1:A:171:SER:CB	2.46	0.60
1:A:67:VAL:HG12	1:A:69:ILE:CD1	2.32	0.60
1:A:46:GLU:HG3	1:A:49:ALA:HB2	1.83	0.60
1:B:118:LEU:HD12	1:B:120:ARG:HH11	1.67	0.60
1:B:5:SER:HA	4:B:932:HOH:O	2.02	0.60
1:B:564:ILE:HB	1:B:565:PRO:HD3	1.83	0.60
1:A:23:TYR:CE2	1:A:74:TYR:HB2	2.37	0.59
1:A:41:ASP:OD2	4:A:960:HOH:O	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LYS:HE3	1:A:467:TYR:CE2	2.37	0.59
1:A:494:GLU:HG2	1:A:498:VAL:CG2	2.31	0.59
1:B:135:LEU:HD21	1:B:387:PRO:HD3	1.85	0.58
1:B:214:ILE:HG21	1:B:605:TRP:CH2	2.38	0.58
1:B:181:TYR:O	1:B:185:MET:HG2	2.02	0.58
1:B:212:VAL:HG12	1:B:214:ILE:HG12	1.84	0.58
1:B:412:GLU:HB3	1:B:414:LEU:HD12	1.86	0.58
1:A:302:LEU:CD1	1:A:305:LEU:CD1	2.80	0.58
1:B:37:LYS:NZ	1:B:70:GLU:OE1	2.21	0.58
1:A:303:GLN:HG3	1:A:360:HIS:NE2	2.19	0.58
1:A:500:GLU:CD	1:A:530:LYS:HD2	2.24	0.58
1:B:462:LYS:NZ	1:B:472:ASP:OD1	2.29	0.58
1:A:70:GLU:OE1	1:A:70:GLU:HA	2.04	0.57
1:B:303:GLN:HG3	1:B:360:HIS:NE2	2.19	0.57
1:A:588:VAL:O	4:A:941:HOH:O	2.17	0.56
1:B:441:LYS:HD2	1:B:441:LYS:H	1.70	0.56
1:B:225:HIS:HB2	1:B:231:MET:CE	2.35	0.56
1:A:38:HIS:CD2	1:A:55:VAL:HG13	2.41	0.56
1:A:430:GLY:N	4:A:970:HOH:O	2.38	0.56
1:B:14:SER:O	1:B:47:ARG:NE	2.27	0.56
1:A:513:TYR:OH	1:A:527:LYS:NZ	2.39	0.55
1:A:25:TYR:HE2	1:A:72:ARG:HG3	1.66	0.55
1:B:557:GLN:O	1:B:561:ALA:HB3	2.07	0.55
1:B:412:GLU:N	1:B:413:GLN:HA	2.22	0.55
1:A:222:VAL:O	1:A:226:TRP:HB3	2.06	0.55
1:B:17:HIS:O	4:B:935:HOH:O	2.17	0.54
1:B:288:LEU:HD21	1:B:365:ILE:HG13	1.89	0.54
1:B:8:VAL:HG22	1:B:87:LEU:CD2	2.37	0.54
1:A:558:TYR:HD1	1:A:604:VAL:CG1	2.16	0.54
3:A:702:ACD:H8	3:A:702:ACD:H42	1.88	0.54
1:A:177:PHE:HB2	1:A:180:ASN:CG	2.27	0.54
1:B:6:TYR:HE2	1:B:57:VAL:HG21	1.72	0.54
1:A:206:ASP:HB3	1:A:209:LYS:HD2	1.89	0.54
1:A:403:THR:HG22	1:A:671:VAL:CG2	2.34	0.54
1:B:635:ALA:O	1:B:639:LYS:HD3	2.08	0.54
1:B:57:VAL:HG11	1:B:61:LEU:HD11	1.90	0.54
1:A:178:VAL:C	1:A:179:LEU:HD23	2.28	0.53
1:A:302:LEU:HD13	1:A:305:LEU:CD1	2.37	0.53
1:A:46:GLU:CG	1:A:49:ALA:HB2	2.36	0.53
1:B:221:ARG:HD3	1:B:225:HIS:CD2	2.44	0.53
1:A:241:ASN:HB2	1:A:362:HIS:CD2	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:GLU:CA	4:A:985:HOH:O	2.56	0.53
1:A:185:MET:CE	1:A:201:TRP:HZ3	2.19	0.53
1:B:494:GLU:OE1	1:B:494:GLU:N	2.37	0.53
1:B:5:SER:CA	4:B:932:HOH:O	2.57	0.53
1:A:406:ILE:CD1	1:A:672:ALA:C	2.77	0.52
1:A:69:ILE:HD11	1:A:85:ILE:HD12	1.91	0.52
1:A:23:TYR:HB2	1:A:72:ARG:HB2	1.90	0.52
1:A:666:ARG:O	1:A:668:PRO:HD3	2.10	0.52
1:B:114:GLY:HA3	1:B:626:ILE:CD1	2.38	0.52
1:A:518:ARG:HA	1:B:330:ILE:HD12	1.92	0.52
1:A:69:ILE:N	1:A:69:ILE:HD12	2.25	0.51
1:A:114:GLY:HA3	1:A:626:ILE:CD1	2.38	0.51
1:B:409:LYS:O	1:B:413:GLN:HA	2.10	0.51
1:A:483:THR:O	1:A:487:GLU:HG3	2.10	0.51
1:B:497:GLN:HG3	4:B:929:HOH:O	2.09	0.51
1:A:610:PHE:CD1	1:A:610:PHE:O	2.63	0.51
1:B:345:TYR:CZ	1:B:584:ILE:HD11	2.46	0.51
1:B:-3:HIS:H	1:B:-3:HIS:CD2	2.27	0.51
1:A:607:LEU:O	1:A:610:PHE:HD2	1.93	0.51
1:A:67:VAL:HG12	1:A:69:ILE:HD12	1.91	0.51
1:A:89:THR:HB	1:A:90:PRO:HD2	1.91	0.51
1:A:607:LEU:O	1:A:610:PHE:CD2	2.64	0.51
1:B:302:LEU:HD21	1:B:574:PRO:HA	1.92	0.51
1:A:177:PHE:C	1:A:177:PHE:CD1	2.84	0.51
1:A:153:LEU:HG	1:A:515:TYR:O	2.11	0.50
1:B:441:LYS:CD	1:B:441:LYS:H	2.23	0.50
1:A:179:LEU:HB3	1:A:183:LYS:CE	2.36	0.50
1:A:671:VAL:O	1:A:672:ALA:C	2.49	0.50
1:B:501:GLU:O	1:B:503:PRO:HD3	2.11	0.50
1:B:302:LEU:CD2	1:B:573:ALA:O	2.60	0.50
1:A:518:ARG:HA	1:B:330:ILE:CD1	2.42	0.50
1:A:302:LEU:HD21	1:A:573:ALA:CA	2.42	0.49
1:A:500:GLU:CG	1:A:530:LYS:HD2	2.42	0.49
1:A:221:ARG:HD3	1:A:225:HIS:HD2	1.77	0.49
1:A:58:ASP:OD1	1:A:59:GLU:N	2.42	0.49
1:B:37:LYS:NZ	1:B:72:ARG:NH2	2.59	0.49
1:B:221:ARG:HG3	1:B:231:MET:HE1	1.95	0.49
1:B:9:THR:HB	1:B:86:THR:OG1	2.13	0.49
1:B:104:THR:O	1:B:106:ASP:N	2.45	0.49
1:B:107:VAL:CG2	1:B:108:GLU:H	2.24	0.49
1:B:73:LYS:CE	1:B:77:ASN:HA	2.36	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:GLU:OE1	1:B:315:ASN:HB2	2.11	0.49
1:A:177:PHE:C	1:A:177:PHE:HD1	2.16	0.49
1:A:288:LEU:HD21	1:A:365:ILE:HG13	1.94	0.49
1:B:169:PHE:C	1:B:171:SER:N	2.66	0.49
1:A:261:MET:HE1	1:A:337:ILE:HG21	1.94	0.49
1:A:41:ASP:OD1	1:A:42:LYS:HD2	2.12	0.49
1:B:167:ILE:O	1:B:405:ALA:HB2	2.12	0.49
1:A:180:ASN:OD1	1:A:180:ASN:C	2.52	0.48
1:B:165:ARG:NH2	1:B:170:ASP:HA	2.23	0.48
1:B:368:LEU:O	1:B:372:HIS:HB2	2.13	0.48
1:A:169:PHE:HB3	1:A:409:LYS:NZ	2.28	0.48
1:B:673:ILE:OXT	4:B:967:HOH:O	2.19	0.48
1:A:302:LEU:HD11	1:A:574:PRO:HA	1.94	0.48
1:A:179:LEU:CB	1:A:183:LYS:HE2	2.37	0.48
1:A:302:LEU:HD21	1:A:574:PRO:N	2.28	0.48
1:B:190:ILE:HB	1:B:193:PHE:CE1	2.49	0.48
1:A:73:LYS:HE2	1:A:77:ASN:CB	2.43	0.48
1:B:443:LEU:HB3	1:B:520:ARG:NH2	2.28	0.48
1:A:107:VAL:CG2	1:A:108:GLU:N	2.77	0.47
1:B:93:ASP:OD2	1:B:95:ILE:HG13	2.14	0.47
1:B:639:LYS:N	1:B:639:LYS:CD	2.75	0.47
1:A:183:LYS:N	1:A:183:LYS:HD3	2.30	0.47
1:A:291:GLY:HA2	1:B:149:PRO:CB	2.44	0.47
1:B:40:LEU:O	1:B:41:ASP:C	2.53	0.47
1:B:479:GLU:OE1	1:B:479:GLU:HA	2.15	0.47
1:A:177:PHE:HZ	3:A:702:ACD:H22	1.79	0.47
1:A:177:PHE:O	1:A:180:ASN:OD1	2.33	0.47
1:A:371:THR:HG23	1:A:372:HIS:N	2.30	0.47
1:A:500:GLU:HG3	1:A:530:LYS:HD2	1.96	0.47
1:B:401:ARG:O	1:B:402:PHE:HB2	2.14	0.47
1:A:67:VAL:HG12	1:A:69:ILE:HD11	1.96	0.47
1:B:107:VAL:CG2	1:B:108:GLU:N	2.75	0.47
1:B:35:SER:HB3	1:B:61:LEU:HD11	1.96	0.47
1:A:564:ILE:HG13	1:A:597:SER:HB3	1.97	0.47
1:A:639:LYS:CD	1:A:639:LYS:N	2.79	0.46
1:B:611:GLN:HG2	1:B:612:GLU:N	2.30	0.46
1:B:6:TYR:HE1	1:B:89:THR:HG22	1.80	0.46
1:B:93:ASP:OD2	1:B:95:ILE:HD11	2.15	0.46
1:B:441:LYS:CD	1:B:441:LYS:N	2.75	0.46
1:B:-3:HIS:N	1:B:-3:HIS:HD2	2.11	0.46
1:A:334:GLU:CD	1:A:334:GLU:H	2.19	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLN:HA	1:A:497:GLN:OE1	2.16	0.46
1:A:500:GLU:HG3	1:A:530:LYS:HD3	1.95	0.46
1:A:70:GLU:OE1	1:A:108:GLU:HA	2.16	0.46
1:A:179:LEU:O	1:A:182:SER:N	2.49	0.46
1:B:165:ARG:HH12	1:B:170:ASP:HA	1.81	0.46
1:B:169:PHE:O	1:B:171:SER:N	2.49	0.46
1:B:302:LEU:C	1:B:302:LEU:HD23	2.36	0.45
1:A:501:GLU:O	1:A:503:PRO:HD3	2.16	0.45
1:A:206:ASP:HB3	1:A:209:LYS:HG3	1.99	0.45
1:A:292:ILE:HG22	1:A:293:ASP:N	2.31	0.45
1:A:368:LEU:O	1:A:372:HIS:HB2	2.17	0.45
1:B:170:ASP:O	1:B:171:SER:C	2.55	0.45
1:B:41:ASP:HB3	1:B:53:TYR:OH	2.16	0.45
1:B:8:VAL:HG22	1:B:87:LEU:HD23	1.98	0.45
1:B:104:THR:C	1:B:106:ASP:H	2.20	0.45
1:B:160:HIS:CD2	1:B:409:LYS:HE2	2.51	0.45
1:B:413:GLN:HG3	1:B:414:LEU:H	1.81	0.45
1:B:26:LEU:HD12	1:B:69:ILE:HD11	1.98	0.45
1:B:414:LEU:HD12	1:B:414:LEU:N	2.32	0.45
1:B:146:GLU:OE2	1:B:149:PRO:HA	2.17	0.44
1:A:107:VAL:CG2	1:A:108:GLU:H	2.25	0.44
1:A:20:THR:HB	1:A:80:TRP:HB2	1.99	0.44
1:B:73:LYS:CE	1:B:77:ASN:OD1	2.65	0.44
1:B:222:VAL:O	1:B:226:TRP:HB3	2.17	0.44
1:A:6:TYR:HE1	1:A:89:THR:HG22	1.83	0.44
1:A:279:GLY:HA2	4:A:883:HOH:O	2.17	0.44
1:B:412:GLU:H	1:B:413:GLN:HA	1.80	0.44
1:A:167:ILE:O	1:A:405:ALA:HB2	2.17	0.44
1:A:73:LYS:HE2	1:A:77:ASN:HB2	1.99	0.44
1:B:302:LEU:HD22	1:B:573:ALA:O	2.17	0.44
1:A:370:ARG:HH22	1:A:447:SER:CB	2.30	0.44
1:A:551:ALA:HA	1:A:555:PHE:CD2	2.52	0.44
1:A:6:TYR:CE1	1:A:89:THR:HG22	2.53	0.43
1:B:628:LYS:HB2	1:B:629:PRO:HD3	1.98	0.43
1:A:42:LYS:HD2	1:A:42:LYS:N	2.30	0.43
1:B:177:PHE:CD2	1:B:177:PHE:C	2.91	0.43
1:B:571:MET:HE3	1:B:590:THR:CG2	2.48	0.43
1:A:527:LYS:NZ	4:A:837:HOH:O	2.48	0.43
1:A:610:PHE:CD1	1:A:610:PHE:C	2.92	0.43
1:A:394:LYS:HG2	1:A:624:HIS:HB3	2.01	0.43
1:B:159:CYS:SG	1:B:161:LYS:CG	3.06	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:ARG:HG3	1:B:523:SER:HB3	1.99	0.43
1:A:104:THR:OG1	1:A:106:ASP:OD1	2.37	0.43
1:A:210:ILE:O	1:A:214:ILE:HG12	2.19	0.43
1:A:402:PHE:HA	4:A:910:HOH:O	2.18	0.43
1:B:26:LEU:HD23	1:B:26:LEU:C	2.38	0.43
1:A:300:CYS:O	1:A:301:THR:CB	2.61	0.42
1:A:596:ARG:HA	1:A:596:ARG:HD2	1.65	0.42
1:A:116:ALA:HB3	1:A:492:TYR:CE1	2.54	0.42
1:A:181:TYR:O	1:A:181:TYR:HD2	2.02	0.42
1:B:273:GLU:CD	1:B:273:GLU:H	2.20	0.42
1:A:149:PRO:HB3	1:B:291:GLY:HA2	2.01	0.42
1:A:319:LYS:CE	1:A:467:TYR:CD2	3.01	0.42
3:A:702:ACD:H8	3:A:702:ACD:C4	2.49	0.42
1:B:533:GLU:OE1	1:B:533:GLU:HA	2.19	0.42
1:A:639:LYS:N	1:A:639:LYS:HD3	2.35	0.42
1:B:73:LYS:HB3	1:B:73:LYS:HE3	1.93	0.42
1:B:20:THR:HA	1:B:78:ASP:OD2	2.19	0.42
1:B:213:LYS:CE	4:B:953:HOH:O	2.65	0.42
1:B:367:HIS:O	1:B:371:THR:OG1	2.28	0.42
1:A:558:TYR:CB	1:A:604:VAL:HG12	2.50	0.42
1:A:291:GLY:HA2	1:B:149:PRO:HB3	2.02	0.42
1:A:302:LEU:HD23	1:A:573:ALA:N	2.34	0.41
1:A:600:HIS:O	1:A:604:VAL:HG23	2.20	0.41
1:A:663:ASP:OD1	1:A:665:ASP:HB2	2.19	0.41
1:B:463:GLU:H	1:B:463:GLU:CD	2.23	0.41
1:B:7:THR:HB	1:B:88:LYS:HB3	2.02	0.41
1:A:135:LEU:HD21	1:A:387:PRO:HD3	2.02	0.41
1:A:184:ALA:O	1:A:188:LEU:HB2	2.20	0.41
1:A:302:LEU:HD23	1:A:572:ARG:C	2.40	0.41
1:B:-3:HIS:H	1:B:-3:HIS:HD2	1.68	0.41
1:B:302:LEU:HD21	1:B:573:ALA:O	2.20	0.41
1:A:455:LYS:HE3	1:A:455:LYS:HB2	1.43	0.41
1:A:663:ASP:C	1:A:663:ASP:OD1	2.59	0.41
1:B:93:ASP:OD2	1:B:95:ILE:CG1	2.68	0.41
1:A:302:LEU:HD12	1:A:302:LEU:C	2.40	0.41
1:A:42:LYS:CD	1:A:42:LYS:H	2.30	0.41
1:A:657:LEU:HA	1:A:657:LEU:HD12	1.83	0.41
1:B:617:LEU:HA	1:B:669:ASN:OD1	2.20	0.41
1:B:6:TYR:CE1	1:B:89:THR:HG22	2.56	0.41
3:A:702:ACD:H14	4:A:922:HOH:O	2.20	0.41
1:B:571:MET:CE	1:B:590:THR:CG2	2.98	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HB	1:A:66:LEU:HB2	2.02	0.41
1:B:288:LEU:CD2	1:B:365:ILE:HG13	2.51	0.41
1:A:154:SER:HB2	1:A:376:GLU:OE2	2.21	0.41
1:A:362:HIS:NE2	1:A:553:VAL:O	2.51	0.40
1:A:22:ASP:OD2	1:A:71:LYS:NZ	2.52	0.40
1:A:260:GLU:N	1:A:260:GLU:OE1	2.49	0.40
1:B:8:VAL:HG22	1:B:87:LEU:HD21	2.04	0.40
1:A:207:PHE:CA	1:A:598:CYS:SG	3.10	0.40
1:A:558:TYR:HE1	1:A:605:TRP:HB2	1.85	0.40
1:B:192:ARG:O	1:B:193:PHE:C	2.59	0.40
1:B:639:LYS:HD3	1:B:639:LYS:H	1.84	0.40
1:A:189:PHE:HZ	1:A:201:TRP:HA	1.87	0.40
1:A:267:GLU:OE1	1:A:315:ASN:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	620/691 (90%)	605 (98%)	15 (2%)	0	100	100
1	B	629/691 (91%)	615 (98%)	11 (2%)	3 (0%)	29	29
All	All	1249/1382 (90%)	1220 (98%)	26 (2%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	ASP
1	B	105	GLY
1	B	43	GLY

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	559/608 (92%)	544 (97%)	15 (3%)	44	54
1	B	565/608 (93%)	552 (98%)	13 (2%)	50	59
All	All	1124/1216 (92%)	1096 (98%)	28 (2%)	47	56

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	40	LEU
1	A	158	LYS
1	A	161	LYS
1	A	171	SER
1	A	177	PHE
1	A	179	LEU
1	A	181	TYR
1	A	185	MET
1	A	250	GLU
1	A	302	LEU
1	A	334	GLU
1	A	468	TYR
1	A	511	ASP
1	A	610	PHE
1	B	-6	HIS
1	B	-5	HIS
1	B	-4	HIS
1	B	-3	HIS
1	B	41	ASP
1	B	57	VAL
1	B	59	GLU
1	B	93	ASP
1	B	113	ASP
1	B	368	LEU
1	B	443	LEU
1	B	468	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	511	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	295	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
3	ACD	A	702	-	18,21,21	0.57	0	17,21,21	0.93	1 (5%)

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
3	ACD	A	702	-	-	7/17/19/19	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	ACD	C2-C3-C4	3.41	118.90	113.09

There are no chirality outliers.

All (7) torsion outliers are listed below:

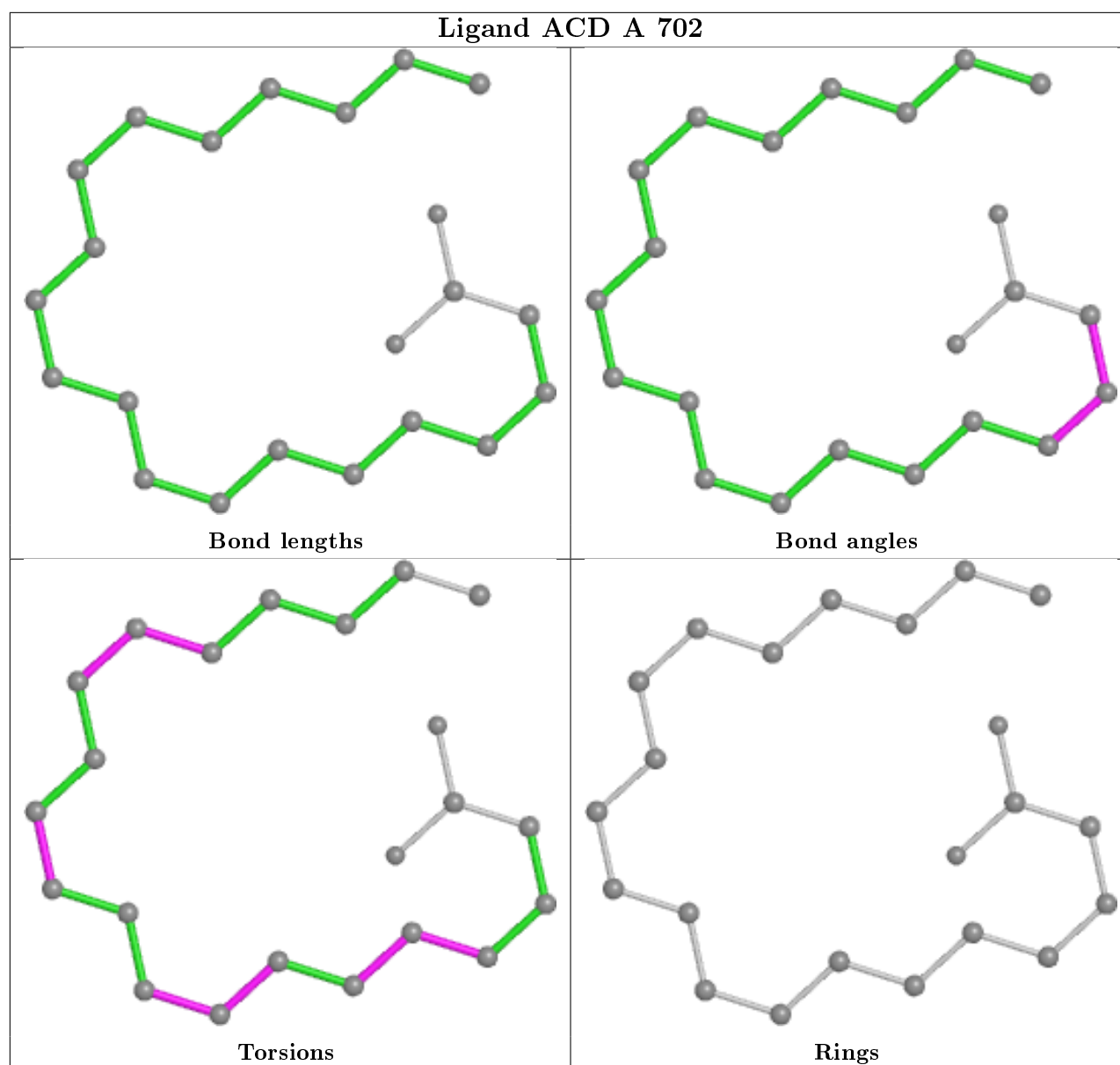
Mol	Chain	Res	Type	Atoms
3	A	702	ACD	C4-C5-C6-C7
3	A	702	ACD	C7-C8-C9-C10
3	A	702	ACD	C6-C7-C8-C9
3	A	702	ACD	C10-C11-C12-C13
3	A	702	ACD	C14-C15-C16-C17
3	A	702	ACD	C13-C14-C15-C16
3	A	702	ACD	C3-C4-C5-C6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	ACD	5	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	630/691 (91%)	0.16	38 (6%)	21 23	13, 28, 65, 113	0
1	B	639/691 (92%)	0.25	49 (7%)	13 14	13, 28, 68, 118	0
All	All	1269/1382 (91%)	0.21	87 (6%)	16 18	13, 28, 65, 118	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	PHE	10.2
1	A	187	ASN	9.2
1	A	42	LYS	7.7
1	B	77	ASN	6.5
1	B	76	SER	6.1
1	A	41	ASP	5.4
1	A	179	LEU	5.3
1	B	74	TYR	5.1
1	A	43	GLY	5.1
1	B	93	ASP	5.0
1	B	106	ASP	4.8
1	B	612	GLU	4.7
1	B	179	LEU	4.7
1	A	558	TYR	4.6
1	A	610	PHE	4.6
1	B	214	ILE	4.3
1	B	75	GLY	4.2
1	A	74	TYR	4.2
1	B	43	GLY	4.1
1	B	414	LEU	4.0
1	A	171	SER	3.9
1	B	171	SER	3.9
1	A	106	ASP	3.8
1	B	91	HIS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	180	ASN	3.5
1	B	41	ASP	3.5
1	A	214	ILE	3.5
1	B	107	VAL	3.3
1	B	42	LYS	3.2
1	B	413	GLN	3.2
1	A	198	GLN	3.2
1	A	158	LYS	3.0
1	A	91	HIS	3.0
1	B	178	VAL	2.9
1	B	44	SER	2.9
1	A	189	PHE	2.9
1	A	16	GLU	2.9
1	B	16	GLU	2.9
1	A	54	ASP	2.9
1	A	649	ALA	2.8
1	A	605	TRP	2.8
1	B	23	TYR	2.7
1	B	21	ASP	2.7
1	A	177	PHE	2.7
1	B	170	ASP	2.7
1	B	213	LYS	2.7
1	A	188	LEU	2.7
1	B	90	PRO	2.5
1	B	581	VAL	2.5
1	B	159	CYS	2.5
1	B	180	ASN	2.5
1	A	293	ASP	2.5
1	B	78	ASP	2.5
1	B	73	LYS	2.5
1	B	177	PHE	2.4
1	A	609	GLN	2.4
1	B	92	GLY	2.4
1	B	158	LYS	2.4
1	B	654	ASN	2.4
1	B	302	LEU	2.4
1	A	639	LYS	2.3
1	A	654	ASN	2.4
1	A	93	ASP	2.3
1	B	-8	HIS	2.3
1	B	58	ASP	2.3
1	B	430	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	56	THR	2.3
1	A	170	ASP	2.3
1	B	5	SER	2.3
1	B	192	ARG	2.3
1	A	199	SER	2.3
1	A	333	ASP	2.2
1	A	76	SER	2.2
1	A	464	ASP	2.2
1	A	181	TYR	2.2
1	B	273	GLU	2.2
1	B	578	ALA	2.2
1	B	653	GLU	2.2
1	B	184	ALA	2.1
1	A	653	GLU	2.1
1	B	278	GLN	2.1
1	A	60	GLU	2.1
1	A	302	LEU	2.1
1	B	46	GLU	2.0
1	A	213	LYS	2.0
1	A	580	GLY	2.0
1	B	545	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 carbohydrates 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.

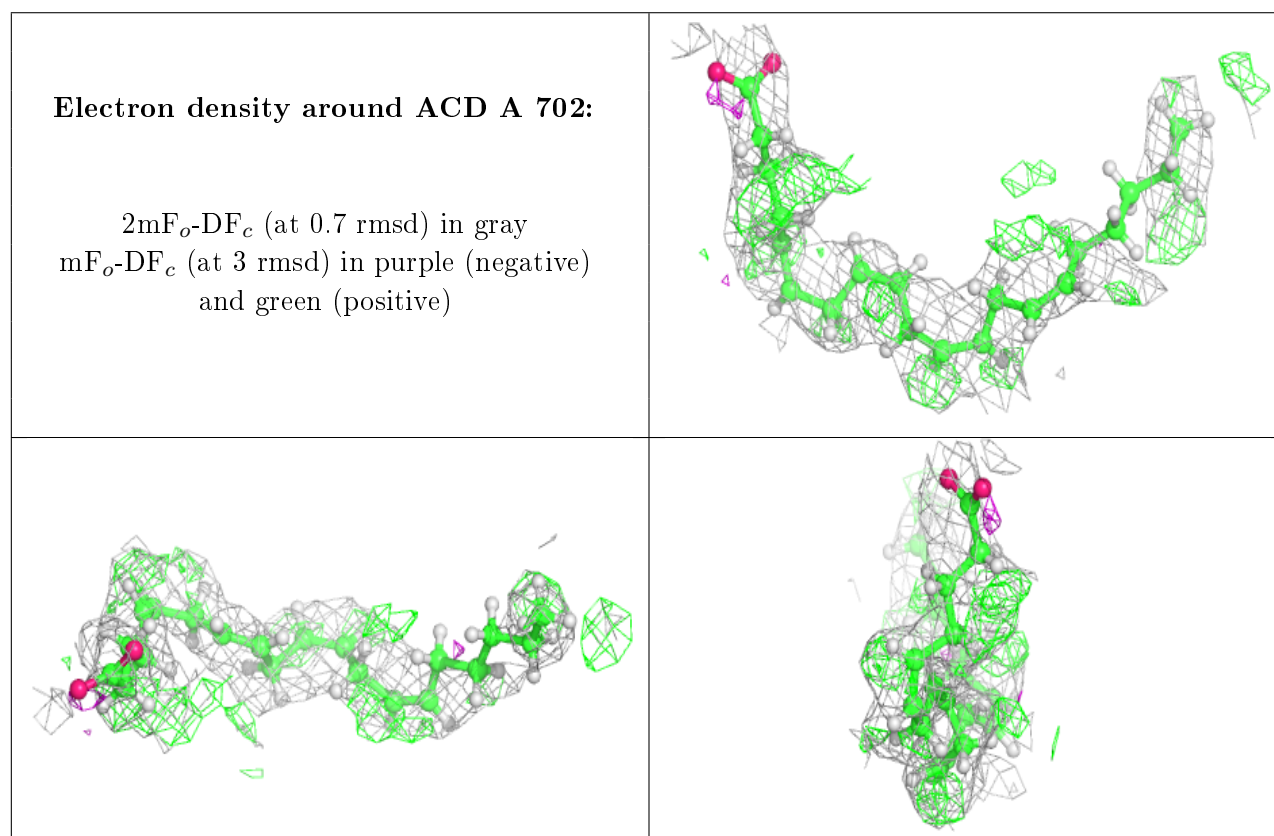
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACD	A	702	22/22	0.51	0.31	50,71,90,98	0
2	FE2	A	701	1/1	0.99	0.14	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE2	B	701	1/1	0.99	0.13	16,16,16,16	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.