



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:51 PM GMT

PDB ID : 1HNE  
Title : Structure of human neutrophil elastase in complex with a peptide chloromethyl ketone inhibitor at 1.84-angstroms resolution  
Authors : Navia, M.A.; Mckeever, B.M.; Springer, J.P.; Lin, T.-Y.; Williams, H.R.; Fluder, E.M.; Dorn, C.P.; Hoogsteen, K.  
Deposited on : 1989-04-10  
Resolution : 1.84 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

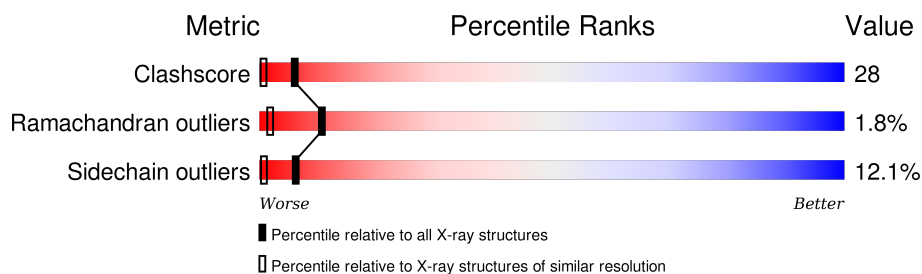
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	218	 66% 23% 9% •
2	I	6	 83% 17%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1892 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 HUMAN LEUCOCYTE ELASTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	218	Total	C	N	O	S	0	0	0
			1636	1026	315	284	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	91	ASP	ASN	CONFLICT	UNP P08246

- Molecule 2 is a protein called METHOXYSUCCINYL-ALA-ALA-PRO-ALA CHLOROMETHYL KETONE INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	6	Total	C	N	O	0	0	1
			31	20	4	7			

- Molecule 3 is water.

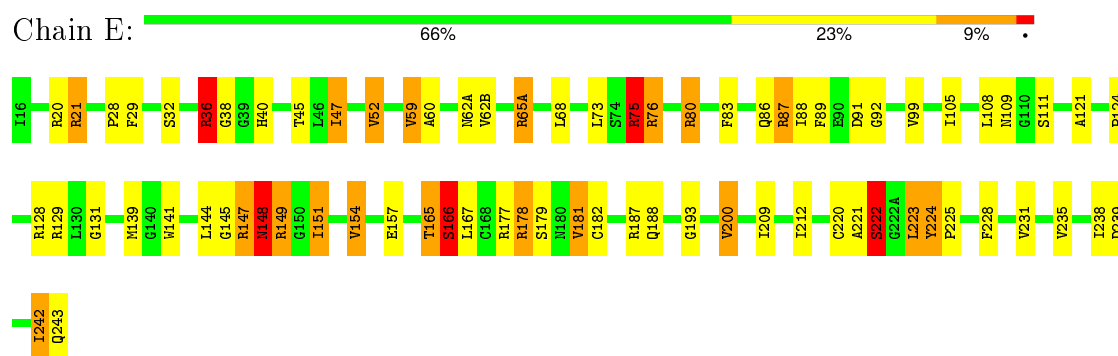
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	220	Total	O	0	0
			220	220		
3	I	5	Total	O	0	0
			5	5		

### 3 Residue-property plots

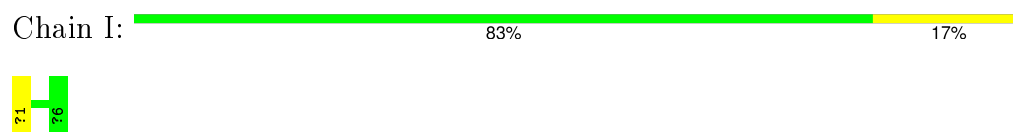
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 LEUCOCYTE ELASTASE



#### • Molecule 2: METHOXYSUCCINYL-ALA-ALA-PRO-ALA CHLOROMETHYL KETONE INHIBITOR



## 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, $\alpha$ , $\beta$ , $\gamma$	74.53Å 74.53Å 70.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.84	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.84)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.164 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ALV, MSU, 0QE

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	1.14	5/1666 (0.3%)	1.75	42/2263 (1.9%)
2	I	1.29	0/17	1.60	0/23
All	All	1.14	5/1683 (0.3%)	1.75	42/2286 (1.8%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	92	GLY	N-CA	10.12	1.61	1.46
1	E	220	CYS	C-O	9.72	1.41	1.23
1	E	222	SER	CA-CB	7.15	1.63	1.52
1	E	157	GLU	CD-OE1	-6.85	1.18	1.25
1	E	223	LEU	C-N	-5.36	1.21	1.34

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	21	ARG	NE-CZ-NH2	13.96	127.28	120.30
1	E	75	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	E	147	ARG	C-N-CA	10.06	146.85	121.70
1	E	20	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	E	220	CYS	N-CA-C	9.44	136.49	111.00
1	E	200	VAL	CA-CB-CG1	9.04	124.47	110.90
1	E	147	ARG	CB-CA-C	8.99	128.38	110.40
1	E	147	ARG	CA-C-O	7.67	136.21	120.10
1	E	47	ILE	CA-CB-CG2	7.51	125.91	110.90
1	E	147	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	E	154	VAL	CA-CB-CG1	7.05	121.47	110.90
1	E	52	VAL	CG1-CB-CG2	7.02	122.13	110.90
1	E	220	CYS	C-N-CA	7.01	139.22	121.70
1	E	91	ASP	CB-CA-C	6.94	124.28	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	59	VAL	N-CA-CB	-6.79	96.55	111.50
1	E	21	ARG	NH1-CZ-NH2	-6.79	111.93	119.40
1	E	91	ASP	CA-C-N	6.70	129.60	116.20
1	E	59	VAL	CG1-CB-CG2	6.62	121.48	110.90
1	E	222	SER	CA-CB-OG	-6.14	94.62	111.20
1	E	220	CYS	CA-CB-SG	-6.08	103.05	114.00
1	E	80	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	E	65(A)	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	E	187	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	E	91	ASP	C-N-CA	-5.98	109.74	122.30
1	E	231	VAL	CA-CB-CG1	5.90	119.75	110.90
1	E	165	THR	CA-C-O	-5.88	107.74	120.10
1	E	36	ARG	CD-NE-CZ	5.81	131.73	123.60
1	E	200	VAL	CB-CA-C	5.69	122.20	111.40
1	E	147	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	E	68	LEU	CB-CG-CD1	5.49	120.34	111.00
1	E	52	VAL	N-CA-CB	-5.42	99.58	111.50
1	E	223	LEU	N-CA-C	-5.38	96.48	111.00
1	E	166	SER	N-CA-CB	-5.33	102.50	110.50
1	E	148	ASN	N-CA-CB	5.29	120.13	110.60
1	E	223	LEU	C-N-CA	5.28	134.89	121.70
1	E	75	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	E	165	THR	CA-C-N	5.26	128.76	117.20
1	E	165	THR	N-CA-C	-5.22	96.89	111.00
1	E	148	ASN	N-CA-C	-5.18	97.01	111.00
1	E	36	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	E	220	CYS	N-CA-CB	-5.14	101.35	110.60
1	E	177	ARG	NE-CZ-NH1	-5.12	117.74	120.30

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	E	1636	0	1646	95	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	31	0	28	2	0
3	E	220	0	0	31	1
3	I	5	0	0	0	0
All	All	1892	0	1674	95	1

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 28.

All (95) 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:E:108:LEU:HB3	3:E:306:HOH:O	1.25	1.29
1:E:87:ARG:HB2	1:E:87:ARG:NH2	1.45	1.27
1:E:87:ARG:CB	1:E:87:ARG:HH21	1.49	1.24
1:E:224:TYR:N	3:E:253:HOH:O	1.71	1.19
1:E:165:THR:O	1:E:166:SER:HB3	1.32	1.12
1:E:121:ALA:HB1	1:E:209:ILE:HD11	1.25	1.12
1:E:222:SER:HB3	1:E:223:LEU:O	1.55	1.06
1:E:165:THR:O	1:E:166:SER:CB	2.02	1.06
1:E:121:ALA:CB	1:E:209:ILE:HD11	1.86	1.04
1:E:121:ALA:HB1	1:E:209:ILE:CD1	1.87	1.04
1:E:148:ASN:O	1:E:149:ARG:HD3	1.59	1.02
1:E:45:THR:HG21	1:E:209:ILE:HD13	1.43	0.99
1:E:139:MET:HE2	3:E:286:HOH:O	1.65	0.94
1:E:36:ARG:HG2	1:E:38:GLY:N	1.83	0.93
1:E:148:ASN:C	1:E:149:ARG:HD3	1.94	0.87
1:E:121:ALA:CB	1:E:209:ILE:CD1	2.52	0.84
1:E:212:ILE:HD12	3:E:402:HOH:O	1.75	0.84
1:E:181:VAL:HG13	1:E:228:PHE:HB2	1.58	0.84
1:E:222:SER:CB	1:E:223:LEU:O	2.26	0.82
1:E:149:ARG:HG2	3:E:416:HOH:O	1.82	0.79
1:E:223:LEU:C	3:E:253:HOH:O	2.06	0.78
1:E:75:ARG:HH11	1:E:76:ARG:H	1.33	0.74
1:E:21:ARG:NH1	3:E:439:HOH:O	2.20	0.73
1:E:62(B):VAL:HG11	1:E:88:ILE:HD11	1.68	0.73
1:E:105:ILE:HD11	1:E:238:ILE:HG12	1.70	0.73
1:E:224:TYR:CZ	2:I:1:MSU:HT1	2.24	0.72
1:E:45:THR:HG21	1:E:209:ILE:CD1	2.18	0.72
1:E:223:LEU:CA	3:E:253:HOH:O	2.36	0.72
1:E:36:ARG:CG	1:E:38:GLY:N	2.51	0.71
1:E:83:PHE:CD2	3:E:306:HOH:O	2.45	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:ARG:HB2	1:E:87:ARG:HH21	0.60	0.70
1:E:139:MET:HB3	3:E:286:HOH:O	1.93	0.68
1:E:60:ALA:O	3:E:329:HOH:O	2.13	0.66
1:E:212:ILE:CD1	3:E:402:HOH:O	2.38	0.66
1:E:222:SER:HB3	1:E:223:LEU:H	1.60	0.65
1:E:21:ARG:NE	3:E:284:HOH:O	2.26	0.65
1:E:75:ARG:NH1	1:E:76:ARG:H	1.94	0.64
1:E:222:SER:HB2	3:E:246:HOH:O	1.97	0.63
1:E:148:ASN:O	1:E:149:ARG:HB2	2.00	0.61
1:E:128:ARG:HD3	3:E:285:HOH:O	1.99	0.61
1:E:36:ARG:CG	1:E:38:GLY:H	2.14	0.61
1:E:83:PHE:HB3	3:E:306:HOH:O	2.02	0.60
1:E:242:ILE:CG2	1:E:243:GLN:N	2.67	0.57
1:E:29:PHE:HZ	3:E:446:HOH:O	1.85	0.57
1:E:29:PHE:CZ	3:E:446:HOH:O	2.52	0.57
1:E:178:ARG:O	1:E:178:ARG:HG2	2.05	0.56
1:E:121:ALA:HB1	1:E:209:ILE:HD12	1.84	0.56
1:E:148:ASN:HB2	1:E:149:ARG:CD	2.35	0.56
1:E:109:ASN:ND2	3:E:406:HOH:O	2.38	0.54
1:E:223:LEU:HA	3:E:253:HOH:O	2.04	0.53
1:E:148:ASN:O	1:E:149:ARG:CB	2.57	0.53
1:E:148:ASN:OD1	1:E:149:ARG:NH1	2.41	0.53
1:E:148:ASN:HB2	1:E:149:ARG:HD3	1.91	0.52
1:E:242:ILE:HG22	1:E:243:GLN:H	1.74	0.52
1:E:179:SER:HB3	3:E:435:HOH:O	2.09	0.52
1:E:65(A):ARG:HG2	3:E:381:HOH:O	2.11	0.51
1:E:148:ASN:CG	1:E:149:ARG:HH11	2.14	0.51
1:E:32:SER:OG	1:E:40:HIS:HD2	1.93	0.51
1:E:178:ARG:NH2	3:E:384:HOH:O	2.43	0.50
1:E:124:PRO:O	1:E:235:VAL:HG21	2.10	0.50
1:E:87:ARG:HD2	1:E:89:PHE:CZ	2.46	0.50
1:E:239:ASP:HA	1:E:242:ILE:HG22	1.94	0.49
1:E:144:LEU:HB2	1:E:149:ARG:CB	2.42	0.49
1:E:242:ILE:HG22	1:E:243:GLN:N	2.26	0.49
1:E:21:ARG:CD	3:E:284:HOH:O	2.61	0.48
1:E:28:PRO:O	3:E:393:HOH:O	2.20	0.48
1:E:148:ASN:O	1:E:149:ARG:CD	2.47	0.47
1:E:76:ARG:HG2	1:E:76:ARG:O	2.14	0.47
1:E:145:GLY:O	1:E:147:ARG:HG2	2.14	0.47
1:E:73:LEU:HA	1:E:80:ARG:HH22	1.80	0.47
1:E:36:ARG:O	3:E:331:HOH:O	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:ARG:HG3	1:E:76:ARG:HH11	1.81	0.46
1:E:80:ARG:HD2	3:E:395:HOH:O	2.16	0.46
1:E:40:HIS:HE1	1:E:193:GLY:O	1.99	0.46
1:E:83:PHE:CG	3:E:306:HOH:O	2.68	0.45
1:E:148:ASN:HB2	1:E:149:ARG:HD2	1.97	0.45
1:E:238:ILE:O	1:E:242:ILE:HB	2.16	0.45
1:E:76:ARG:HG3	1:E:76:ARG:NH1	2.31	0.45
1:E:128:ARG:NH2	3:E:394:HOH:O	2.50	0.45
1:E:144:LEU:HB2	1:E:149:ARG:HB3	1.98	0.44
1:E:121:ALA:CB	1:E:209:ILE:HD12	2.43	0.44
1:E:62(B):VAL:HG11	1:E:88:ILE:CD1	2.43	0.44
1:E:148:ASN:C	1:E:149:ARG:CD	2.77	0.43
1:E:86:GLN:HG3	3:E:440:HOH:O	2.18	0.43
1:E:141:TRP:O	1:E:151:ILE:HG23	2.18	0.43
1:E:131:GLY:N	3:E:291:HOH:O	2.01	0.43
1:E:87:ARG:CG	1:E:87:ARG:HH21	2.21	0.43
1:E:76:ARG:CG	1:E:76:ARG:O	2.67	0.42
1:E:62(B):VAL:CG1	1:E:88:ILE:HD11	2.42	0.42
1:E:87:ARG:CB	1:E:87:ARG:NH2	2.34	0.41
1:E:144:LEU:HB2	1:E:149:ARG:HB2	2.02	0.41
1:E:182:CYS:HB3	1:E:225:PRO:HB2	2.02	0.41
1:E:62(B):VAL:HG21	1:E:88:ILE:HD11	2.03	0.40
1:E:75:ARG:HA	1:E:75:ARG:HD2	1.58	0.40
1:E:224:TYR:CZ	2:I:1:MSU:CT	3.02	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:ALA:N	3:E:249:HOH:O[3_665]	1.88	0.32

## 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%)	10	1
2	I	2/6 (33%)	2 (100%)	0	0	100	100
All	All	218/224 (97%)	203 (93%)	11 (5%)	4 (2%)	11	2

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	166	SER
1	E	224	TYR
1	E	148	ASN
1	E	149	ARG

### 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%)	151 (88%)	21 (12%)	6	1
2	I	1/1 (100%)	1 (100%)	0	100	100
All	All	173/173 (100%)	152 (88%)	21 (12%)	6	1

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	36	ARG
1	E	47	ILE
1	E	52	VAL
1	E	59	VAL
1	E	62(A)	ASN
1	E	75	ARG
1	E	76	ARG
1	E	87	ARG
1	E	99	VAL
1	E	111	SER

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Mol	Chain	Res	Type
1	E	129	ARG
1	E	148	ASN
1	E	151	ILE
1	E	154	VAL
1	E	167	LEU
1	E	178	ARG
1	E	181	VAL
1	E	188	GLN
1	E	200	VAL
1	E	222	SER
1	E	242	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	34	GLN
1	E	40	HIS
1	E	62(A)	ASN
1	E	101	ASN
1	E	117	ASN
1	E	119	GLN
1	E	210	HIS
1	E	236	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	ALV	I	5	1,2	4,4,5	0.37	0	2,4,6	0.21	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	ALV	I	5	1,2	-	0/2/2/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 ⓘ

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.