



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6APR / pdb_00006apr
Title : STRUCTURES OF COMPLEXES OF RHIZOPUSPEPSIN WITH PEP-STATIN AND OTHER STATINE-CONTAINING INHIBITORS
Authors : Suguna, K.; Davies, D.R.
Deposited on : 1989-08-03
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

<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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

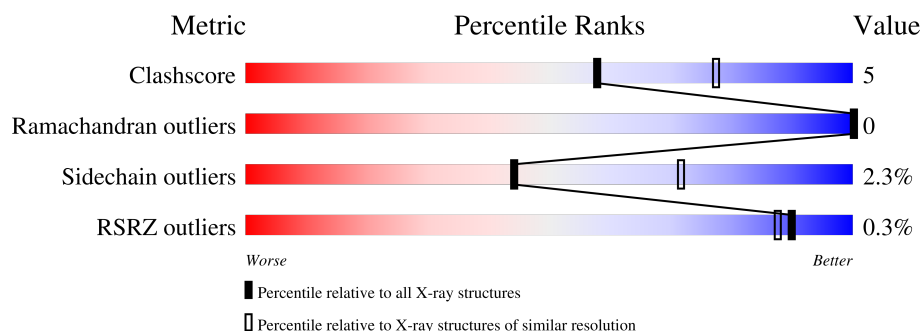
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	E	325	
2	I	6	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2686 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 RHIZOPUSPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	325	Total	C	N	O	S	0	4	0
			2417	1524	399	488	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	15	ILE	VAL	conflict	UNP P06026
E	54	GLY	ARG	conflict	UNP P06026
E	61	ASN	LYS	conflict	UNP P06026
E	116	SER	ASN	conflict	UNP P06026
E	162	LYS	SER	conflict	UNP P06026
E	230	ILE	VAL	conflict	UNP P06026
E	256	ALA	ARG	conflict	UNP P06026
E	281	PHE	TYR	conflict	UNP P06026
E	294	TRP	PHE	conflict	UNP P06026
E	295	GLY	ASP	conflict	UNP P06026

- Molecule 2 is a protein called PEPSTATIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	6	Total	C	N	O	0	0	0
			47	34	5	8			

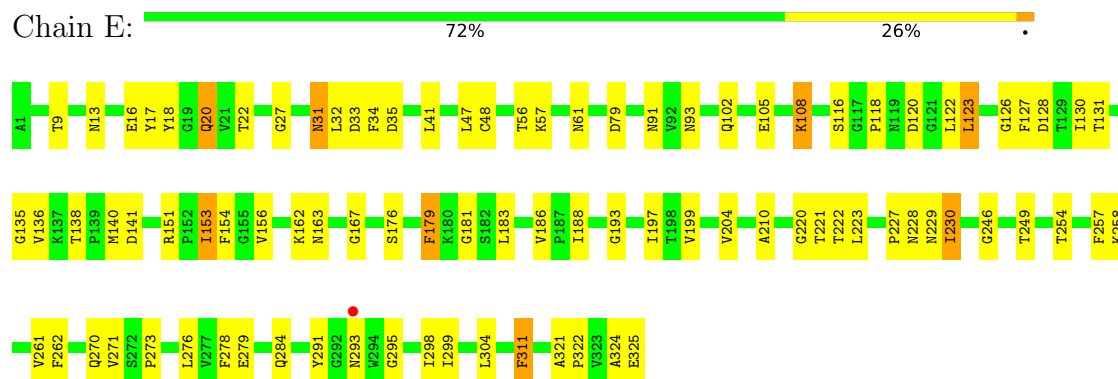
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	220	Total	O	0	0
			220	220		
3	I	2	Total	O	0	0
			2	2		

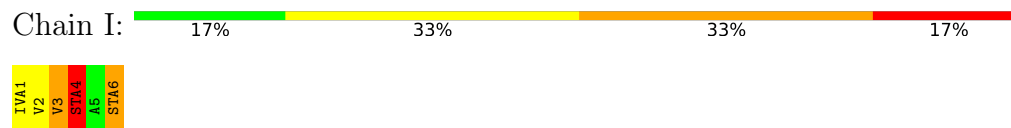
3 Residue-property plots

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 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.

• Molecule 1: RHIZOPUSPEPSIN



• Molecule 2: PEPSTATIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.33Å 60.66Å 107.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 82.1 (8.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.149 , (Not available) 0.134 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.5	EDS
L-test for twinning ¹	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.065 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2686	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IVA, STA

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	3/2488 (0.1%)	1.95	80/3381 (2.4%)
2	I	0.80	0/17	2.46	0/21
All	All	1.05	3/2505 (0.1%)	1.95	80/3402 (2.4%)

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
2	I	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	13	ASN	CG-OD1	6.20	1.35	1.23
1	E	228	ASN	CG-OD1	6.11	1.35	1.23
1	E	61	ASN	CG-OD1	5.19	1.33	1.23

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	199	VAL	CA-C-O	-8.39	111.44	120.59
1	E	123	LEU	CA-C-O	-8.00	112.00	120.40
1	E	105	GLU	CB-CG-CD	7.94	126.09	112.60
1	E	35	ASP	N-CA-C	7.64	121.52	107.99
1	E	284	GLN	OE1-CD-NE2	-7.60	115.00	122.60
1	E	270	GLN	CA-C-O	7.59	130.01	121.51
1	E	220	GLY	CA-C-N	7.46	133.52	123.00
1	E	220	GLY	C-N-CA	7.46	133.52	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	230	ILE	O-C-N	7.34	129.54	121.90
1	E	304	LEU	CA-C-O	-6.99	112.20	120.10
1	E	228	ASN	CA-CB-CG	6.96	119.56	112.60
1	E	27	GLY	CA-C-N	6.82	133.26	122.62
1	E	27	GLY	C-N-CA	6.82	133.26	122.62
1	E	179	PHE	CA-CB-CG	6.80	120.60	113.80
1	E	108	LYS	N-CA-C	-6.65	105.70	113.88
1	E	321	ALA	O-C-N	6.64	127.01	121.83
1	E	120	ASP	N-CA-C	-6.63	105.23	113.38
1	E	322	PRO	CA-C-O	-6.60	113.81	121.34
1	E	299	ILE	CA-C-N	6.57	128.77	122.27
1	E	299	ILE	C-N-CA	6.57	128.77	122.27
1	E	221	THR	N-CA-CB	6.55	120.86	110.65
1	E	284	GLN	CB-CG-CD	6.51	123.67	112.60
1	E	222	THR	N-CA-C	6.48	118.00	111.07
1	E	102	GLN	CG-CD-NE2	6.40	126.00	116.40
1	E	204	VAL	CB-CA-C	6.39	117.69	110.41
1	E	123	LEU	CA-C-N	-6.36	115.41	121.57
1	E	123	LEU	C-N-CA	-6.36	115.41	121.57
1	E	16	GLU	O-C-N	6.31	129.60	123.29
1	E	249	THR	N-CA-CB	6.30	120.46	110.57
1	E	153	ILE	N-CA-C	6.19	119.16	108.95
1	E	271	VAL	N-CA-C	-6.16	98.25	107.37
1	E	279	GLU	CA-CB-CG	6.12	126.34	114.10
1	E	229	ASN	CA-C-O	-6.11	114.07	120.55
1	E	311	PHE	CA-CB-CG	6.02	119.82	113.80
1	E	167	GLY	N-CA-C	-5.87	103.29	111.09
1	E	156	VAL	N-CA-C	5.81	116.24	107.75
1	E	325	GLU	CB-CG-CD	5.76	122.40	112.60
1	E	262	PHE	CA-CB-CG	5.73	119.53	113.80
1	E	228	ASN	CA-C-O	-5.70	114.36	121.02
1	E	183	LEU	CA-C-O	-5.67	114.94	121.47
1	E	57	LYS	O-C-N	5.63	130.00	123.30
1	E	32	LEU	CA-C-O	-5.63	114.75	121.11
1	E	181	GLY	CA-C-N	5.61	130.38	122.09
1	E	181	GLY	C-N-CA	5.61	130.38	122.09
1	E	270	GLN	N-CA-C	5.56	117.43	109.14
1	E	295	GLY	N-CA-C	-5.49	108.13	115.32
1	E	34	PHE	CB-CA-C	5.48	119.92	110.77
1	E	154	PHE	N-CA-CB	5.46	119.78	110.71
1	E	20	GLN	OE1-CD-NE2	5.45	128.05	122.60
1	E	258	LYS	N-CA-C	-5.45	102.78	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	249	THR	N-CA-C	-5.40	100.38	109.07
1	E	151[A]	ARG	CB-CA-C	5.38	116.95	108.88
1	E	151[B]	ARG	CB-CA-C	5.38	116.95	108.88
1	E	140	MET	N-CA-CB	5.37	118.11	110.16
1	E	324	ALA	N-CA-C	-5.37	100.43	108.96
1	E	136	VAL	CB-CA-C	5.33	117.52	110.91
1	E	47	LEU	CA-C-N	5.32	128.39	120.95
1	E	47	LEU	C-N-CA	5.32	128.39	120.95
1	E	126	GLY	N-CA-C	-5.29	104.51	112.60
1	E	229	ASN	O-C-N	5.28	127.72	122.12
1	E	91	ASN	CA-CB-CG	5.28	117.88	112.60
1	E	199	VAL	CB-CA-C	5.25	118.17	110.98
1	E	199	VAL	N-CA-C	-5.24	100.34	107.99
1	E	56	THR	N-CA-C	-5.23	100.77	109.46
1	E	141	ASP	CB-CG-OD2	5.22	130.41	118.40
1	E	199	VAL	O-C-N	5.22	129.86	122.97
1	E	34	PHE	CA-CB-CG	5.21	119.01	113.80
1	E	47	LEU	N-CA-C	-5.20	106.99	113.38
1	E	223	LEU	O-C-N	5.18	130.22	122.76
1	E	131	THR	N-CA-C	-5.17	103.21	110.50
1	E	186	VAL	O-C-N	5.17	126.99	121.10
1	E	31	ASN	O-C-N	5.16	129.19	123.05
1	E	33	ASP	CA-CB-CG	5.15	117.75	112.60
1	E	261	VAL	N-CA-C	5.09	115.30	108.17
1	E	118	PRO	CA-C-N	5.04	129.76	121.39
1	E	118	PRO	C-N-CA	5.04	129.76	121.39
1	E	135	GLY	CA-C-N	-5.03	115.88	122.37
1	E	135	GLY	C-N-CA	-5.03	115.88	122.37
1	E	127	PHE	CB-CA-C	5.00	119.72	109.76
1	E	230	ILE	CA-C-O	-5.00	115.50	121.05

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	4	STA	Mainchain,Peptide

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	2417	0	2331	22	0
2	I	47	0	60	4	0
3	E	220	0	0	0	0
3	I	2	0	0	0	0
All	All	2686	0	2391	22	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 5.

All (22) 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:79:ASP:HB3	2:I:3:VAL:HG13	1.81	0.61
1:E:122:LEU:HD21	2:I:4:STA:HD12	1.83	0.61
1:E:188:ILE:HD13	1:E:197:ILE:HG22	1.85	0.58
1:E:162:LYS:NZ	1:E:163:ASN:HD21	2.07	0.53
1:E:273:PRO:HA	1:E:276:LEU:HD12	1.91	0.52
1:E:18:TYR:CD1	1:E:31:ASN:HB3	2.45	0.52
1:E:162:LYS:HG3	1:E:163:ASN:ND2	2.26	0.51
1:E:210:ALA:HB2	1:E:230:ILE:HG23	1.93	0.50
1:E:278:PHE:CE2	2:I:1:IVA:HG11	2.47	0.50
1:E:162:LYS:HZ3	1:E:163:ASN:HD21	1.60	0.50
1:E:298:ILE:HD13	2:I:6:STA:HD21	1.98	0.45
1:E:246:GLY:HA2	1:E:291:TYR:CE1	2.53	0.44
1:E:128:ASP:HB3	1:E:138:THR:HG23	1.99	0.44
1:E:176:SER:HA	1:E:179:PHE:CE1	2.53	0.43
1:E:130:ILE:HG23	1:E:193:GLY:HA3	2.01	0.43
1:E:22:THR:HB	1:E:93:ASN:HB3	2.01	0.43
1:E:254:THR:HA	1:E:257:PHE:CD1	2.54	0.42
1:E:153:ILE:HA	1:E:311:PHE:O	2.20	0.42
1:E:9:THR:O	1:E:17:TYR:HA	2.19	0.42
1:E:227:PRO:HD2	1:E:230:ILE:HD12	2.01	0.41
1:E:48:CYS:HA	1:E:108:LYS:O	2.22	0.40
1:E:20:GLN:HG2	1:E:31:ASN:OD1	2.22	0.40

There are no symmetry-related clashes.

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	327/325 (101%)	322 (98%)	5 (2%)	0	100	100
2	I	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	330/331 (100%)	324 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	259/255 (102%)	254 (98%)	5 (2%)	50	76
2	I	2/2 (100%)	0	2 (100%)	0	0
All	All	261/257 (102%)	254 (97%)	7 (3%)	44	67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	41	LEU
1	E	116[A]	SER
1	E	116[B]	SER
1	E	123	LEU
1	E	293	ASN
2	I	2	VAL
2	I	3	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	20	GLN
1	E	119	ASN
1	E	163	ASN
1	E	243	ASN
1	E	282	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	STA	I	4	2	10,10,11	0.87	0	9,12,14	2.08	3 (33%)
2	STA	I	6	2	10,10,11	1.46	2 (20%)	9,12,14	2.66	3 (33%)

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	STA	I	4	2	-	2/11/11/12	-
2	STA	I	6	2	-	5/11/11/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	6	STA	CH-CA	3.46	1.56	1.53
2	I	6	STA	CB-CA	-2.45	1.49	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	6	STA	CG-CB-CA	5.55	127.70	115.76
2	I	4	STA	CM-CH-CA	4.34	119.64	112.93
2	I	6	STA	CM-CH-CA	3.48	118.30	112.93
2	I	4	STA	O-C-CM	-3.19	116.09	125.38
2	I	6	STA	OH-CH-CM	3.17	116.53	109.24
2	I	4	STA	CH-CM-C	-2.92	108.05	113.02

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	4	STA	N-CA-CB-CG
2	I	4	STA	O-C-CM-CH
2	I	6	STA	CA-CH-CM-C
2	I	6	STA	O-C-CM-CH
2	I	6	STA	CA-CB-CG-CD1
2	I	6	STA	CA-CB-CG-CD2
2	I	6	STA	OH-CH-CM-C

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	4	STA	1	0
2	I	6	STA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	325/325 (100%)	-0.98	1 (0%) 90 87	2, 11, 22, 35	4 (1%)
2	I	3/6 (50%)	-0.68	0 100 100	13, 13, 16, 19	0
All	All	328/331 (99%)	-0.98	1 (0%) 90 87	2, 11, 22, 35	4 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	293	ASN	3.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	STA	I	6	11/12	0.84	0.10	23,25,30,32	0
2	STA	I	4	11/12	0.96	0.05	10,12,15,15	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.