



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:06 AM UTC

PDB ID : 1SGR / pdb_00001sgr
Title : LEU 18 VARIANT OF TURKEY OVOMUCOID INHIBITOR THIRD DOMAIN COMPLEXED WITH STREPTOMYCES GRISEUS PROTEINASE B
Authors : Huang, K.; James, M.N.G.
Deposited on : 1995-05-26
Resolution : 1.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

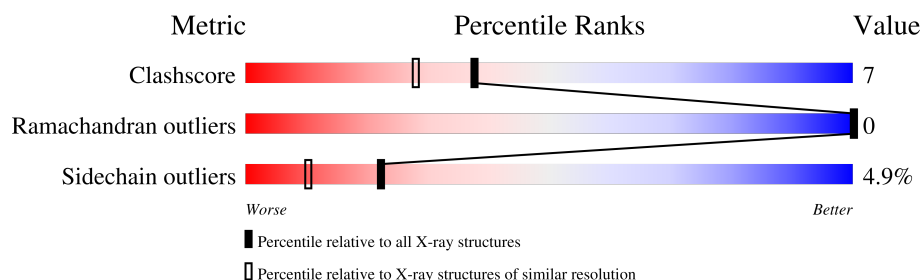
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	185	
2	I	51	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1871 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 STREPTOMYCES GRISEUS PROTEINASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	185	1310	801	228	275	6	0	0	0

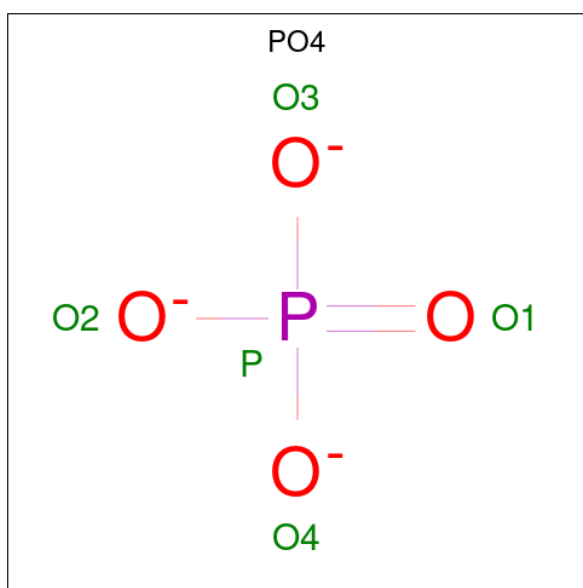
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	235A	VAL	SER	conflict	UNP P00777

- Molecule 2 is a protein called TURKEY OVOMUCOID INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	51	387	238	65	78	6	0	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

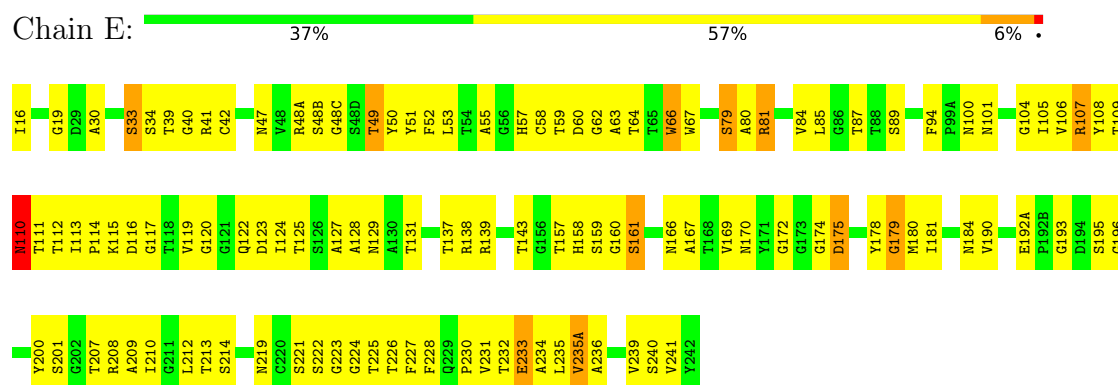
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	125	Total	O	0	0
			125	125		
4	I	44	Total	O	0	0
			44	44		

3 Residue-property plots [i](#)

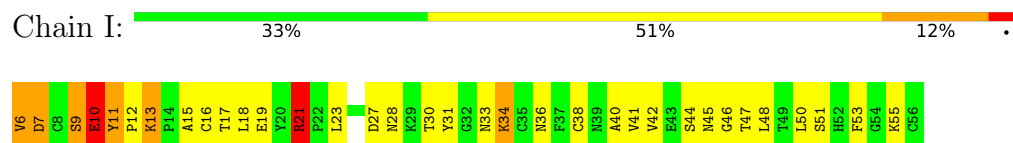
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: TURKEY OVOMUCOID INHIBITOR



4 Data and refinement statistics

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	45.53Å 54.66Å 45.59Å 90.00° 119.19° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.136 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1871	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: PO4

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	1.33	2/1335 (0.1%)	3.14	209/1820 (11.5%)
2	I	1.29	1/395 (0.3%)	3.19	64/533 (12.0%)
All	All	1.32	3/1730 (0.2%)	3.15	273/2353 (11.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	104	GLY	N-CA	5.76	1.51	1.45
1	E	233	GLU	CD-OE2	5.55	1.35	1.25
2	I	10	GLU	CD-OE1	5.06	1.34	1.25

All (273) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	120	GLY	CA-C-N	-14.06	93.84	121.41
1	E	120	GLY	C-N-CA	-14.06	93.84	121.41
1	E	129	ASN	CA-CB-CG	-13.03	99.57	112.60
1	E	100	ASN	CA-CB-CG	-12.21	100.39	112.60
1	E	123	ASP	CA-C-O	-10.96	108.87	121.47
1	E	235(A)	VAL	N-CA-CB	-10.80	90.54	110.95
1	E	81	ARG	NE-CZ-NH2	10.61	128.75	119.20
2	I	17	THR	O-C-N	-10.36	110.98	122.79
1	E	110	ASN	CA-CB-CG	10.26	122.86	112.60
2	I	9	SER	O-C-N	-9.80	110.22	122.27
1	E	39	THR	N-CA-CB	-9.73	96.23	110.53
1	E	235(A)	VAL	CG1-CB-CG2	-9.69	89.49	110.80
1	E	127	ALA	CA-C-O	-9.40	110.49	121.11
2	I	51	SER	CA-CB-OG	-9.39	92.33	111.10
1	E	120	GLY	O-C-N	-9.27	112.33	122.62
1	E	47	ASN	O-C-N	-9.27	112.20	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	180	MET	CG-SD-CE	-9.25	80.55	100.90
1	E	227	PHE	CA-CB-CG	-9.14	104.66	113.80
2	I	23	LEU	CD1-CG-CD2	-8.61	91.86	110.80
1	E	55	ALA	CA-C-N	8.48	129.39	119.98
1	E	55	ALA	C-N-CA	8.48	129.39	119.98
2	I	16	CYS	CA-C-O	-8.47	111.56	120.70
1	E	105	ILE	CA-C-O	8.45	130.24	121.28
1	E	104	GLY	O-C-N	-8.34	115.87	123.54
1	E	84	VAL	CA-C-O	-8.31	111.40	121.54
1	E	210	ILE	N-CA-CB	-8.25	100.59	111.90
1	E	81	ARG	NE-CZ-NH1	-8.25	113.25	121.50
2	I	10	GLU	N-CA-CB	-8.24	98.95	110.65
1	E	109	THR	N-CA-C	-8.21	102.70	114.12
1	E	64	THR	N-CA-C	-8.13	101.22	112.12
1	E	60	ASP	CA-C-N	-8.06	105.81	121.78
1	E	60	ASP	C-N-CA	-8.06	105.81	121.78
1	E	167	ALA	N-CA-CB	-8.01	97.36	110.41
1	E	241	VAL	N-CA-C	-8.00	101.33	110.05
2	I	45	ASN	OD1-CG-ND2	-7.93	114.67	122.60
1	E	125	THR	OG1-CB-CG2	-7.88	93.53	109.30
2	I	55	LYS	O-C-N	-7.88	113.56	122.86
1	E	120	GLY	N-CA-C	-7.84	97.99	111.47
1	E	79	SER	N-CA-CB	7.80	122.23	110.22
2	I	55	LYS	CA-C-O	7.70	129.95	121.56
1	E	87	THR	OG1-CB-CG2	-7.63	94.03	109.30
2	I	21	ARG	NE-CZ-NH1	7.63	129.13	121.50
1	E	116	ASP	CA-CB-CG	-7.62	104.98	112.60
1	E	120	GLY	CA-C-O	7.61	131.10	121.67
1	E	33	SER	CA-CB-OG	-7.57	95.97	111.10
1	E	81	ARG	CA-C-N	-7.55	108.86	121.92
1	E	81	ARG	C-N-CA	-7.55	108.86	121.92
2	I	9	SER	CA-C-O	7.53	128.62	119.97
1	E	87	THR	CA-CB-OG1	-7.43	98.45	109.60
2	I	50	LEU	CB-CA-C	-7.41	97.64	109.80
2	I	46	GLY	CA-C-O	-7.41	110.09	119.13
1	E	100	ASN	OD1-CG-ND2	-7.40	115.20	122.60
2	I	11	TYR	CA-CB-CG	-7.40	100.58	113.90
1	E	84	VAL	CG1-CB-CG2	-7.38	94.56	110.80
1	E	85	LEU	N-CA-C	-7.36	103.15	112.93
1	E	109	THR	OG1-CB-CG2	-7.36	94.59	109.30
2	I	41	VAL	N-CA-C	-7.36	103.36	110.42
1	E	19	GLY	CA-C-O	-7.35	111.41	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	66	TRP	CD2-CE2-CZ2	-7.34	115.06	122.40
2	I	55	LYS	CB-CA-C	-7.24	96.23	109.54
2	I	36	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	E	184	ASN	OD1-CG-ND2	-7.13	115.47	122.60
1	E	57	HIS	N-CA-CB	7.12	122.21	110.39
1	E	169	VAL	CB-CA-C	-7.11	100.82	110.42
1	E	159	SER	CA-C-O	-7.11	113.30	121.68
2	I	47	THR	OG1-CB-CG2	-7.08	95.14	109.30
1	E	143	THR	OG1-CB-CG2	-7.07	95.17	109.30
1	E	208	ARG	CD-NE-CZ	7.01	134.21	124.40
2	I	34	LYS	CG-CD-CE	6.98	127.35	111.30
1	E	47	ASN	CA-CB-CG	-6.96	105.64	112.60
1	E	49	THR	O-C-N	6.91	131.44	123.29
1	E	159	SER	N-CA-C	6.89	120.36	109.81
1	E	39	THR	CA-CB-CG2	-6.87	98.82	110.50
2	I	30	THR	CA-C-N	6.87	131.87	122.19
2	I	30	THR	C-N-CA	6.87	131.87	122.19
1	E	131	THR	CA-CB-OG1	6.86	119.89	109.60
1	E	240	SER	CA-CB-OG	-6.85	97.40	111.10
1	E	87	THR	CA-C-O	6.83	129.10	121.11
2	I	15	ALA	N-CA-CB	6.82	123.32	111.39
1	E	63	ALA	O-C-N	-6.81	115.27	123.10
1	E	40	GLY	CA-C-N	-6.81	111.70	122.73
1	E	40	GLY	C-N-CA	-6.81	111.70	122.73
1	E	89	SER	N-CA-CB	6.80	120.12	110.67
1	E	207	THR	CA-C-O	6.80	127.87	119.78
1	E	111	THR	CA-C-N	-6.76	111.51	122.26
1	E	111	THR	C-N-CA	-6.76	111.51	122.26
2	I	33	ASN	OD1-CG-ND2	-6.76	115.84	122.60
2	I	38	CYS	O-C-N	-6.75	113.96	122.27
2	I	46	GLY	CA-C-N	-6.75	109.77	121.66
2	I	46	GLY	C-N-CA	-6.75	109.77	121.66
1	E	108	TYR	CA-C-O	-6.70	113.11	120.81
1	E	161	SER	CB-CA-C	6.68	124.77	110.07
1	E	79	SER	CA-CB-OG	-6.67	97.76	111.10
1	E	158	HIS	CA-CB-CG	-6.66	107.14	113.80
1	E	100	ASN	N-CA-CB	6.65	121.73	110.49
1	E	66	TRP	CA-CB-CG	-6.64	100.98	113.60
1	E	169	VAL	CA-C-N	-6.64	113.68	123.11
1	E	169	VAL	C-N-CA	-6.64	113.68	123.11
1	E	59	THR	CA-CB-OG1	-6.63	99.66	109.60
1	E	225	THR	CA-CB-OG1	-6.59	99.72	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	34	SER	CA-CB-OG	-6.58	97.93	111.10
2	I	9	SER	CA-C-N	-6.56	111.97	122.66
2	I	9	SER	C-N-CA	-6.56	111.97	122.66
1	E	16	ILE	CA-C-N	-6.55	111.98	122.53
1	E	16	ILE	C-N-CA	-6.55	111.98	122.53
1	E	175	ASP	CA-C-N	-6.55	114.03	123.06
1	E	175	ASP	C-N-CA	-6.55	114.03	123.06
1	E	138	ARG	O-C-N	-6.51	114.72	123.19
1	E	201	SER	CA-C-N	-6.50	108.68	121.41
1	E	201	SER	C-N-CA	-6.50	108.68	121.41
2	I	21	ARG	N-CA-C	-6.49	96.93	108.55
1	E	200	TYR	CA-C-N	-6.49	113.61	122.95
1	E	200	TYR	C-N-CA	-6.49	113.61	122.95
1	E	143	THR	O-C-N	6.48	130.44	122.34
2	I	45	ASN	CB-CG-OD1	6.45	133.70	120.80
1	E	239	VAL	O-C-N	6.44	130.09	123.00
1	E	52	PHE	N-CA-CB	6.43	123.08	111.37
2	I	12	PRO	O-C-N	6.43	133.31	121.10
1	E	170	ASN	N-CA-CB	-6.42	99.80	110.47
1	E	193	GLY	CA-C-O	6.42	125.76	119.27
1	E	196	GLY	CA-C-N	-6.41	111.83	121.64
1	E	196	GLY	C-N-CA	-6.41	111.83	121.64
1	E	178	TYR	CA-C-N	-6.37	109.66	121.07
1	E	178	TYR	C-N-CA	-6.37	109.66	121.07
1	E	224	GLY	CA-C-O	-6.36	115.40	121.38
1	E	181	ILE	CB-CA-C	-6.35	102.90	111.15
1	E	48(C)	GLY	CA-C-O	6.35	129.89	121.51
2	I	13	LYS	CD-CE-NZ	-6.35	91.59	111.90
2	I	41	VAL	CB-CA-C	-6.31	103.90	111.97
2	I	45	ASN	CA-CB-CG	-6.29	106.31	112.60
1	E	57	HIS	O-C-N	-6.28	114.02	122.43
1	E	34	SER	N-CA-CB	6.24	120.57	110.40
1	E	33	SER	CB-CA-C	-6.17	103.43	113.37
1	E	30	ALA	CA-C-O	6.09	128.20	121.56
1	E	48(C)	GLY	N-CA-C	-6.09	99.69	111.02
1	E	161	SER	CA-CB-OG	-6.08	98.94	111.10
1	E	58	CYS	N-CA-C	-6.08	104.94	112.90
2	I	28	ASN	CA-CB-CG	-6.08	106.52	112.60
1	E	143	THR	CA-C-O	-6.06	112.26	119.35
1	E	236	ALA	CB-CA-C	-6.05	100.74	110.79
2	I	48	LEU	N-CA-CB	-6.05	100.93	110.06
2	I	13	LYS	CB-CG-CD	-6.04	97.42	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	235	LEU	CD1-CG-CD2	-6.03	97.54	110.80
1	E	50	TYR	CA-C-O	6.03	127.49	120.80
1	E	123	ASP	N-CA-CB	-6.02	101.14	110.29
1	E	123	ASP	N-CA-C	6.01	119.37	110.48
1	E	47	ASN	CA-C-N	6.00	131.19	123.03
1	E	47	ASN	C-N-CA	6.00	131.19	123.03
1	E	94	PHE	CA-CB-CG	-6.00	107.80	113.80
1	E	221	SER	N-CA-C	-5.99	104.09	111.40
2	I	44	SER	N-CA-C	-5.99	105.55	112.92
1	E	235(A)	VAL	CA-CB-CG1	-5.98	100.23	110.40
1	E	227	PHE	CD1-CG-CD2	-5.98	109.63	118.60
2	I	40	ALA	CB-CA-C	-5.97	99.20	110.67
1	E	222	SER	CA-CB-OG	5.96	123.01	111.10
1	E	234	ALA	N-CA-CB	-5.94	101.07	110.28
1	E	101	ASN	N-CA-C	-5.93	100.59	109.96
1	E	129	ASN	OD1-CG-ND2	5.93	128.53	122.60
1	E	89	SER	CB-CA-C	-5.92	99.12	109.07
1	E	169	VAL	O-C-N	5.88	129.29	123.18
2	I	6	VAL	N-CA-CB	5.87	121.48	111.50
1	E	116	ASP	CA-C-O	-5.85	114.61	121.16
1	E	34	SER	O-C-N	5.84	130.52	122.46
1	E	226	THR	OG1-CB-CG2	-5.83	97.65	109.30
2	I	48	LEU	CA-C-O	-5.82	114.41	121.05
1	E	174	GLY	CA-C-N	-5.82	113.03	122.34
1	E	174	GLY	C-N-CA	-5.82	113.03	122.34
1	E	207	THR	O-C-N	-5.80	115.22	122.35
1	E	41	ARG	NE-CZ-NH1	5.79	127.29	121.50
1	E	80	ALA	N-CA-CB	-5.79	101.05	110.42
2	I	15	ALA	O-C-N	5.79	129.96	123.48
1	E	119	VAL	N-CA-C	-5.78	96.33	106.61
1	E	122	GLN	CA-C-N	-5.78	111.80	121.39
1	E	122	GLN	C-N-CA	-5.78	111.80	121.39
1	E	230	PRO	CB-CA-C	-5.77	104.37	111.64
2	I	12	PRO	N-CA-CB	-5.75	96.27	102.60
2	I	55	LYS	CA-CB-CG	-5.75	102.60	114.10
1	E	84	VAL	O-C-N	5.75	129.66	122.59
1	E	84	VAL	N-CA-CB	-5.74	100.44	110.49
1	E	214	SER	CA-C-N	-5.73	112.37	121.03
1	E	214	SER	C-N-CA	-5.73	112.37	121.03
2	I	30	THR	CA-CB-CG2	-5.73	100.75	110.50
1	E	48(B)	SER	N-CA-C	-5.73	98.75	108.26
1	E	239	VAL	CG1-CB-CG2	-5.71	98.23	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	13	LYS	CB-CA-C	5.71	117.12	109.42
1	E	227	PHE	CG-CD1-CE1	5.71	130.40	120.70
1	E	231	VAL	CA-C-O	-5.69	112.79	119.85
2	I	7	ASP	CA-CB-CG	5.69	118.29	112.60
1	E	119	VAL	CA-CB-CG1	-5.66	100.78	110.40
1	E	128	ALA	O-C-N	5.66	129.70	123.25
1	E	125	THR	CA-CB-OG1	5.64	118.06	109.60
1	E	63	ALA	CB-CA-C	-5.62	100.00	109.50
1	E	157	THR	N-CA-CB	-5.62	101.75	110.57
1	E	124	ILE	CA-CB-CG2	-5.61	100.96	110.50
1	E	41	ARG	CD-NE-CZ	-5.61	116.55	124.40
1	E	213	THR	CA-C-N	-5.61	112.81	122.79
1	E	213	THR	C-N-CA	-5.61	112.81	122.79
2	I	18	LEU	N-CA-C	5.61	119.32	111.30
2	I	31	TYR	CG-CD2-CE2	-5.59	112.81	121.20
2	I	51	SER	N-CA-CB	-5.59	101.42	110.14
1	E	81	ARG	CG-CD-NE	5.58	124.27	112.00
1	E	63	ALA	CA-C-O	5.56	127.84	121.28
1	E	174	GLY	N-CA-C	-5.55	107.67	115.32
1	E	62	GLY	N-CA-C	5.54	122.73	115.47
1	E	106	VAL	CA-CB-CG1	5.52	119.78	110.40
1	E	137	THR	CA-C-N	-5.52	114.15	122.81
1	E	137	THR	C-N-CA	-5.52	114.15	122.81
2	I	19	GLU	O-C-N	-5.50	116.58	122.85
1	E	212	LEU	CD1-CG-CD2	-5.49	98.72	110.80
1	E	107	ARG	N-CA-CB	-5.48	101.50	110.43
1	E	179	GLY	CA-C-O	5.46	126.54	119.44
2	I	31	TYR	N-CA-CB	5.45	119.16	110.16
1	E	105	ILE	CB-CG1-CD1	-5.45	102.36	113.80
2	I	28	ASN	OD1-CG-ND2	-5.42	117.17	122.60
2	I	13	LYS	CA-C-O	5.42	125.22	119.69
1	E	232	THR	CA-CB-OG1	-5.42	101.47	109.60
1	E	110	ASN	CB-CG-ND2	-5.41	108.29	116.40
1	E	89	SER	CA-CB-OG	-5.41	100.29	111.10
1	E	223	GLY	CA-C-N	-5.36	111.51	121.15
1	E	223	GLY	C-N-CA	-5.36	111.51	121.15
1	E	42	CYS	O-C-N	5.35	129.71	122.59
1	E	137	THR	O-C-N	5.34	129.80	123.33
2	I	45	ASN	CA-C-O	5.34	127.64	121.28
1	E	53	LEU	CA-C-O	5.32	127.56	121.28
1	E	116	ASP	N-CA-C	5.32	118.15	110.28
1	E	170	ASN	OD1-CG-ND2	-5.31	117.29	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	11	TYR	CA-C-O	-5.31	116.36	121.08
1	E	41	ARG	O-C-N	5.30	129.74	123.27
1	E	209	ALA	CA-C-N	-5.29	117.21	122.77
1	E	209	ALA	C-N-CA	-5.29	117.21	122.77
1	E	122	GLN	CG-CD-NE2	5.29	124.33	116.40
2	I	23	LEU	CB-CG-CD2	-5.26	94.92	110.70
1	E	129	ASN	CB-CA-C	-5.25	100.86	109.53
1	E	192(A)	GLU	CA-CB-CG	-5.25	103.61	114.10
2	I	53	PHE	CA-CB-CG	-5.25	108.56	113.80
1	E	195	SER	CB-CA-C	-5.24	101.26	109.70
1	E	210	ILE	CB-CA-C	-5.24	105.77	110.91
1	E	63	ALA	N-CA-CB	-5.24	102.09	110.63
1	E	207	THR	CA-CB-OG1	-5.24	101.74	109.60
1	E	219	ASN	N-CA-C	-5.22	101.33	108.38
1	E	160	GLY	N-CA-C	-5.22	100.81	113.18
1	E	190	VAL	CB-CA-C	-5.22	104.06	111.21
1	E	226	THR	CA-C-O	-5.22	114.66	120.66
1	E	112	THR	CA-CB-CG2	-5.21	101.65	110.50
1	E	158	HIS	ND1-CG-CD2	5.19	111.29	106.10
1	E	64	THR	O-C-N	-5.16	115.91	121.95
1	E	184	ASN	CA-C-O	5.16	126.81	120.15
1	E	210	ILE	CA-C-O	-5.16	115.65	120.34
1	E	235	LEU	C-N-CA	-5.15	108.83	121.70
1	E	34	SER	CA-C-N	-5.15	113.01	121.92
1	E	34	SER	C-N-CA	-5.15	113.01	121.92
1	E	233	GLU	N-CA-CB	-5.14	102.55	110.16
2	I	42	VAL	CB-CA-C	-5.13	105.21	112.14
1	E	139	ARG	CG-CD-NE	-5.12	100.74	112.00
2	I	21	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	E	158	HIS	CG-CD2-NE2	-5.11	102.09	107.20
1	E	81	ARG	CB-CG-CD	5.10	123.03	111.30
1	E	63	ALA	N-CA-C	-5.10	101.96	110.17
1	E	228	PHE	CA-CB-CG	-5.10	108.70	113.80
1	E	110	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	E	180	MET	O-C-N	5.09	128.77	123.06
1	E	87	THR	CA-CB-CG2	-5.07	101.88	110.50
1	E	117	GLY	CA-C-N	-5.07	114.37	122.53
1	E	117	GLY	C-N-CA	-5.07	114.37	122.53
1	E	101	ASN	CB-CA-C	-5.07	102.75	112.43
2	I	19	GLU	N-CA-C	-5.04	103.74	110.55
1	E	81	ARG	CA-C-O	5.04	127.28	121.28
1	E	48(A)	ARG	CD-NE-CZ	5.04	131.45	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	40	GLY	O-C-N	5.03	129.24	122.70
2	I	27	ASP	N-CA-C	-5.03	106.99	112.72
2	I	9	SER	N-CA-C	5.02	117.64	111.82
2	I	34	LYS	N-CA-CB	-5.00	102.77	110.12
1	E	157	THR	CA-CB-OG1	-5.00	102.10	109.60

There are no chirality outliers.

There are no planarity outliers.

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	1310	0	1231	13	0
2	I	387	0	358	10	0
3	I	5	0	0	0	0
4	E	125	0	0	2	0
4	I	44	0	0	0	0
All	All	1871	0	1589	23	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 (23) 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)
2:I:11:TYR:CE2	2:I:13:LYS:HD2	2.24	0.73
1:E:110:ASN:HD22	1:E:110:ASN:C	2.00	0.69
1:E:235(A):VAL:HG23	4:E:364:HOH:O	1.92	0.68
2:I:10:GLU:H	2:I:10:GLU:CD	1.97	0.66
2:I:10:GLU:OE1	2:I:10:GLU:N	2.30	0.59
2:I:21:ARG:NH1	2:I:21:ARG:HG2	2.19	0.58
2:I:21:ARG:HG2	2:I:21:ARG:HH11	1.68	0.58
1:E:166:ASN:HD22	1:E:179:GLY:HA2	1.74	0.53
2:I:21:ARG:HH11	2:I:21:ARG:CG	2.25	0.49
1:E:172:GLY:O	1:E:175:ASP:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:ASN:ND2	1:E:179:GLY:HA2	2.29	0.48
1:E:110:ASN:ND2	1:E:113:ILE:H	2.12	0.48
1:E:161:SER:HB3	4:E:267:HOH:O	2.14	0.48
1:E:49:THR:HG22	1:E:51:TYR:CE1	2.50	0.47
1:E:33:SER:HB3	1:E:66:TRP:CH2	2.53	0.43
1:E:67:TRP:CD2	1:E:81:ARG:HG3	2.55	0.42
1:E:113:ILE:O	1:E:115:LYS:NZ	2.49	0.42
2:I:9:SER:N	2:I:10:GLU:OE1	2.54	0.41
2:I:21:ARG:HH11	2:I:21:ARG:HB3	1.85	0.41
2:I:21:ARG:NH1	2:I:21:ARG:CG	2.82	0.41
1:E:110:ASN:C	1:E:110:ASN:ND2	2.75	0.41
1:E:113:ILE:HA	1:E:114:PRO:HD3	1.90	0.40
2:I:11:TYR:CZ	2:I:13:LYS:HD2	2.56	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	183/185 (99%)	176 (96%)	7 (4%)	0	100	100
2	I	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
All	All	232/236 (98%)	224 (97%)	8 (3%)	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	138/138 (100%)	134 (97%)	4 (3%)	37	25
2	I	45/45 (100%)	40 (89%)	5 (11%)	6	1
All	All	183/183 (100%)	174 (95%)	9 (5%)	22	10

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	79	SER
1	E	107	ARG
1	E	110	ASN
1	E	233	GLU
2	I	6	VAL
2	I	7	ASP
2	I	10	GLU
2	I	21	ARG
2	I	34	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	110	ASN
1	E	166	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
3	PO4	I	500	-	4,4,4	1.86	2 (50%)	6,6,6	1.25	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	500	PO4	P-O4	-2.42	1.47	1.54
3	I	500	PO4	P-O1	-2.00	1.46	1.50

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.

5.7 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.