Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 01:54 AM GMT

PDB ID	:	2EST
Title	:	Crystallographic study of the binding of a trifluoroacetyl dipeptide anilide inhibitor with elastase
Authors	:	Sieker, L.C.; Hughes, D.L.
Deposited on	:	1986-03-24
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/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:

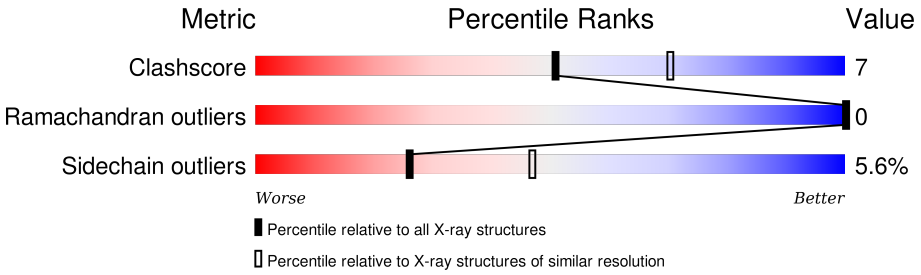
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	240	31% 56% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1899 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.

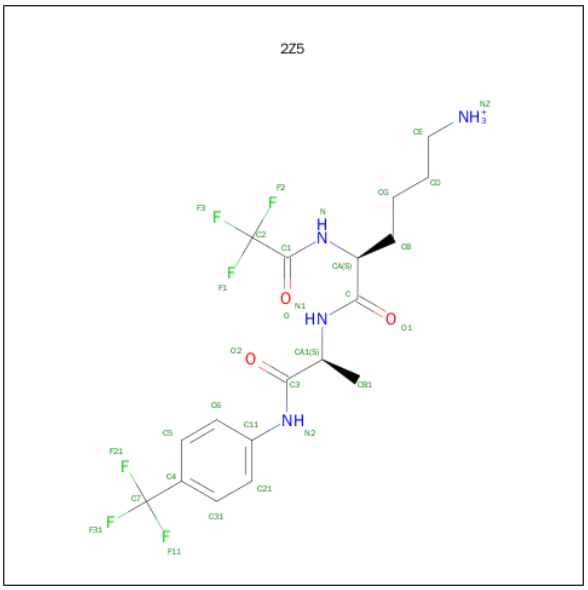
- Molecule 1 is a protein called ELASTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	240	1822	1135	330	347	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

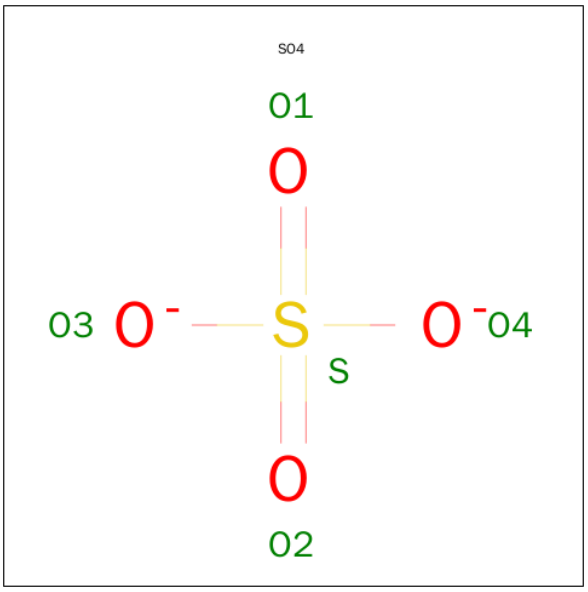
Chain	Residue	Modelled	Actual	Comment	Reference
E	77	ASN	ASP	CONFLICT	UNP P00772

- Molecule 2 is 6-AMMONIO-N-(TRIFLUOROACETYL)-L-NORLEUCYL-N-[4-(TRIFLUOROMETHYL)PHENYL]-L-ALANINAMIDE (three-letter code: 2Z5) (formula: $C_{18}H_{23}F_6N_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	E	1	31	18	6	4	3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total S 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	45	Total O 45 45	0	0

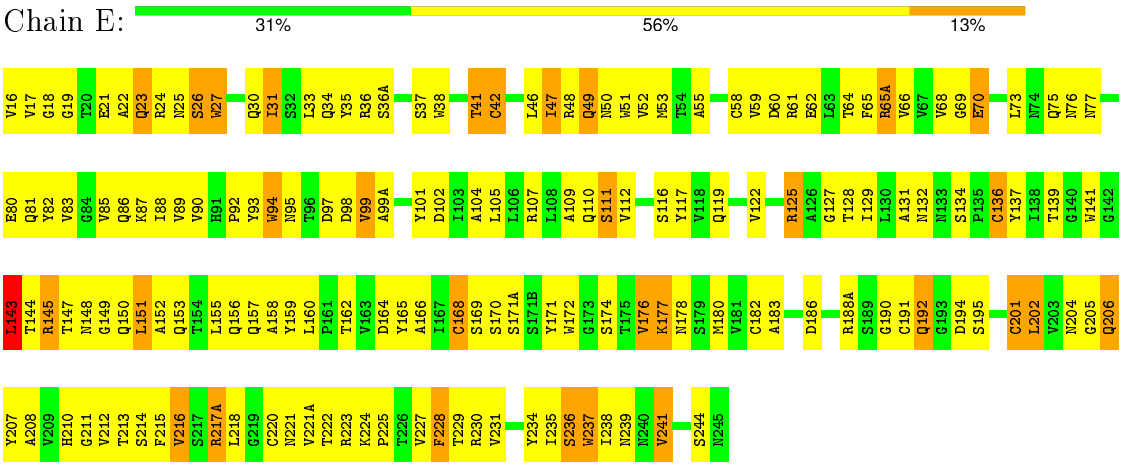
3 Residue-property plots (i)

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: ELASTASE

Chain E:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.53Å 57.47Å 75.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1899	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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: 2Z5, SO4

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	2.01	48/1862 (2.6%)	3.61	301/2543 (11.8%)

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

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	62	GLU	CD-OE2	-9.26	1.15	1.25
1	E	174	SER	CB-OG	8.70	1.53	1.42
1	E	171(A)	SER	CB-OG	8.14	1.52	1.42
1	E	94	TRP	NE1-CE2	-7.34	1.28	1.37
1	E	237	TRP	NE1-CE2	-7.28	1.28	1.37
1	E	51	TRP	NE1-CE2	-7.11	1.28	1.37
1	E	36	ARG	CZ-NH1	7.10	1.42	1.33
1	E	172	TRP	NE1-CE2	-7.09	1.28	1.37
1	E	37	SER	CB-OG	7.06	1.51	1.42
1	E	93	TYR	CG-CD1	7.02	1.48	1.39
1	E	61	ARG	NE-CZ	6.70	1.41	1.33
1	E	82	TYR	CD1-CE1	6.57	1.49	1.39
1	E	210	HIS	C-O	6.38	1.35	1.23
1	E	80	GLU	CD-OE2	-6.35	1.18	1.25
1	E	42	CYS	CB-SG	6.30	1.93	1.82
1	E	153	GLN	CD-OE1	6.22	1.37	1.24
1	E	61	ARG	CZ-NH1	6.17	1.41	1.33
1	E	110	GLN	CD-OE1	6.17	1.37	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	141	TRP	NE1-CE2	-6.16	1.29	1.37
1	E	62	GLU	CD-OE1	-6.15	1.18	1.25
1	E	38	TRP	CB-CG	6.08	1.61	1.50
1	E	223	ARG	NE-CZ	6.01	1.40	1.33
1	E	159	TYR	CE1-CZ	-5.88	1.30	1.38
1	E	172	TRP	CB-CG	5.80	1.60	1.50
1	E	27	TRP	NE1-CE2	-5.79	1.30	1.37
1	E	137	TYR	CD1-CE1	5.75	1.48	1.39
1	E	69	GLY	N-CA	-5.64	1.37	1.46
1	E	149	GLY	C-O	5.61	1.32	1.23
1	E	50	ASN	CG-ND2	5.61	1.46	1.32
1	E	93	TYR	CD1-CE1	5.61	1.47	1.39
1	E	36	ARG	NE-CZ	5.52	1.40	1.33
1	E	129	ILE	C-O	5.49	1.33	1.23
1	E	178	ASN	CG-ND2	5.48	1.46	1.32
1	E	38	TRP	NE1-CE2	-5.48	1.30	1.37
1	E	214	SER	CB-OG	5.37	1.49	1.42
1	E	36	ARG	CZ-NH2	5.37	1.40	1.33
1	E	125	ARG	NE-CZ	5.35	1.40	1.33
1	E	215	PHE	CG-CD2	-5.30	1.30	1.38
1	E	48	ARG	CZ-NH1	5.28	1.40	1.33
1	E	149	GLY	N-CA	-5.25	1.38	1.46
1	E	101	TYR	CD2-CE2	5.21	1.47	1.39
1	E	24	ARG	NE-CZ	5.19	1.39	1.33
1	E	225	PRO	N-CD	-5.18	1.40	1.47
1	E	152	ALA	C-O	5.18	1.33	1.23
1	E	159	TYR	CG-CD1	5.17	1.45	1.39
1	E	223	ARG	CZ-NH1	5.16	1.39	1.33
1	E	165	TYR	CG-CD1	5.14	1.45	1.39
1	E	21	GLU	CG-CD	5.13	1.59	1.51

All (301) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	107	ARG	NE-CZ-NH2	40.32	140.46	120.30
1	E	230	ARG	NE-CZ-NH1	-26.96	106.82	120.30
1	E	107	ARG	NE-CZ-NH1	-23.64	108.48	120.30
1	E	164	ASP	CB-CG-OD1	22.15	138.24	118.30
1	E	36	ARG	NE-CZ-NH1	22.03	131.32	120.30
1	E	194	ASP	CB-CG-OD2	20.25	136.52	118.30
1	E	223	ARG	NE-CZ-NH1	18.54	129.57	120.30
1	E	207	TYR	CB-CG-CD1	17.94	131.76	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	82	TYR	CB-CG-CD1	-17.34	110.60	121.00
1	E	60	ASP	CB-CG-OD2	-17.19	102.83	118.30
1	E	186	ASP	CB-CG-OD1	17.13	133.72	118.30
1	E	207	TYR	CB-CG-CD2	-15.82	111.50	121.00
1	E	217(A)	ARG	CD-NE-CZ	15.36	145.11	123.60
1	E	234	TYR	CB-CG-CD1	14.86	129.91	121.00
1	E	230	ARG	CD-NE-CZ	14.50	143.90	123.60
1	E	125	ARG	NE-CZ-NH2	14.14	127.37	120.30
1	E	117	TYR	CB-CG-CD1	-13.44	112.94	121.00
1	E	223	ARG	NH1-CZ-NH2	-13.21	104.87	119.40
1	E	61	ARG	CD-NE-CZ	13.01	141.82	123.60
1	E	145	ARG	NE-CZ-NH1	-12.70	113.95	120.30
1	E	164	ASP	CB-CG-OD2	-12.59	106.97	118.30
1	E	82	TYR	CB-CG-CD2	12.26	128.36	121.00
1	E	101	TYR	CB-CG-CD2	-12.20	113.68	121.00
1	E	168	CYS	CA-CB-SG	-11.87	92.64	114.00
1	E	145	ARG	CD-NE-CZ	11.83	140.16	123.60
1	E	50	ASN	CB-CG-OD1	11.66	144.93	121.60
1	E	217(A)	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	E	36	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	E	107	ARG	CD-NE-CZ	10.85	138.79	123.60
1	E	230	ARG	NH1-CZ-NH2	10.84	131.33	119.40
1	E	62	GLU	CG-CD-OE1	-10.74	96.82	118.30
1	E	62	GLU	CG-CD-OE2	10.67	139.64	118.30
1	E	75	GLN	CA-CB-CG	10.66	136.85	113.40
1	E	215	PHE	CB-CG-CD2	10.64	128.25	120.80
1	E	223	ARG	NE-CZ-NH2	10.48	125.54	120.30
1	E	159	TYR	CG-CD1-CE1	-10.24	113.11	121.30
1	E	52	VAL	CA-CB-CG1	10.20	126.20	110.90
1	E	87	LYS	CA-CB-CG	10.15	135.72	113.40
1	E	48	ARG	NE-CZ-NH2	10.02	125.31	120.30
1	E	125	ARG	NH1-CZ-NH2	-9.81	108.61	119.40
1	E	220	CYS	CA-CB-SG	-9.80	96.36	114.00
1	E	236	SER	N-CA-CB	-9.68	95.98	110.50
1	E	212	VAL	CA-CB-CG2	9.63	125.34	110.90
1	E	239	ASN	O-C-N	9.58	138.02	122.70
1	E	215	PHE	CG-CD1-CE1	9.56	131.32	120.80
1	E	70	GLU	OE1-CD-OE2	9.55	134.76	123.30
1	E	80	GLU	O-C-N	9.53	137.94	122.70
1	E	194	ASP	OD1-CG-OD2	-9.49	105.28	123.30
1	E	206	GLN	O-C-N	-9.18	108.02	122.70
1	E	82	TYR	O-C-N	9.12	137.29	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	148	ASN	C-N-CA	9.11	141.42	122.30
1	E	236	SER	CB-CA-C	9.01	127.22	110.10
1	E	176	VAL	CG1-CB-CG2	-9.00	96.50	110.90
1	E	117	TYR	CB-CG-CD2	8.87	126.32	121.00
1	E	101	TYR	CZ-CE2-CD2	-8.84	111.85	119.80
1	E	93	TYR	CD1-CE1-CZ	-8.78	111.90	119.80
1	E	228	PHE	O-C-N	-8.71	108.77	122.70
1	E	212	VAL	CG1-CB-CG2	-8.68	97.02	110.90
1	E	186	ASP	OD1-CG-OD2	-8.52	107.12	123.30
1	E	236	SER	O-C-N	-8.50	109.09	122.70
1	E	81	GLN	O-C-N	-8.46	109.17	122.70
1	E	217(A)	ARG	NH1-CZ-NH2	8.43	128.68	119.40
1	E	41	THR	CA-CB-CG2	8.38	124.12	112.40
1	E	137	TYR	CB-CG-CD1	-8.26	116.04	121.00
1	E	145	ARG	NH1-CZ-NH2	8.23	128.45	119.40
1	E	18	GLY	C-N-CA	8.19	139.49	122.30
1	E	122	VAL	CA-CB-CG2	8.18	123.17	110.90
1	E	62	GLU	N-CA-CB	-8.12	95.98	110.60
1	E	192	GLN	N-CA-CB	-8.12	95.98	110.60
1	E	38	TRP	CD1-CG-CD2	8.08	112.77	106.30
1	E	153	GLN	CG-CD-OE1	-8.07	105.45	121.60
1	E	227	VAL	CA-CB-CG2	8.00	122.90	110.90
1	E	228	PHE	C-N-CA	7.97	141.63	121.70
1	E	99(A)	ALA	CB-CA-C	-7.96	98.17	110.10
1	E	102	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	E	97	ASP	CB-CG-OD1	7.93	125.44	118.30
1	E	141	TRP	N-CA-CB	-7.88	96.41	110.60
1	E	112	VAL	CA-CB-CG2	7.78	122.58	110.90
1	E	238	ILE	CB-CG1-CD1	7.69	135.43	113.90
1	E	107	ARG	NH1-CZ-NH2	-7.64	111.00	119.40
1	E	141	TRP	C-N-CA	7.64	138.34	122.30
1	E	81	GLN	CA-C-O	7.63	136.12	120.10
1	E	24	ARG	CG-CD-NE	-7.63	95.78	111.80
1	E	61	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	E	136	CYS	O-C-N	7.62	134.89	122.70
1	E	150	GLN	CG-CD-OE1	-7.59	106.43	121.60
1	E	176	VAL	CA-CB-CG2	7.58	122.27	110.90
1	E	61	ARG	NE-CZ-NH1	-7.55	116.53	120.30
1	E	42	CYS	CA-CB-SG	-7.50	100.50	114.00
1	E	177	LYS	CD-CE-NZ	7.50	128.95	111.70
1	E	119	GLN	OE1-CD-NE2	-7.47	104.72	121.90
1	E	82	TYR	CA-C-N	-7.45	100.82	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	48	ARG	CD-NE-CZ	7.35	133.88	123.60
1	E	75	GLN	CA-C-N	7.34	133.35	117.20
1	E	111	SER	N-CA-CB	7.33	121.49	110.50
1	E	125	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	E	208	ALA	N-CA-CB	7.22	120.21	110.10
1	E	110	GLN	CB-CG-CD	7.22	130.37	111.60
1	E	41	THR	CA-CB-OG1	-7.22	93.84	109.00
1	E	222	THR	O-C-N	-7.19	111.19	122.70
1	E	22	ALA	O-C-N	-7.16	111.24	122.70
1	E	216	VAL	CA-CB-CG2	7.15	121.63	110.90
1	E	102	ASP	CB-CG-OD1	7.14	124.72	118.30
1	E	183	ALA	CB-CA-C	7.14	120.80	110.10
1	E	166	ALA	CB-CA-C	-7.06	99.51	110.10
1	E	65(A)	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	E	127	GLY	N-CA-C	7.04	130.70	113.10
1	E	171	TYR	CD1-CE1-CZ	-7.02	113.48	119.80
1	E	217(A)	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	E	201	CYS	CA-C-N	-7.02	101.77	117.20
1	E	236	SER	CA-C-N	6.99	132.59	117.20
1	E	55	ALA	CA-C-O	6.94	134.67	120.10
1	E	234	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	E	90	VAL	CA-CB-CG2	6.93	121.30	110.90
1	E	159	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	E	153	GLN	OE1-CD-NE2	6.92	137.82	121.90
1	E	202	LEU	CA-CB-CG	6.91	131.19	115.30
1	E	137	TYR	CZ-CE2-CD2	-6.90	113.59	119.80
1	E	65	PHE	CA-C-N	-6.86	102.12	117.20
1	E	128	THR	C-N-CA	6.85	138.82	121.70
1	E	55	ALA	N-CA-CB	6.84	119.68	110.10
1	E	47	ILE	CA-CB-CG1	6.82	123.96	111.00
1	E	229	THR	O-C-N	6.82	133.61	122.70
1	E	165	TYR	CA-C-O	-6.82	105.78	120.10
1	E	169	SER	C-N-CA	6.80	138.69	121.70
1	E	80	GLU	CG-CD-OE2	6.75	131.79	118.30
1	E	224	LYS	O-C-N	-6.74	108.30	121.10
1	E	225	PRO	CA-N-CD	6.72	121.11	111.70
1	E	70	GLU	O-C-N	6.71	133.43	122.70
1	E	99	VAL	CA-CB-CG2	6.71	120.96	110.90
1	E	239	ASN	CA-C-O	-6.70	106.02	120.10
1	E	25	ASN	OD1-CG-ND2	-6.65	106.61	121.90
1	E	221	ASN	CA-C-O	6.63	134.03	120.10
1	E	125	ARG	CA-CB-CG	-6.54	99.00	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	23	GLN	CB-CG-CD	6.52	128.56	111.60
1	E	195	SER	CA-C-N	6.51	129.22	116.20
1	E	97	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	E	36(A)	SER	CA-C-O	6.49	133.73	120.10
1	E	23	GLN	CG-CD-OE1	6.48	134.56	121.60
1	E	98	ASP	CB-CG-OD1	6.47	124.12	118.30
1	E	88	ILE	O-C-N	6.46	133.03	122.70
1	E	244	SER	N-CA-CB	-6.45	100.83	110.50
1	E	166	ALA	N-CA-CB	6.43	119.10	110.10
1	E	180	MET	C-N-CA	6.41	137.72	121.70
1	E	50	ASN	CA-C-N	6.40	131.28	117.20
1	E	221(A)	VAL	CA-CB-CG2	6.39	120.49	110.90
1	E	217(A)	ARG	CA-C-O	-6.38	106.69	120.10
1	E	158	ALA	N-CA-CB	6.38	119.04	110.10
1	E	222	THR	C-N-CA	6.36	137.60	121.70
1	E	165	TYR	CA-C-N	6.34	131.16	117.20
1	E	60	ASP	OD1-CG-OD2	6.32	135.31	123.30
1	E	129	ILE	CA-C-N	-6.29	103.36	117.20
1	E	23	GLN	O-C-N	-6.27	112.67	122.70
1	E	229	THR	CA-CB-CG2	6.26	121.17	112.40
1	E	99	VAL	O-C-N	-6.26	112.68	122.70
1	E	81	GLN	C-N-CA	6.23	137.28	121.70
1	E	215	PHE	O-C-N	6.23	132.66	122.70
1	E	65	PHE	CA-CB-CG	6.22	128.83	113.90
1	E	65(A)	ARG	CA-CB-CG	6.21	127.07	113.40
1	E	221	ASN	O-C-N	-6.20	112.79	122.70
1	E	38	TRP	CB-CG-CD2	-6.18	118.57	126.60
1	E	206	GLN	CG-CD-OE1	-6.17	109.26	121.60
1	E	165	TYR	CG-CD2-CE2	-6.16	116.37	121.30
1	E	215	PHE	CD1-CE1-CZ	-6.16	112.71	120.10
1	E	159	TYR	CD1-CE1-CZ	6.14	125.33	119.80
1	E	49	GLN	C-N-CA	6.14	137.05	121.70
1	E	86	GLN	CG-CD-OE1	-6.12	109.37	121.60
1	E	241	VAL	CA-CB-CG2	6.09	120.04	110.90
1	E	36	ARG	N-CA-CB	6.09	121.56	110.60
1	E	170	SER	CA-CB-OG	-6.07	94.82	111.20
1	E	27	TRP	CB-CG-CD2	-6.06	118.72	126.60
1	E	36	ARG	CG-CD-NE	-6.04	99.12	111.80
1	E	36(A)	SER	C-N-CA	6.03	134.96	122.30
1	E	52	VAL	CA-C-O	6.03	132.75	120.10
1	E	38	TRP	CG-CD1-NE1	-6.01	104.08	110.10
1	E	70	GLU	CB-CA-C	-6.00	98.39	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	48	ARG	CG-CD-NE	5.98	124.35	111.80
1	E	25	ASN	CB-CG-OD1	5.97	133.54	121.60
1	E	205	GLY	C-N-CA	5.96	136.59	121.70
1	E	218	LEU	CB-CG-CD1	-5.94	100.90	111.00
1	E	195	SER	O-C-N	-5.94	113.10	123.20
1	E	229	THR	CA-CB-OG1	-5.91	96.58	109.00
1	E	222	THR	CA-CB-CG2	5.91	120.67	112.40
1	E	19	GLY	O-C-N	-5.87	113.30	122.70
1	E	93	TYR	CG-CD1-CE1	5.85	125.98	121.30
1	E	202	LEU	O-C-N	5.84	132.05	122.70
1	E	129	ILE	CA-C-O	5.84	132.37	120.10
1	E	190	GLY	O-C-N	5.83	132.03	122.70
1	E	75	GLN	CB-CG-CD	5.83	126.75	111.60
1	E	36	ARG	O-C-N	5.83	132.02	122.70
1	E	165	TYR	CZ-CE2-CD2	5.77	124.99	119.80
1	E	178	ASN	CA-C-N	5.76	129.87	117.20
1	E	36	ARG	CA-CB-CG	5.75	126.05	113.40
1	E	139	THR	CA-CB-CG2	-5.75	104.35	112.40
1	E	94	TRP	CD2-CE3-CZ3	-5.72	111.36	118.80
1	E	17	VAL	CA-CB-CG2	5.71	119.46	110.90
1	E	68	VAL	CA-CB-CG1	5.71	119.46	110.90
1	E	24	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	E	119	GLN	CG-CD-OE1	5.71	133.01	121.60
1	E	86	GLN	N-CA-CB	5.70	120.86	110.60
1	E	111	SER	O-C-N	5.70	131.82	122.70
1	E	111	SER	CB-CA-C	-5.70	99.28	110.10
1	E	188(A)	ARG	CG-CD-NE	-5.69	99.85	111.80
1	E	83	VAL	CA-CB-CG1	5.69	119.43	110.90
1	E	223	ARG	CB-CG-CD	-5.68	96.83	111.60
1	E	46	LEU	CA-C-O	-5.67	108.18	120.10
1	E	65	PHE	CA-C-O	5.67	132.02	120.10
1	E	38	TRP	O-C-N	-5.66	113.64	122.70
1	E	134	SER	N-CA-CB	5.66	118.99	110.50
1	E	110	GLN	CA-CB-CG	-5.65	100.97	113.40
1	E	162	THR	O-C-N	5.63	131.71	122.70
1	E	172	TRP	CB-CG-CD1	-5.63	119.68	127.00
1	E	86	GLN	OE1-CD-NE2	5.62	134.81	121.90
1	E	229	THR	CA-C-O	-5.61	108.32	120.10
1	E	51	TRP	N-CA-CB	5.61	120.70	110.60
1	E	212	VAL	O-C-N	-5.61	113.73	122.70
1	E	31	ILE	CB-CG1-CD1	5.60	129.59	113.90
1	E	104	ALA	O-C-N	-5.60	113.73	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	172	TRP	CD2-CE2-CZ2	5.60	129.02	122.30
1	E	50	ASN	OD1-CG-ND2	-5.58	109.07	121.90
1	E	186	ASP	CA-CB-CG	5.58	125.67	113.40
1	E	51	TRP	CB-CA-C	-5.57	99.26	110.40
1	E	145	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	E	101	TYR	CE1-CZ-CE2	5.56	128.70	119.80
1	E	204	ASN	CB-CG-ND2	5.56	130.04	116.70
1	E	215	PHE	CB-CG-CD1	-5.55	116.92	120.80
1	E	204	ASN	CA-CB-CG	-5.54	101.21	113.40
1	E	92	PRO	O-C-N	-5.54	113.84	122.70
1	E	101	TYR	CG-CD1-CE1	-5.53	116.87	121.30
1	E	77	ASN	C-N-CA	5.53	133.91	122.30
1	E	143	LEU	CA-CB-CG	5.53	128.01	115.30
1	E	93	TYR	CB-CG-CD1	5.51	124.31	121.00
1	E	97	ASP	O-C-N	5.51	131.52	122.70
1	E	206	GLN	C-N-CA	5.51	135.48	121.70
1	E	109	ALA	N-CA-CB	5.51	117.81	110.10
1	E	137	TYR	CG-CD2-CE2	5.51	125.71	121.30
1	E	73	LEU	C-N-CA	5.49	135.42	121.70
1	E	176	VAL	CA-CB-CG1	5.47	119.11	110.90
1	E	36(A)	SER	N-CA-CB	5.47	118.71	110.50
1	E	155	LEU	C-N-CA	5.47	135.37	121.70
1	E	170	SER	N-CA-CB	5.46	118.69	110.50
1	E	117	TYR	CG-CD1-CE1	-5.45	116.94	121.30
1	E	172	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	E	157	GLN	CG-CD-OE1	5.41	132.42	121.60
1	E	50	ASN	CA-CB-CG	5.41	125.30	113.40
1	E	66	VAL	CA-CB-CG1	5.40	119.00	110.90
1	E	174	SER	O-C-N	-5.40	114.06	122.70
1	E	201	CYS	CA-CB-SG	-5.39	104.29	114.00
1	E	144	THR	O-C-N	5.39	131.32	122.70
1	E	213	THR	CA-C-N	-5.38	105.36	117.20
1	E	35	TYR	CG-CD1-CE1	-5.38	117.00	121.30
1	E	164	ASP	CA-CB-CG	5.38	125.23	113.40
1	E	230	ARG	CG-CD-NE	-5.38	100.50	111.80
1	E	172	TRP	CH2-CZ2-CE2	-5.37	112.03	117.40
1	E	16	VAL	CA-CB-CG1	5.35	118.93	110.90
1	E	73	LEU	O-C-N	-5.35	114.15	122.70
1	E	22	ALA	N-CA-CB	-5.32	102.66	110.10
1	E	132	ASN	CB-CG-OD1	5.31	132.22	121.60
1	E	147	THR	OG1-CB-CG2	-5.30	97.81	110.00
1	E	235	ILE	CB-CG1-CD1	5.30	128.74	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	85	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	E	85	VAL	CA-CB-CG1	5.28	118.81	110.90
1	E	141	TRP	CD1-NE1-CE2	5.26	113.73	109.00
1	E	156	GLN	CG-CD-OE1	-5.25	111.11	121.60
1	E	141	TRP	CE3-CZ3-CH2	5.24	126.96	121.20
1	E	27	TRP	CB-CG-CD1	5.23	133.79	127.00
1	E	191	CYS	CA-CB-SG	5.22	123.39	114.00
1	E	125	ARG	N-CA-CB	5.21	119.98	110.60
1	E	223	ARG	CA-CB-CG	-5.20	101.96	113.40
1	E	105	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	E	30	GLN	CG-CD-NE2	5.18	129.13	116.70
1	E	201	CYS	CA-C-O	5.18	130.97	120.10
1	E	131	ALA	N-CA-CB	5.16	117.33	110.10
1	E	215	PHE	CZ-CE2-CD2	5.16	126.29	120.10
1	E	141	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	E	65(A)	ARG	CG-CD-NE	-5.15	100.98	111.80
1	E	151	LEU	CA-C-O	-5.14	109.30	120.10
1	E	75	GLN	N-CA-CB	-5.13	101.36	110.60
1	E	77	ASN	CA-C-N	5.12	126.44	116.20
1	E	89	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	E	177	LYS	N-CA-C	-5.12	97.19	111.00
1	E	51	TRP	CD1-CG-CD2	-5.10	102.22	106.30
1	E	151	LEU	CB-CG-CD1	-5.09	102.35	111.00
1	E	224	LYS	CA-C-N	5.09	131.34	117.10
1	E	59	VAL	O-C-N	-5.08	114.56	122.70
1	E	83	VAL	CA-C-N	-5.08	106.04	116.20
1	E	157	GLN	CA-C-O	5.08	130.76	120.10
1	E	95	ASN	CB-CA-C	5.07	120.53	110.40
1	E	21	GLU	C-N-CA	5.06	134.36	121.70
1	E	36	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
1	E	195	SER	N-CA-CB	-5.06	102.91	110.50
1	E	217(A)	ARG	CA-C-N	5.06	128.33	117.20
1	E	24	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	E	42	CYS	N-CA-CB	-5.05	101.52	110.60
1	E	234	TYR	CG-CD2-CE2	5.04	125.33	121.30
1	E	36	ARG	C-N-CA	5.04	134.30	121.70
1	E	64	THR	N-CA-C	-5.03	97.42	111.00
1	E	27	TRP	CA-CB-CG	5.01	123.22	113.70
1	E	51	TRP	NE1-CE2-CZ2	-5.01	124.89	130.40
1	E	231	VAL	O-C-N	5.01	130.71	122.70
1	E	230	ARG	CA-C-O	5.01	130.61	120.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	125	ARG	Sidechain
1	E	145	ARG	Sidechain
1	E	217(A)	ARG	Sidechain

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	1822	0	1763	25	0
2	E	31	0	21	6	0
3	E	1	0	0	0	0
4	E	45	0	0	0	0
All	All	1899	0	1784	25	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 7.

All (25) 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:99:VAL:HG11	2:E:1:2Z5:HD2	1.59	0.82
1:E:99:VAL:HG11	2:E:1:2Z5:CD	2.15	0.76
1:E:168:CYS:HG	1:E:182:CYS:HG	1.40	0.68
1:E:49:GLN:HB3	1:E:111:SER:HB3	1.76	0.68
1:E:136:CYS:HG	1:E:201:CYS:HG	1.35	0.68
1:E:216:VAL:O	2:E:1:2Z5:H6	2.01	0.60
1:E:94:TRP:HH2	1:E:99:VAL:HG12	1.71	0.54
1:E:99:VAL:CG1	2:E:1:2Z5:HD2	2.34	0.53
1:E:47:ILE:HD13	1:E:53:MET:HB2	1.91	0.53
1:E:34:GLN:HB2	1:E:65(A):ARG:HG2	1.92	0.51
1:E:42:CYS:SG	1:E:58:CYS:SG	3.00	0.51
1:E:168:CYS:SG	1:E:182:CYS:SG	3.01	0.51
1:E:99:VAL:HG11	2:E:1:2Z5:HD3	1.93	0.50
1:E:26:SER:HB3	1:E:27:TRP:CD1	2.46	0.50
1:E:41:THR:C	1:E:42:CYS:SG	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:TRP:O	1:E:241:VAL:HG23	2.13	0.48
1:E:136:CYS:HB2	1:E:160:LEU:O	2.14	0.48
1:E:41:THR:O	1:E:42:CYS:SG	2.71	0.47
1:E:192:GLN:NE2	2:E:1:2Z5:HB31	2.31	0.46
1:E:94:TRP:CH2	1:E:99:VAL:HG12	2.52	0.44
1:E:23:GLN:O	1:E:26:SER:HB2	2.18	0.43
1:E:211:GLY:HA3	1:E:228:PHE:HB3	1.99	0.43
1:E:136:CYS:SG	1:E:201:CYS:SG	3.00	0.43
1:E:33:LEU:HD23	1:E:42:CYS:HB2	2.00	0.42
1:E:143:LEU:HD23	1:E:151:LEU:HD23	2.00	0.42

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	238/240 (99%)	223 (94%)	15 (6%)	0	100 100

There are no Ramachandran outliers to report.

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	198/198 (100%)	187 (94%)	11 (6%)	26 47

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	26	SER
1	E	31	ILE
1	E	70	GLU
1	E	76	ASN
1	E	116	SER
1	E	143	LEU
1	E	176	VAL
1	E	177	LYS
1	E	202	LEU
1	E	206	GLN
1	E	236	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	119	GLN
1	E	153	GLN
1	E	240	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 2 ligands modelled in this entry, 1 is modelled with single atom - 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	$\#\|Z\| > 2$
2	2Z5	E	1	-	31,31,31	1.95	8 (25%)	44,44,44	3.19	23 (52%)

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	2Z5	E	1	-	-	0/37/37/37	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	2Z5	C3-N2	-3.79	1.28	1.35
2	E	1	2Z5	C2-C1	-2.92	1.45	1.53
2	E	1	2Z5	C1-N	-2.22	1.29	1.33
2	E	1	2Z5	CA1-N1	2.09	1.50	1.46
2	E	1	2Z5	C6-C5	2.20	1.42	1.38
2	E	1	2Z5	CA1-C3	2.40	1.59	1.52
2	E	1	2Z5	CB-CA	2.94	1.60	1.53
2	E	1	2Z5	O2-C3	6.33	1.35	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	2Z5	O-C1-N	-5.30	111.30	122.66
2	E	1	2Z5	C6-C11-C21	-5.16	111.90	119.06
2	E	1	2Z5	F31-C7-C4	-3.68	105.09	112.95
2	E	1	2Z5	F21-C7-F11	-2.93	95.14	105.71
2	E	1	2Z5	C31-C4-C7	-2.91	115.62	119.99
2	E	1	2Z5	C3-CA1-N1	-2.87	104.50	111.67
2	E	1	2Z5	CB-CA-N	-2.68	105.77	110.87
2	E	1	2Z5	F3-C2-C1	-2.53	104.00	111.97
2	E	1	2Z5	F1-C2-C1	-2.00	105.66	111.97
2	E	1	2Z5	F11-C7-C4	2.04	117.32	112.95
2	E	1	2Z5	C21-C11-N2	2.10	127.43	120.41
2	E	1	2Z5	F31-C7-F11	2.17	113.56	105.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	2Z5	C11-N2-C3	2.74	132.33	127.40
2	E	1	2Z5	CA-C-N1	3.11	123.96	116.78
2	E	1	2Z5	C31-C21-C11	3.46	124.18	120.28
2	E	1	2Z5	CD-CG-CB	3.61	126.50	113.66
2	E	1	2Z5	F21-C7-C4	4.03	121.58	112.95
2	E	1	2Z5	F2-C2-C1	4.09	124.84	111.97
2	E	1	2Z5	C5-C6-C11	4.40	125.24	120.28
2	E	1	2Z5	CB1-CA1-N1	5.18	120.09	110.31
2	E	1	2Z5	CA-N-C1	5.45	132.40	121.61
2	E	1	2Z5	C5-C4-C7	5.74	128.60	119.99
2	E	1	2Z5	C2-C1-N	10.45	129.93	115.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	2Z5	6	0

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.