Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 09:56 PM EDT

PDB ID	:	1SGR
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 (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:

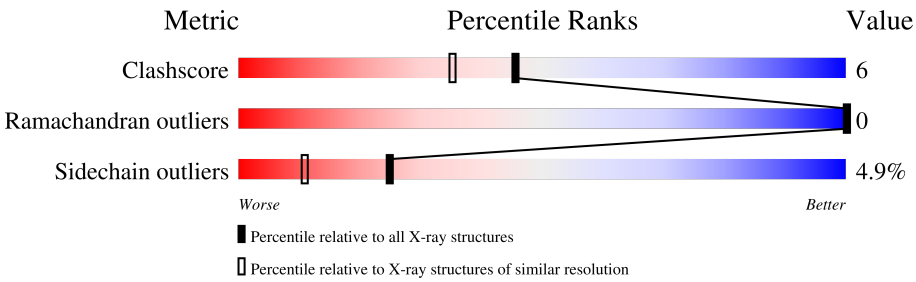
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	185	58% 35% 6%
2	I	51	43% 45% 8% •

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

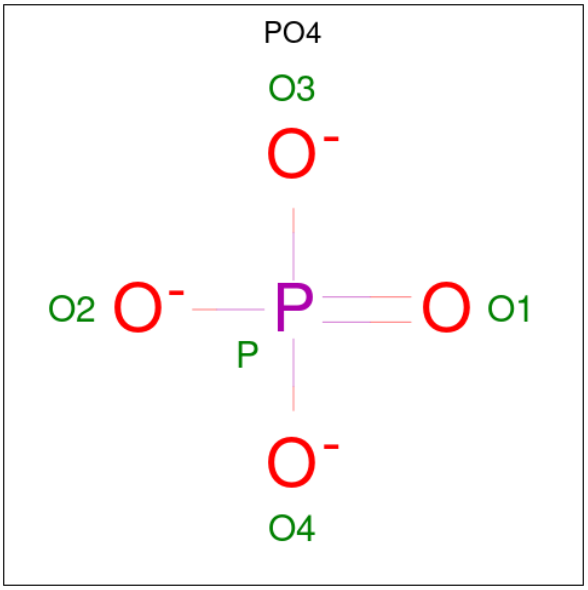
There is a discrepancy between the modelled and reference sequences:

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 (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is water.

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

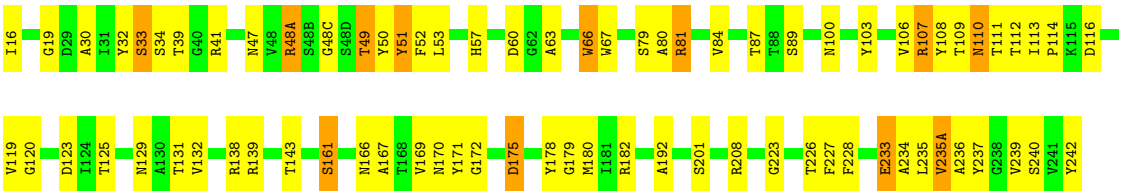
3 Residue-property plots (i)

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.

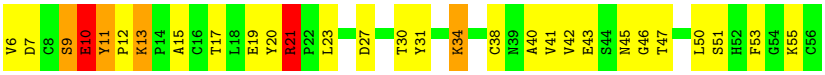
• Molecule 1: STREPTOMYCES GRISEUS PROTEINASE B

Chain E: 58% 35% 6%



• Molecule 2: TURKEY OVOMUCOID INHIBITOR

Chain I: 43% 45% 8% •



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	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 (i)

5.1 Standard geometry (i)

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	1.06	1/1335 (0.1%)	2.75	118/1820 (6.5%)
2	I	1.15	3/395 (0.8%)	3.00	49/533 (9.2%)
All	All	1.08	4/1730 (0.2%)	2.81	167/2353 (7.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	233	GLU	CD-OE2	9.31	1.35	1.25
2	I	10	GLU	CD-OE1	8.47	1.34	1.25
2	I	43	GLU	CD-OE1	6.41	1.32	1.25
2	I	19	GLU	CD-OE2	5.68	1.31	1.25

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	21	ARG	NE-CZ-NH1	17.67	129.13	120.30
1	E	81	ARG	NE-CZ-NH2	16.89	128.75	120.30
1	E	81	ARG	NE-CZ-NH1	-14.10	113.25	120.30
1	E	41	ARG	NE-CZ-NH1	13.98	127.29	120.30
1	E	120	GLY	C-N-CA	-13.55	93.84	122.30
1	E	235(A)	VAL	CG1-CB-CG2	-13.38	89.49	110.90
1	E	180	MET	CG-SD-CE	-12.28	80.55	100.20
2	I	21	ARG	NE-CZ-NH2	-11.41	114.59	120.30
2	I	31	TYR	CG-CD2-CE2	-10.61	112.81	121.30
1	E	116	ASP	CB-CG-OD1	10.29	127.56	118.30
1	E	84	VAL	CG1-CB-CG2	-10.21	94.56	110.90
1	E	39	THR	CA-CB-CG2	-9.70	98.82	112.40
2	I	20	TYR	CB-CG-CD2	-9.67	115.20	121.00
1	E	235(A)	VAL	N-CA-CB	-9.53	90.54	111.50
2	I	23	LEU	CB-CG-CD2	-9.46	94.92	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	15	ALA	N-CA-CB	9.44	123.32	110.10
1	E	167	ALA	N-CA-CB	-9.10	97.36	110.10
1	E	123	ASP	CB-CG-OD2	-9.07	110.13	118.30
1	E	123	ASP	CB-CG-OD1	9.06	126.45	118.30
1	E	108	TYR	CD1-CE1-CZ	-8.92	111.77	119.80
1	E	103	TYR	CZ-CE2-CD2	-8.88	111.81	119.80
2	I	13	LYS	CD-CE-NZ	-8.74	91.59	111.70
1	E	227	PHE	CG-CD1-CE1	8.73	130.40	120.80
2	I	31	TYR	CZ-CE2-CD2	8.51	127.46	119.80
2	I	11	TYR	CD1-CE1-CZ	-8.50	112.15	119.80
2	I	30	THR	CA-CB-CG2	-8.32	100.75	112.40
1	E	175	ASP	CB-CG-OD2	8.29	125.76	118.30
2	I	31	TYR	CB-CG-CD2	-8.12	116.13	121.00
1	E	242	TYR	CG-CD2-CE2	-8.11	114.81	121.30
1	E	239	VAL	CG1-CB-CG2	-7.92	98.23	110.90
1	E	60	ASP	C-N-CA	-7.85	105.81	122.30
1	E	237	TYR	CG-CD1-CE1	-7.84	115.03	121.30
1	E	79	SER	N-CA-CB	7.82	122.23	110.50
2	I	9	SER	O-C-N	-7.80	110.22	122.70
1	E	161	SER	CB-CA-C	7.72	124.77	110.10
1	E	60	ASP	CB-CG-OD2	-7.68	111.38	118.30
1	E	112	THR	CA-CB-CG2	-7.68	101.65	112.40
1	E	227	PHE	CB-CG-CD1	7.67	126.17	120.80
1	E	178	TYR	CD1-CE1-CZ	-7.64	112.93	119.80
2	I	11	TYR	CG-CD1-CE1	7.62	127.39	121.30
1	E	208	ARG	CD-NE-CZ	7.58	134.21	123.60
1	E	87	THR	CA-CB-CG2	-7.52	101.88	112.40
1	E	39	THR	N-CA-CB	-7.41	96.23	110.30
2	I	31	TYR	CD1-CE1-CZ	-7.33	113.20	119.80
2	I	17	THR	O-C-N	-7.32	110.98	122.70
2	I	27	ASP	CB-CG-OD1	7.30	124.87	118.30
2	I	40	ALA	CB-CA-C	-7.27	99.20	110.10
1	E	125	THR	OG1-CB-CG2	-7.16	93.53	110.00
1	E	237	TYR	CB-CG-CD1	-7.15	116.71	121.00
1	E	66	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	E	235(A)	VAL	CA-CB-CG1	-7.11	100.23	110.90
2	I	55	LYS	CB-CA-C	-7.09	96.23	110.40
2	I	53	PHE	CB-CG-CD1	-7.04	115.88	120.80
1	E	111	THR	CA-CB-CG2	-7.02	102.58	112.40
2	I	51	SER	CA-CB-OG	-6.99	92.33	111.20
1	E	87	THR	OG1-CB-CG2	-6.94	94.03	110.00
1	E	52	PHE	N-CA-CB	6.93	123.08	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	12	PRO	CA-C-N	-6.93	101.96	117.20
2	I	23	LEU	CB-CG-CD1	-6.86	99.33	111.00
2	I	11	TYR	CA-CB-CG	-6.75	100.58	113.40
1	E	119	VAL	CA-CB-CG1	-6.75	100.78	110.90
2	I	31	TYR	CG-CD1-CE1	6.74	126.69	121.30
1	E	63	ALA	CB-CA-C	-6.73	100.00	110.10
1	E	34	SER	N-CA-CB	6.72	120.57	110.50
1	E	109	THR	OG1-CB-CG2	-6.70	94.59	110.00
1	E	66	TRP	CA-CB-CG	-6.70	100.98	113.70
2	I	41	VAL	CG1-CB-CG2	-6.69	100.19	110.90
1	E	51	TYR	CB-CG-CD1	-6.68	116.99	121.00
1	E	227	PHE	CD1-CG-CD2	-6.67	109.63	118.30
1	E	237	TYR	CZ-CE2-CD2	-6.65	113.81	119.80
2	I	12	PRO	O-C-N	6.63	133.31	122.70
2	I	53	PHE	CZ-CE2-CD2	-6.62	112.15	120.10
2	I	50	LEU	CB-CA-C	-6.61	97.64	110.20
1	E	47	ASN	O-C-N	-6.56	112.20	122.70
1	E	171	TYR	CZ-CE2-CD2	-6.55	113.91	119.80
1	E	171	TYR	CG-CD2-CE2	6.53	126.52	121.30
1	E	201	SER	C-N-CA	-6.49	108.68	122.30
2	I	10	GLU	N-CA-CB	-6.47	98.95	110.60
1	E	80	ALA	N-CA-CB	-6.46	101.05	110.10
2	I	47	THR	OG1-CB-CG2	-6.46	95.14	110.00
1	E	57	HIS	N-CA-CB	6.45	122.21	110.60
1	E	143	THR	OG1-CB-CG2	-6.45	95.17	110.00
1	E	234	ALA	N-CA-CB	-6.45	101.07	110.10
1	E	242	TYR	CD1-CE1-CZ	-6.42	114.02	119.80
1	E	89	SER	N-CA-CB	6.42	120.12	110.50
1	E	120	GLY	O-C-N	-6.40	112.33	123.20
1	E	242	TYR	CG-CD1-CE1	6.38	126.40	121.30
1	E	129	ASN	CA-CB-CG	-6.29	99.57	113.40
1	E	51	TYR	CD1-CE1-CZ	-6.24	114.18	119.80
1	E	236	ALA	CB-CA-C	-6.24	100.74	110.10
1	E	138	ARG	NE-CZ-NH1	-6.24	117.18	120.30
2	I	23	LEU	CD1-CG-CD2	-6.21	91.86	110.50
2	I	34	LYS	CD-CE-NZ	6.21	125.97	111.70
1	E	103	TYR	CG-CD2-CE2	6.20	126.26	121.30
1	E	100	ASN	N-CA-CB	6.18	121.73	110.60
1	E	242	TYR	CZ-CE2-CD2	6.13	125.31	119.80
2	I	51	SER	N-CA-CB	-6.06	101.42	110.50
2	I	45	ASN	CB-CG-OD1	6.05	133.70	121.60
1	E	120	GLY	N-CA-C	-6.04	97.99	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	66	TRP	CD2-CE2-CZ2	-6.03	115.06	122.30
1	E	178	TYR	C-N-CA	-6.02	109.66	122.30
1	E	170	ASN	N-CA-CB	-6.00	99.80	110.60
1	E	132	VAL	CA-CB-CG2	-5.98	101.94	110.90
1	E	30	ALA	CB-CA-C	-5.96	101.16	110.10
1	E	81	ARG	CG-CD-NE	5.94	124.27	111.80
1	E	106	VAL	CA-CB-CG1	5.92	119.78	110.90
1	E	100	ASN	CA-CB-CG	-5.91	100.39	113.40
1	E	84	VAL	CA-CB-CG2	-5.91	102.03	110.90
1	E	138	ARG	NE-CZ-NH2	5.85	123.23	120.30
1	E	66	TRP	CH2-CZ2-CE2	5.84	123.25	117.40
2	I	46	GLY	CA-C-O	-5.84	110.09	120.60
1	E	120	GLY	CA-C-O	5.83	131.10	120.60
1	E	139	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	E	51	TYR	CB-CG-CD2	5.78	124.47	121.00
1	E	89	SER	CB-CA-C	-5.78	99.12	110.10
1	E	66	TRP	CE2-CD2-CG	-5.75	102.70	107.30
2	I	12	PRO	N-CA-CB	-5.75	96.27	102.60
1	E	63	ALA	N-CA-CB	-5.72	102.09	110.10
2	I	55	LYS	O-C-N	-5.71	113.56	122.70
2	I	42	VAL	CG1-CB-CG2	5.70	120.02	110.90
2	I	11	TYR	CB-CG-CD1	5.69	124.42	121.00
1	E	108	TYR	CG-CD2-CE2	-5.65	116.78	121.30
1	E	33	SER	CA-CB-OG	-5.64	95.97	111.20
1	E	39	THR	CA-C-N	5.61	127.41	116.20
1	E	48(A)	ARG	CD-NE-CZ	5.61	131.45	123.60
1	E	182	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	E	169	VAL	CB-CA-C	-5.57	100.82	111.40
2	I	41	VAL	CA-CB-CG2	-5.56	102.56	110.90
1	E	139	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	E	50	TYR	CG-CD1-CE1	5.54	125.73	121.30
2	I	11	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	E	41	ARG	NH1-CZ-NH2	-5.48	113.37	119.40
1	E	49	THR	O-C-N	5.46	131.44	122.70
2	I	38	CYS	O-C-N	-5.46	113.96	122.70
2	I	13	LYS	CB-CG-CD	-5.45	97.42	111.60
1	E	228	PHE	CB-CG-CD2	-5.45	116.99	120.80
1	E	119	VAL	N-CA-C	-5.43	96.33	111.00
1	E	57	HIS	O-C-N	-5.43	114.02	122.70
1	E	32	TYR	CZ-CE2-CD2	-5.42	114.92	119.80
1	E	226	THR	OG1-CB-CG2	-5.37	97.65	110.00
1	E	48(C)	GLY	N-CA-C	-5.36	99.69	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	123	ASP	CA-C-O	-5.35	108.87	120.10
1	E	50	TYR	CB-CG-CD1	5.34	124.20	121.00
1	E	139	ARG	CG-CD-NE	-5.27	100.74	111.80
1	E	16	ILE	CG1-CB-CG2	5.26	122.98	111.40
1	E	123	ASP	N-CA-CB	-5.26	101.14	110.60
2	I	50	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	E	50	TYR	CA-C-N	-5.21	105.74	117.20
2	I	21	ARG	N-CA-C	-5.21	96.93	111.00
1	E	169	VAL	CG1-CB-CG2	-5.21	102.57	110.90
1	E	131	THR	CA-CB-OG1	5.19	119.89	109.00
2	I	23	LEU	CB-CA-C	-5.18	100.35	110.20
2	I	11	TYR	CG-CD2-CE2	-5.18	117.16	121.30
1	E	48(C)	GLY	CA-C-O	5.16	129.89	120.60
1	E	235	LEU	C-N-CA	-5.15	108.83	121.70
2	I	34	LYS	CG-CD-CE	5.15	127.35	111.90
1	E	223	GLY	C-N-CA	-5.14	111.51	122.30
1	E	81	ARG	C-N-CA	-5.13	108.86	121.70
1	E	240	SER	CA-CB-OG	-5.11	97.40	111.20
1	E	19	GLY	CA-C-O	-5.11	111.41	120.60
1	E	53	LEU	CB-CG-CD2	-5.09	102.34	111.00
1	E	107	ARG	N-CA-CB	-5.05	101.50	110.60
1	E	41	ARG	CD-NE-CZ	-5.04	116.55	123.60
1	E	84	VAL	N-CA-CB	-5.03	100.44	111.50
1	E	192	ALA	N-CA-CB	5.03	117.14	110.10
2	I	19	GLU	CG-CD-OE2	-5.03	108.25	118.30
1	E	87	THR	CA-CB-OG1	-5.02	98.45	109.00

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	11	0
2	I	387	0	358	10	0
3	I	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	125	0	0	2	0
4	I	44	0	0	0	0
All	All	1871	0	1589	21	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 6.

All (21) 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:235(A):VAL:HG23	4:E:364:HOH:O	1.92	0.68
1:E:110:ASN:HD22	1:E:110:ASN:C	2.00	0.65
2:I:10:GLU:H	2:I:10:GLU:CD	1.97	0.62
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
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
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: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%)	42	29
2	I	45/45 (100%)	40 (89%)	5 (11%)	6	1
All	All	183/183 (100%)	174 (95%)	9 (5%)	25	11

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

Mol	Chain	Res	Type
1	E	48(A)	ARG
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 monosaccharides 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 (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.