Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 02:23 PM EDT

PDB ID	:	2ER0
Title	:	X-RAY STUDIES OF ASPARTIC PROTEINASE-STATINE INHIBITOR COMPLEXES
Authors	:	Cooper, J.B.; Foundling, S.I.; Boger, J.; Blundell, T.L.
Deposited on	:	1990-10-20
Resolution	:	3.00 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

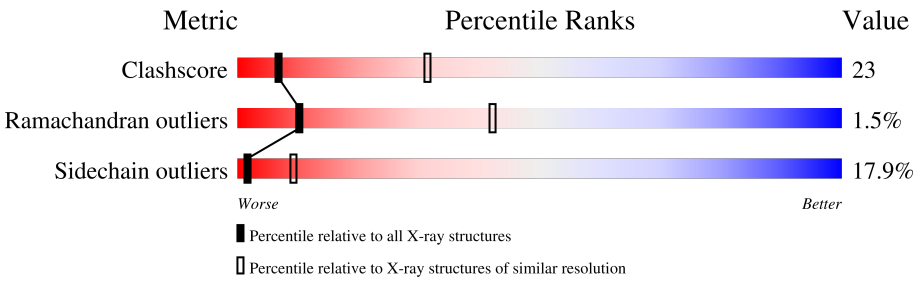
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	330	55% 35% 8% •
2	I	8	38% 38% 12% 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2456 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 ENDOTHIAPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	330	2389	1514	366	507	2	0	0	0

- Molecule 2 is a protein called L364,099.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	8	67	48	11	8	0	0	1

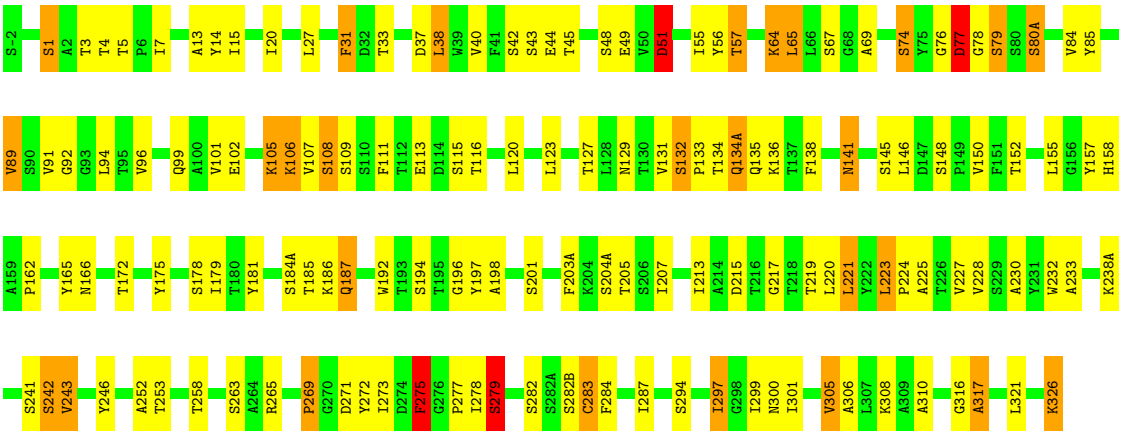
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

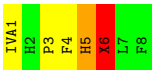
• Molecule 1: ENDOTHIAPEPSIN

Chain E: 55% 35% 8%



• Molecule 2: L364,099

Chain I: 38% 38% 12% 12%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.00Å 75.80Å 42.80Å 90.00° 97.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.280 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2456	wwPDB-VP
Average B, all atoms ($Å^2$)	0.0	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: IVA, CHS

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	1.03	7/2445 (0.3%)	1.50	27/3345 (0.8%)
2	I	1.05	0/49	1.09	0/65
All	All	1.03	7/2494 (0.3%)	1.49	27/3410 (0.8%)

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	3
2	I	0	2
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	187	GLN	CD-OE1	6.46	1.38	1.24
1	E	242	SER	CB-OG	6.31	1.50	1.42
1	E	44	GLU	C-N	-6.20	1.19	1.34
1	E	192	TRP	NE1-CE2	-5.34	1.30	1.37
1	E	141	ASN	CG-OD1	5.16	1.35	1.24
1	E	232	TRP	NE1-CE2	-5.13	1.30	1.37
1	E	326	LYS	C-OXT	5.06	1.32	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	275	PHE	CB-CG-CD1	-10.01	113.80	120.80
1	E	227	VAL	CA-CB-CG2	8.65	123.87	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	150	VAL	CA-CB-CG1	8.28	123.32	110.90
1	E	96	VAL	CA-CB-CG2	8.24	123.26	110.90
1	E	101	VAL	CA-CB-CG2	7.68	122.42	110.90
1	E	265	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	E	89	VAL	CA-CB-CG2	7.32	121.88	110.90
1	E	40	VAL	CA-CB-CG2	6.63	120.85	110.90
1	E	271	ASP	CB-CG-OD1	6.55	124.20	118.30
1	E	91	VAL	CA-CB-CG2	6.47	120.60	110.90
1	E	283	CYS	N-CA-CB	-6.43	99.02	110.60
1	E	51	ASP	CB-CG-OD2	6.22	123.90	118.30
1	E	275	PHE	CG-CD2-CE2	-6.17	114.01	120.80
1	E	84	VAL	CA-CB-CG2	6.10	120.04	110.90
1	E	85	TYR	CB-CG-CD2	-5.89	117.46	121.00
1	E	275	PHE	CA-CB-CG	-5.75	100.11	113.90
1	E	165	TYR	O-C-N	5.64	131.73	122.70
1	E	275	PHE	CD1-CG-CD2	5.63	125.62	118.30
1	E	225	ALA	O-C-N	-5.43	114.00	122.70
1	E	243	VAL	CA-CB-CG2	5.38	118.97	110.90
1	E	279	SER	O-C-N	-5.36	114.12	122.70
1	E	51	ASP	CA-CB-CG	5.33	125.14	113.40
1	E	284	PHE	CB-CG-CD1	-5.26	117.12	120.80
1	E	185	THR	CA-CB-CG2	-5.20	105.12	112.40
1	E	284	PHE	CG-CD2-CE2	-5.12	115.17	120.80
1	E	279	SER	C-N-CA	-5.10	108.94	121.70
1	E	165	TYR	C-N-CA	5.06	134.35	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	115	SER	Mainchain
1	E	31	PHE	Mainchain
1	E	38	LEU	Mainchain
2	I	6	CHS	Mainchain,Peptide

5.2 Too-close contacts (i)

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	2389	0	2279	110	0
2	I	67	0	68	15	0
All	All	2456	0	2347	112	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 23.

All (112) 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:64:LYS:HD2	1:E:65:LEU:N	1.34	1.43
1:E:64:LYS:CD	1:E:65:LEU:H	1.61	1.11
1:E:120:LEU:HD21	2:I:6:CHS:HD23	1.28	1.10
1:E:64:LYS:CD	1:E:65:LEU:N	2.21	1.02
1:E:301:ILE:CD1	2:I:5:HIS:CE1	2.44	1.00
2:I:1:IVA:HG13	2:I:3:PRO:HD3	1.55	0.89
1:E:64:LYS:HD2	1:E:64:LYS:C	1.75	0.87
1:E:20:ILE:HD12	1:E:27:LEU:HD13	1.58	0.86
1:E:310:ALA:C	1:E:326:LYS:HD3	1.97	0.84
1:E:205:THR:O	1:E:205:THR:HG23	1.75	0.84
1:E:301:ILE:CD1	2:I:5:HIS:HE1	1.88	0.83
1:E:107:VAL:CG1	1:E:111:PHE:HB2	2.09	0.83
1:E:297:ILE:HD13	2:I:5:HIS:NE2	1.95	0.82
1:E:4:THR:O	1:E:4:THR:CG2	2.28	0.81
1:E:129:ASN:HB3	1:E:134(A):GLN:HG2	1.64	0.80
1:E:77:ASP:HB3	1:E:79:SER:HB2	1.64	0.79
1:E:64:LYS:CE	1:E:65:LEU:H	1.98	0.76
1:E:269:PRO:O	1:E:273:ILE:HD12	1.86	0.75
1:E:64:LYS:HE3	1:E:65:LEU:HB2	1.69	0.75
1:E:301:ILE:HD13	2:I:5:HIS:HE1	1.49	0.75
1:E:220:LEU:HA	1:E:305:VAL:CG1	2.16	0.74
1:E:64:LYS:HD2	1:E:65:LEU:H	0.94	0.74
1:E:219:THR:O	1:E:305:VAL:HG12	1.87	0.74
1:E:107:VAL:HG11	1:E:111:PHE:HB2	1.71	0.73
1:E:301:ILE:HD12	2:I:5:HIS:CE1	2.24	0.72
1:E:136:LYS:HE3	1:E:141:ASN:ND2	2.06	0.69
1:E:277:PRO:HA	1:E:283:CYS:HA	1.72	0.69
1:E:221:LEU:HD13	1:E:223:LEU:HD22	1.76	0.68
1:E:1:SER:HB3	1:E:166:ASN:ND2	2.11	0.66
1:E:129:ASN:ND2	1:E:131:VAL:H	1.94	0.65
1:E:4:THR:O	1:E:4:THR:HG23	1.95	0.65
1:E:294:SER:O	1:E:297:ILE:HG23	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:ALA:HB2	2:I:4:PHE:CD2	2.33	0.64
1:E:38:LEU:O	1:E:102:GLU:HG3	1.99	0.62
1:E:207:ILE:HG22	1:E:207:ILE:O	1.99	0.62
1:E:77:ASP:HB3	1:E:79:SER:H	1.64	0.62
1:E:7:ILE:HG23	1:E:13:ALA:O	2.01	0.61
1:E:152:THR:OG1	1:E:166:ASN:HB2	2.01	0.60
1:E:179:ILE:HG21	1:E:181:TYR:CZ	2.37	0.60
1:E:129:ASN:HD21	1:E:131:VAL:HB	1.67	0.59
1:E:310:ALA:O	1:E:326:LYS:HD3	2.02	0.59
1:E:220:LEU:HA	1:E:305:VAL:HG12	1.85	0.59
1:E:301:ILE:HD11	2:I:5:HIS:CE1	2.38	0.58
1:E:64:LYS:HE3	1:E:65:LEU:H	1.67	0.57
1:E:278:ILE:HG13	1:E:279:SER:N	2.19	0.57
1:E:224:PRO:HD3	1:E:300:ASN:ND2	2.19	0.57
1:E:51:ASP:OD1	1:E:113:GLU:HA	2.04	0.57
1:E:273:ILE:HG22	1:E:273:ILE:O	2.06	0.56
1:E:220:LEU:HA	1:E:305:VAL:HG11	1.88	0.55
1:E:4:THR:O	1:E:4:THR:HG22	2.03	0.55
1:E:205:THR:O	1:E:205:THR:CG2	2.50	0.55
1:E:99:GLN:NE2	1:E:138:PHE:HA	2.23	0.54
1:E:301:ILE:HD13	2:I:5:HIS:CE1	2.30	0.53
1:E:43:SER:HB3	1:E:57:THR:HG23	1.89	0.53
1:E:31:PHE:CD2	1:E:31:PHE:N	2.77	0.53
1:E:219:THR:HG22	1:E:275:PHE:CZ	2.44	0.53
1:E:13:ALA:HB2	2:I:4:PHE:CE2	2.45	0.52
1:E:31:PHE:N	1:E:31:PHE:HD2	2.07	0.52
1:E:38:LEU:C	1:E:38:LEU:HD23	2.31	0.52
1:E:221:LEU:HD13	1:E:223:LEU:CD2	2.39	0.51
1:E:132:SER:CB	1:E:133:PRO:HA	2.40	0.51
1:E:111:PHE:HE1	2:I:6:CHS:HZ3	1.77	0.50
1:E:301:ILE:CD1	2:I:5:HIS:NE2	2.74	0.50
1:E:77:ASP:CB	1:E:79:SER:HB2	2.40	0.49
1:E:74:SER:HA	1:E:79:SER:O	2.12	0.49
1:E:76:GLY:C	1:E:78:GLY:H	2.16	0.49
1:E:7:ILE:CG2	1:E:15:ILE:HG23	2.43	0.48
1:E:197:TYR:HA	1:E:258:THR:O	2.13	0.48
1:E:228:VAL:HG22	1:E:287:ILE:CG2	2.44	0.48
1:E:69:ALA:HA	1:E:132:SER:O	2.14	0.48
1:E:172:THR:HA	1:E:175:TYR:CE1	2.48	0.48
1:E:129:ASN:ND2	1:E:135:GLN:H	2.11	0.48
2:I:1:IVA:HG13	2:I:3:PRO:CD	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:VAL:HG11	1:E:111:PHE:CB	2.41	0.47
1:E:219:THR:CG2	1:E:275:PHE:CZ	2.98	0.47
1:E:228:VAL:HG12	1:E:246:TYR:CE1	2.49	0.47
1:E:230:ALA:O	1:E:233:ALA:HB3	2.15	0.47
1:E:316:GLY:C	1:E:317:ALA:O	2.52	0.46
1:E:42:SER:HB2	1:E:56:TYR:O	2.16	0.46
1:E:129:ASN:ND2	1:E:131:VAL:HB	2.31	0.46
1:E:111:PHE:CE1	2:I:6:CHS:HZ3	2.50	0.46
1:E:94:LEU:CD2	1:E:146:LEU:HD21	2.45	0.46
1:E:221:LEU:HG	1:E:306:ALA:HB2	1.98	0.46
1:E:77:ASP:HB3	1:E:79:SER:N	2.31	0.46
1:E:157:TYR:CE1	1:E:158:HIS:NE2	2.85	0.45
1:E:157:TYR:CZ	1:E:158:HIS:CD2	3.05	0.44
1:E:278:ILE:HG13	1:E:279:SER:H	1.81	0.44
1:E:3:THR:CG2	1:E:4:THR:N	2.80	0.44
1:E:1:SER:HB3	1:E:166:ASN:HD21	1.82	0.44
1:E:297:ILE:CD1	1:E:301:ILE:HD11	2.48	0.43
1:E:94:LEU:HD21	1:E:146:LEU:HD21	2.01	0.43
1:E:3:THR:HG22	1:E:4:THR:N	2.34	0.43
1:E:196:GLY:HA3	1:E:203(A):PHE:CZ	2.54	0.43
1:E:198:ALA:HB2	1:E:203(A):PHE:HA	2.01	0.43
1:E:49:GLU:OE2	1:E:106:LYS:HE3	2.19	0.42
1:E:64:LYS:HD3	1:E:64:LYS:HA	1.74	0.42
1:E:243:VAL:O	1:E:243:VAL:HG12	2.20	0.42
1:E:14:TYR:CD2	1:E:155:LEU:HD22	2.55	0.41
1:E:33:THR:HG22	1:E:123:LEU:HB2	2.01	0.41
1:E:45:THR:HA	1:E:105:LYS:O	2.20	0.41
1:E:42:SER:HA	1:E:55:ILE:HB	2.02	0.41
1:E:228:VAL:HG22	1:E:287:ILE:HG23	2.03	0.41
1:E:194:SER:HB3	1:E:207:ILE:HB	2.02	0.41
1:E:197:TYR:CD2	1:E:197:TYR:C	2.93	0.41
1:E:213:ILE:HD12	1:E:215:ASP:HB2	2.02	0.41
1:E:215:ASP:C	1:E:217:GLY:H	2.24	0.41
1:E:89:VAL:HG23	1:E:99:GLN:HB3	2.03	0.40
1:E:136:LYS:HE3	1:E:141:ASN:HD22	1.81	0.40
1:E:273:ILE:O	1:E:273:ILE:CG2	2.68	0.40
1:E:1:SER:O	1:E:92:GLY:HA3	2.20	0.40
1:E:269:PRO:HB2	1:E:272:TYR:CD1	2.56	0.40
1:E:321:LEU:HD12	1:E:321:LEU:HA	1.91	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	E	328/330 (99%)	308 (94%)	15 (5%)	5 (2%)	10 42
2	I	5/8 (62%)	5 (100%)	0	0	100 100
All	All	333/338 (98%)	313 (94%)	15 (4%)	5 (2%)	10 42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	77	ASP
1	E	108	SER
1	E	252	ALA
1	E	317	ALA
1	E	80(A)	SER

5.3.2 Protein sidechains (i)

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	263/263 (100%)	216 (82%)	47 (18%)	2 9
2	I	5/6 (83%)	4 (80%)	1 (20%)	1 7
All	All	268/269 (100%)	220 (82%)	48 (18%)	2 9

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1	SER

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Mol	Chain	Res	Type
1	E	5	THR
1	E	37	ASP
1	E	48	SER
1	E	51	ASP
1	E	57	THR
1	E	64	LYS
1	E	65	LEU
1	E	67	SER
1	E	74	SER
1	E	77	ASP
1	E	79	SER
1	E	80(A)	SER
1	E	105	LYS
1	E	106	LYS
1	E	108	SER
1	E	109	SER
1	E	116	THR
1	E	127	THR
1	E	132	SER
1	E	134	THR
1	E	134(A)	GLN
1	E	145	SER
1	E	148	SER
1	E	162	PRO
1	E	178	SER
1	E	184(A)	SER
1	E	186	LYS
1	E	187	GLN
1	E	201	SER
1	E	204(A)	SER
1	E	221	LEU
1	E	223	LEU
1	E	238(A)	LYS
1	E	241	SER
1	E	242	SER
1	E	253	THR
1	E	263	SER
1	E	269	PRO
1	E	275	PHE
1	E	279	SER
1	E	282	SER
1	E	282(B)	SER

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Mol	Chain	Res	Type
1	E	297	ILE
1	E	299	ILE
1	E	305	VAL
1	E	308	LYS
2	I	5	HIS

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

Mol	Chain	Res	Type
1	E	99	GLN
1	E	129	ASN
1	E	134(A)	GLN
1	E	135	GLN
1	E	141	ASN
1	E	166	ASN
1	E	300	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	CHS	I	6	2	14,14,15	1.24	1 (7%)	13,17,19	0.81	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	CHS	I	6	2	-	3/11/19/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	6	CHS	CD2-CG	-3.88	1.41	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	6	CHS	O-C-CM-CH
2	I	6	CHS	CA-CH-CM-C
2	I	6	CHS	OH-CH-CM-C

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	6	CHS	3	0

5.5 Carbohydrates (i)

There are no monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	44:GLU	C	45:THR	N	1.19

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.