



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:01 PM GMT

PDB ID : 1PPG
Title : The refined 2.3 angstroms crystal structure of human leukocyte elastase in a complex with a valine chloromethyl ketone inhibitor
Authors : Bode, W.; Wei, A-Z.
Deposited on : 1991-10-24
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

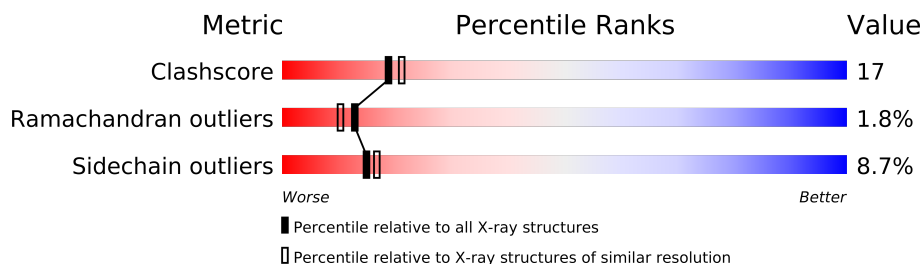
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.


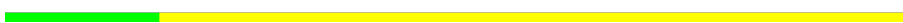
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	218	
2	I	6	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2053 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HUMAN LEUKOCYTE ELASTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	218	Total	C	N	O	S	43	0	0
			1636	1026	316	283	11			

- Molecule 2 is a protein called MEO-SUCCINYLA-ALA-PRO-VALCHLOROMETHYLKETONE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	6	Total	C	N	O	0	0	1
			33	22	4	7			

- Molecule 3 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	8	Total	C	N	O	60	0
			96	54	3	39		

- Molecule 4 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	8	Total	C	N	O	72	0
			96	54	3	39		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	189	Total	O	29	0
			189	189		
5	I	3	Total	O	1	0
			3	3		

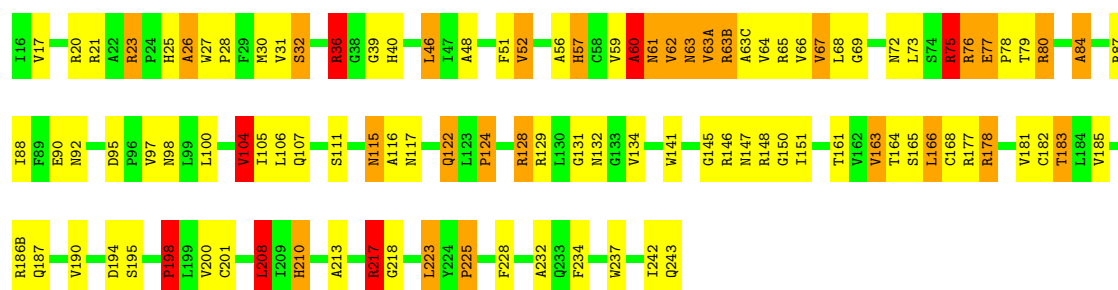
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: HUMAN LEUKOCYTE ELASTASE

Chain E: 



• Molecule 2: MEO-SUCCINYL-ALA-ALA-PRO-VALCHLOROMETHYLKETONE

Chain I: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	74.20Å 74.20Å 70.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.145 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2053	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VAI, OQE, GLC, NAG, NDG, GAL, BMA, MAN, HMB, FUC

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	E	1.35	9/1666 (0.5%)	1.81	37/2263 (1.6%)
2	I	1.24	0/17	1.27	0/23
All	All	1.35	9/1683 (0.5%)	1.81	37/2286 (1.6%)

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	E	0	24
2	I	1	0
4	E	2	0
All	All	3	24

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	141	TRP	NE1-CE2	-7.82	1.27	1.37
1	E	237	TRP	NE1-CE2	-6.85	1.28	1.37
1	E	75	ARG	NE-CZ	6.25	1.41	1.33
1	E	76	ARG	CZ-NH1	5.95	1.40	1.33
1	E	27	TRP	NE1-CE2	-5.91	1.29	1.37
1	E	32	SER	CB-OG	-5.89	1.34	1.42
1	E	40	HIS	CE1-NE2	5.77	1.46	1.32
1	E	57	HIS	CE1-NE2	5.63	1.45	1.32
1	E	76	ARG	CZ-NH2	5.23	1.39	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	217	ARG	NE-CZ-NH1	11.60	126.10	120.30
1	E	23	ARG	NE-CZ-NH1	-10.33	115.14	120.30
1	E	177	ARG	NE-CZ-NH2	-9.85	115.37	120.30
1	E	217	ARG	NH1-CZ-NH2	-8.41	110.15	119.40
1	E	194	ASP	CB-CG-OD2	7.70	125.23	118.30
1	E	87	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	E	208	LEU	N-CA-CB	-7.12	96.17	110.40
1	E	129	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	E	190	VAL	CA-CB-CG2	6.57	120.76	110.90
1	E	76	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	E	65	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	E	210	HIS	C-N-CA	-5.98	109.73	122.30
1	E	60	ALA	N-CA-CB	-5.83	101.94	110.10
1	E	36	ARG	CD-NE-CZ	-5.71	115.61	123.60
1	E	194	ASP	CA-CB-CG	-5.70	100.86	113.40
1	E	128	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	E	242	ILE	C-N-CA	5.65	135.82	121.70
1	E	223	LEU	CB-CG-CD2	5.62	120.56	111.00
1	E	181	VAL	CA-CB-CG1	5.61	119.31	110.90
1	E	90	GLU	N-CA-CB	-5.60	100.53	110.60
1	E	104	VAL	CA-CB-CG1	5.49	119.13	110.90
1	E	65	ARG	CA-CB-CG	-5.46	101.38	113.40
1	E	62	VAL	CG1-CB-CG2	5.42	119.57	110.90
1	E	63	ASN	CA-CB-CG	-5.40	101.52	113.40
1	E	190	VAL	CA-CB-CG1	5.36	118.93	110.90
1	E	104	VAL	CG1-CB-CG2	5.26	119.31	110.90
1	E	77	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	E	178	ARG	O-C-N	-5.16	114.44	122.70
1	E	183	THR	CA-CB-CG2	-5.14	105.20	112.40
1	E	198	PRO	N-CA-CB	-5.13	96.95	102.60
1	E	20	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	E	75	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	E	67	VAL	CA-CB-CG2	-5.07	103.30	110.90
1	E	186(B)	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	E	80	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	E	198	PRO	N-CD-CG	-5.05	95.62	103.20
1	E	59	VAL	CG1-CB-CG2	5.03	118.95	110.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	416	NDG	C3
4	E	417	GLC	C3

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Mol	Chain	Res	Type	Atom
2	I	1	HMB	CG

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	104	VAL	Mainchain
1	E	107	GLN	Mainchain
1	E	111	SER	Mainchain
1	E	122	GLN	Mainchain
1	E	163	VAL	Mainchain
1	E	165	SER	Mainchain
1	E	168	CYS	Mainchain
1	E	178	ARG	Mainchain
1	E	185	VAL	Mainchain
1	E	198	PRO	Mainchain
1	E	217	ARG	Sidechain
1	E	225	PRO	Mainchain
1	E	234	PHE	Mainchain
1	E	26	ALA	Mainchain
1	E	28	PRO	Mainchain
1	E	46	LEU	Mainchain
1	E	52	VAL	Mainchain
1	E	60	ALA	Mainchain
1	E	61	ASN	Mainchain
1	E	63	ASN	Mainchain
1	E	63(B)	ARG	Mainchain
1	E	63(C)	ALA	Mainchain
1	E	69	GLY	Mainchain
1	E	84	ALA	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1636	0	1650	54	37
2	I	33	0	33	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	96	0	82	0	37
4	E	96	0	82	1	0
5	E	189	0	0	3	28
5	I	3	0	0	0	0
All	All	2053	0	1847	55	53

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (55) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:195:SER:OG	2:I:6:0QE:C1	1.78	1.28
1:E:218:GLY:H	2:I:1:HMB:HB1	1.36	0.90
1:E:88:ILE:HG22	1:E:106:LEU:HD22	1.56	0.87
1:E:195:SER:CB	2:I:6:0QE:C1	2.55	0.85
1:E:105:ILE:HG13	5:E:1239:HOH:O	1.85	0.77
1:E:57:HIS:CE1	1:E:195:SER:OG	2.40	0.74
1:E:23:ARG:HB3	1:E:26:ALA:HB2	1.71	0.72
1:E:124:PRO:HG2	1:E:232:ALA:HB2	1.73	0.71
1:E:195:SER:CB	2:I:5:VAI:C	2.69	0.71
1:E:63(A):VAL:HA	1:E:64:VAL:HG23	1.74	0.68
1:E:201:CYS:HB2	1:E:210:HIS:HD2	1.59	0.68
1:E:115:ASN:HD22	1:E:117:ASN:H	1.44	0.65
1:E:201:CYS:HB2	1:E:210:HIS:CD2	2.33	0.64
1:E:21:ARG:HD2	5:E:740:HOH:O	2.01	0.61
1:E:39:GLY:HA2	5:E:972:HOH:O	2.00	0.60
1:E:57:HIS:HE1	1:E:195:SER:OG	1.84	0.60
1:E:72:ASN:ND2	1:E:75:ARG:NH1	2.50	0.59
1:E:166:LEU:HB3	1:E:225:PRO:HD2	1.85	0.58
1:E:182:CYS:HB3	1:E:225:PRO:HB2	1.85	0.57
1:E:218:GLY:N	2:I:1:HMB:HB1	2.14	0.56
1:E:84:ALA:HB2	4:E:412:FUC:H5	1.89	0.54
1:E:131:GLY:O	1:E:134:VAL:HG23	2.07	0.54
1:E:31:VAL:HG21	1:E:52:VAL:HG11	1.90	0.54
1:E:105:ILE:O	1:E:106:LEU:HD23	2.07	0.53
1:E:31:VAL:HG11	1:E:66:VAL:HG13	1.91	0.53
1:E:195:SER:HB2	2:I:6:0QE:C1	2.41	0.51
1:E:88:ILE:HG22	1:E:106:LEU:CD2	2.35	0.50
1:E:122:GLN:HB2	1:E:208:LEU:HD12	1.94	0.49
1:E:183:THR:HG1	1:E:228:PHE:HE1	1.59	0.49
1:E:95:ASP:HB3	1:E:100:LEU:HB2	1.94	0.49
1:E:63(A):VAL:HA	1:E:64:VAL:CG2	2.41	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:163:VAL:HG21	1:E:225:PRO:HB3	1.95	0.48
1:E:17:VAL:HG22	1:E:145:GLY:HA2	1.95	0.48
1:E:73:LEU:HA	1:E:80:ARG:NH2	2.28	0.48
1:E:166:LEU:HB3	1:E:225:PRO:CD	2.44	0.47
1:E:56:ALA:HA	1:E:104:VAL:HG22	1.96	0.47
1:E:115:ASN:C	1:E:115:ASN:HD22	2.19	0.47
1:E:217:ARG:HA	2:I:1:HMB:O	2.15	0.46
1:E:161:THR:O	1:E:183:THR:HA	2.15	0.46
1:E:31:VAL:HG22	1:E:68:LEU:HD22	1.99	0.45
1:E:115:ASN:ND2	1:E:117:ASN:H	2.10	0.45
1:E:25:HIS:CE1	1:E:79:THR:HG21	2.52	0.44
1:E:48:ALA:HB3	1:E:51:PHE:HB2	1.99	0.44
1:E:132:ASN:ND2	1:E:164:THR:H	2.17	0.43
1:E:31:VAL:HG21	1:E:52:VAL:CG1	2.49	0.43
1:E:31:VAL:CG1	1:E:66:VAL:HG13	2.49	0.43
1:E:77:GLU:O	1:E:80:ARG:HG3	2.19	0.43
1:E:30:MET:SD	1:E:198:PRO:HD2	2.59	0.42
1:E:77:GLU:HA	1:E:78:PRO:HD2	1.72	0.42
1:E:32:SER:HB3	1:E:67:VAL:HB	2.01	0.42
1:E:132:ASN:HD22	1:E:164:THR:H	1.68	0.41
2:I:3:ALA:HA	2:I:4:PRO:HD2	1.87	0.41
1:E:166:LEU:HA	1:E:166:LEU:HD12	1.79	0.40
1:E:46:LEU:HD12	1:E:46:LEU:HA	1.92	0.40
1:E:60:ALA:O	1:E:61:ASN:HB2	2.22	0.40

All (53) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:408:MAN:C3	5:E:744:HOH:O[2_565]	0.28	1.92
1:E:97:VAL:CB	3:E:406:NAG:C5[4_564]	0.32	1.88
1:E:97:VAL:CA	3:E:406:NAG:C6[4_564]	0.62	1.58
1:E:243:GLN:C	5:E:1278:HOH:O[6_554]	0.63	1.57
1:E:243:GLN:CB	5:E:1276:HOH:O[6_554]	0.63	1.57
3:E:405:MAN:C3	5:E:1234:HOH:O[4_565]	0.74	1.46
1:E:97:VAL:CG1	3:E:406:NAG:O5[4_564]	0.86	1.34
1:E:97:VAL:CG2	3:E:406:NAG:C4[4_564]	0.89	1.31
1:E:243:GLN:CG	5:E:1276:HOH:O[6_554]	1.09	1.11
1:E:243:GLN:CA	5:E:1278:HOH:O[6_554]	1.22	0.98
3:E:408:MAN:O3	5:E:744:HOH:O[2_565]	1.22	0.98
1:E:97:VAL:CG2	3:E:406:NAG:C5[4_564]	1.23	0.97
1:E:100:LEU:CG	5:E:1168:HOH:O[4_564]	1.31	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:97:VAL:CB	3:E:406:NAG:C6[4_564]	1.33	0.87
1:E:243:GLN:O	5:E:1278:HOH:O[6_554]	1.34	0.86
3:E:405:MAN:C2	5:E:1234:HOH:O[4_565]	1.34	0.86
1:E:147:ASN:O	1:E:187:GLN:NE2[2_665]	1.35	0.85
1:E:98:ASN:N	3:E:406:NAG:O6[4_564]	1.39	0.81
3:E:401:NAG:N2	5:E:975:HOH:O[4_565]	1.40	0.80
1:E:97:VAL:CB	3:E:406:NAG:O5[4_564]	1.41	0.79
1:E:100:LEU:CD1	5:E:1168:HOH:O[4_564]	1.41	0.79
1:E:100:LEU:CB	5:E:1168:HOH:O[4_564]	1.45	0.75
1:E:97:VAL:N	3:E:406:NAG:C6[4_564]	1.50	0.70
5:E:708:HOH:O	5:E:838:HOH:O[4_565]	1.55	0.65
1:E:97:VAL:C	3:E:406:NAG:C6[4_564]	1.56	0.64
3:E:401:NAG:C2	5:E:975:HOH:O[4_565]	1.56	0.64
1:E:116:ALA:O	3:E:408:MAN:O4[3_455]	1.57	0.63
1:E:97:VAL:CG1	3:E:406:NAG:C5[4_564]	1.58	0.62
1:E:97:VAL:CG2	3:E:406:NAG:C3[4_564]	1.59	0.61
1:E:97:VAL:CG2	3:E:406:NAG:O4[4_564]	1.60	0.60
1:E:97:VAL:C	3:E:406:NAG:O6[4_564]	1.65	0.55
3:E:408:MAN:C4	5:E:744:HOH:O[2_565]	1.69	0.51
3:E:408:MAN:C2	5:E:744:HOH:O[2_565]	1.72	0.48
1:E:97:VAL:CA	3:E:406:NAG:C5[4_564]	1.74	0.46
1:E:243:GLN:OXT	5:E:1278:HOH:O[6_554]	1.74	0.46
1:E:97:VAL:CB	3:E:406:NAG:C4[4_564]	1.83	0.37
1:E:97:VAL:O	3:E:407:GAL:C1[4_564]	1.84	0.36
1:E:243:GLN:CA	5:E:1276:HOH:O[6_554]	1.85	0.35
1:E:25:HIS:O	3:E:408:MAN:O3[3_455]	1.88	0.32
3:E:405:MAN:C4	5:E:1234:HOH:O[4_565]	1.90	0.30
3:E:401:NAG:C3	5:E:975:HOH:O[4_565]	1.94	0.26
3:E:405:MAN:C1	5:E:1234:HOH:O[4_565]	1.94	0.26
1:E:97:VAL:CA	3:E:406:NAG:O6[4_564]	1.95	0.25
1:E:243:GLN:N	5:E:1278:HOH:O[6_554]	1.96	0.24
1:E:150:GLY:CA	5:E:592:HOH:O[2_665]	2.03	0.17
3:E:405:MAN:O3	5:E:1234:HOH:O[4_565]	2.05	0.15
3:E:404:BMA:O6	5:E:1234:HOH:O[4_565]	2.06	0.14
1:E:36:ARG:NH2	1:E:164:THR:OG1[2_665]	2.09	0.11
1:E:97:VAL:CG1	3:E:406:NAG:C6[4_564]	2.09	0.11
1:E:97:VAL:CG1	3:E:406:NAG:C1[4_564]	2.11	0.09
1:E:97:VAL:CG1	3:E:406:NAG:O6[4_564]	2.15	0.05
5:E:570:HOH:O	5:E:1271:HOH:O[3_565]	2.17	0.03
3:E:407:GAL:O2	5:E:1129:HOH:O[4_565]	2.19	0.01

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	E	216/218 (99%)	201 (93%)	11 (5%)	4 (2%)	12	9
2	I	3/6 (50%)	3 (100%)	0	0	100	100
All	All	219/224 (98%)	204 (93%)	11 (5%)	4 (2%)	13	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	36	ARG
1	E	146	ARG
1	E	213	ALA
1	E	124	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	E	172/172 (100%)	157 (91%)	15 (9%)	15	17
2	I	1/1 (100%)	1 (100%)	0	100	100
All	All	173/173 (100%)	158 (91%)	15 (9%)	15	17

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	62	VAL
1	E	63(A)	VAL
1	E	63(B)	ARG
1	E	75	ARG
1	E	76	ARG

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Mol	Chain	Res	Type
1	E	92	ASN
1	E	104	VAL
1	E	115	ASN
1	E	128	ARG
1	E	148	ARG
1	E	151	ILE
1	E	166	LEU
1	E	200	VAL
1	E	208	LEU
1	E	223	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	92	ASN
1	E	115	ASN
1	E	117	ASN
1	E	132	ASN
1	E	135	GLN
1	E	156	GLN
1	E	210	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	VAI	I	5	1,2	6,6,7	7.65	1 (16%)	4,7,9	0.45	0

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	VAI	I	5	1,2	-	0/4/6/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	5	VAI	O-C	18.72	1.46	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

16 carbohydrates 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	$\# Z > 2$
3	NAG	E	401	1,3	12,14,15	1.07	0	15,19,21	2.21	6 (40%)
3	FUC	E	402	3	9,10,11	1.24	1 (11%)	10,14,16	1.32	3 (30%)
3	NAG	E	403	3	12,14,15	0.77	0	15,19,21	1.52	3 (20%)
3	BMA	E	404	3	10,11,12	0.51	0	11,15,17	0.92	0
3	MAN	E	405	3	10,11,12	0.49	0	11,15,17	1.01	1 (9%)
3	NAG	E	406	3	12,14,15	0.68	0	15,19,21	1.03	1 (6%)
3	GAL	E	407	3	10,11,12	0.60	0	11,15,17	0.80	0
3	MAN	E	408	3	10,11,12	0.56	0	11,15,17	0.85	0
4	NAG	E	411	1,4	12,14,15	1.64	5 (41%)	15,19,21	1.89	2 (13%)
4	FUC	E	412	4	9,10,11	1.22	1 (11%)	10,14,16	2.15	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	413	4	12,14,15	0.96	1 (8%)	15,19,21	2.13	3 (20%)
4	BMA	E	414	4	10,11,12	0.63	0	11,15,17	2.75	4 (36%)
4	BMA	E	415	4	10,11,12	0.64	0	11,15,17	1.32	1 (9%)
4	NDG	E	416	4	12,14,15	0.88	1 (8%)	15,19,21	3.13	7 (46%)
4	GLC	E	417	4	10,11,12	0.59	0	11,15,17	1.20	1 (9%)
4	MAN	E	418	4	10,11,12	0.55	0	11,15,17	1.51	1 (9%)

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	NAG	E	401	1,3	-	0/6/23/26	0/1/1/1
3	FUC	E	402	3	-	0/0/17/20	0/1/1/1
3	NAG	E	403	3	-	0/6/23/26	0/1/1/1
3	BMA	E	404	3	-	0/2/19/22	0/1/1/1
3	MAN	E	405	3	-	0/2/19/22	0/1/1/1
3	NAG	E	406	3	-	0/6/23/26	0/1/1/1
3	GAL	E	407	3	-	0/2/19/22	0/1/1/1
3	MAN	E	408	3	-	0/2/19/22	0/1/1/1
4	NAG	E	411	1,4	-	0/6/23/26	0/1/1/1
4	FUC	E	412	4	-	0/0/17/20	0/1/1/1
4	NAG	E	413	4	-	0/6/23/26	0/1/1/1
4	BMA	E	414	4	-	0/2/19/22	0/1/1/1
4	BMA	E	415	4	-	0/2/19/22	0/1/1/1
4	NDG	E	416	4	1/1/5/7	0/6/23/26	0/1/1/1
4	GLC	E	417	4	1/1/4/5	0/2/19/22	1/1/1/1
4	MAN	E	418	4	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	411	NAG	C3-C2	2.55	1.57	1.52
3	E	402	FUC	O5-C5	-2.37	1.41	1.45
4	E	411	NAG	C4-C3	2.31	1.58	1.52
4	E	413	NAG	O5-C5	-2.29	1.41	1.45
4	E	411	NAG	O3-C3	2.27	1.48	1.43
4	E	411	NAG	C8-C7	2.23	1.55	1.50
4	E	412	FUC	O3-C3	2.18	1.48	1.43
4	E	411	NAG	C2-N2	2.17	1.48	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	416	NDG	C2-N2	2.01	1.48	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	414	BMA	O5-C5-C6	7.54	114.89	106.98
4	E	416	NDG	O-C5-C6	6.79	114.11	106.98
4	E	413	NAG	O5-C5-C6	-6.41	100.26	106.98
4	E	416	NDG	C3-C4-C5	-5.70	100.02	110.20
4	E	412	FUC	C4-C3-C2	-5.33	103.35	110.50
4	E	418	MAN	O5-C5-C6	4.73	111.94	106.98
4	E	416	NDG	C3-C2-N2	-4.67	104.66	111.76
4	E	411	NAG	C2-N2-C7	-4.24	115.97	123.09
3	E	401	NAG	O4-C4-C3	-4.02	101.33	110.35
3	E	401	NAG	O7-C7-N2	3.84	129.93	121.90
4	E	416	NDG	O-C5-C4	-3.68	105.98	110.65
4	E	411	NAG	O5-C5-C6	3.62	110.78	106.98
4	E	415	BMA	C3-C4-C5	3.52	116.49	110.20
4	E	417	GLC	O5-C5-C6	3.51	110.67	106.98
4	E	416	NDG	O3-C3-C2	-3.51	101.73	109.09
3	E	403	NAG	C2-N2-C7	-3.30	117.54	123.09
4	E	413	NAG	C3-C2-N2	-3.25	106.81	111.76
3	E	401	NAG	C8-C7-N2	-3.22	109.81	116.11
3	E	401	NAG	O7-C7-C8	-3.19	115.82	122.04
4	E	416	NDG	C2-N2-C7	2.95	128.05	123.09
3	E	403	NAG	O4-C4-C3	-2.94	103.77	110.35
3	E	403	NAG	C3-C2-N2	-2.89	107.36	111.76
3	E	401	NAG	C2-N2-C7	-2.84	118.32	123.09
4	E	413	NAG	O5-C5-C4	-2.79	107.11	110.65
4	E	414	BMA	O5-C5-C4	-2.61	107.34	110.65
4	E	412	FUC	O2-C2-C3	2.57	115.73	110.18
4	E	414	BMA	O6-C6-C5	-2.30	103.43	111.36
4	E	414	BMA	C3-C4-C5	-2.29	106.11	110.20
3	E	401	NAG	O6-C6-C5	-2.27	103.55	111.36
4	E	416	NDG	O3-C3-C4	-2.24	105.34	110.35
3	E	405	MAN	C4-C3-C2	-2.17	107.59	110.50
3	E	402	FUC	O3-C3-C2	-2.10	106.09	109.94
3	E	402	FUC	C4-C3-C2	-2.06	107.74	110.50
3	E	406	NAG	O5-C5-C4	-2.06	108.04	110.65
3	E	402	FUC	O5-C5-C4	-2.01	107.19	110.22

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	416	NDG	C3
4	E	417	GLC	C3

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	417	GLC	C1-C2-C3-C4-C5-O5

5.6 Ligand geometry

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.