Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 06:13 AM EST

PDB ID	:	1SIB
Title	:	REFINED CRYSTAL STRUCTURES OF SUBTILISIN NOVO IN COMPLEX WITH WILD-TYPE AND TWO MUTANT EGLINS. COMPARISON WITH OTHER SERINE PROTEINASE INHIBITOR COMPLEXES
Authors	:	Gruetter, M.G.; Heinz, D.W.; Priestle, J.P.
Deposited on	:	1993-08-02
Resolution	:	2.40 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:

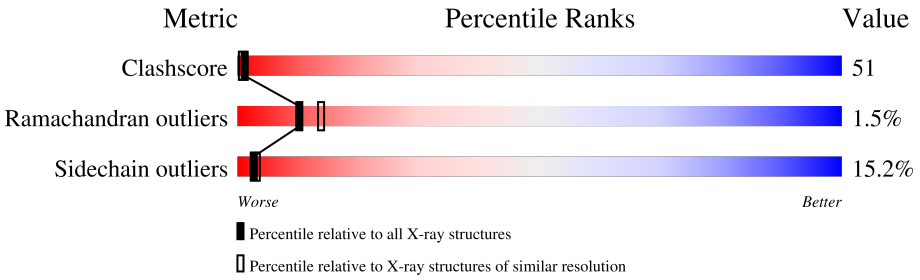
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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	275	39% 47% 13% ·
2	I	70	14% 50% 21% · 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2655 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 SUBTILISIN NOVO BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	275	Total	C	N	O	S	0	0	0
			1938	1204	335	394	5			

- Molecule 2 is a protein called EGLIN C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	63	Total	C	N	O	0	0	0
			520	339	87	94			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	53	LYS	ARG	conflict	UNP P01051

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	155	Total	O	0	0
			155	155		
4	I	40	Total	O	0	0
			40	40		

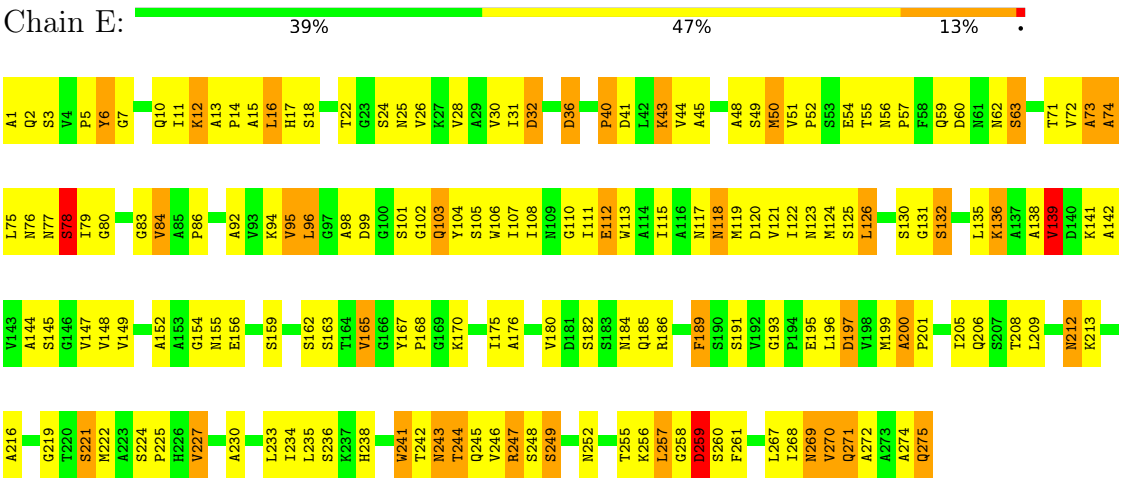
3 Residue-property plots (i)

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.

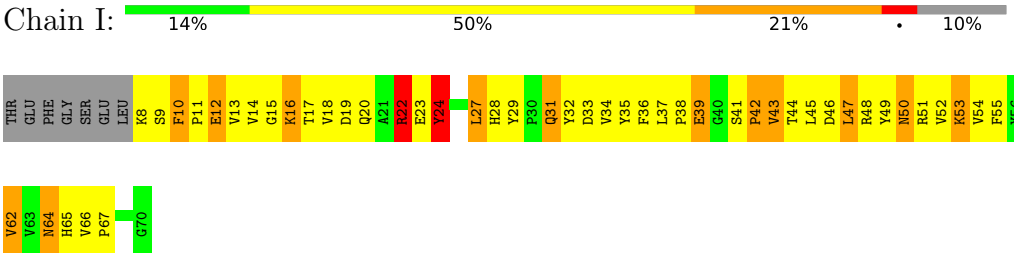
• Molecule 1: SUBTILISIN NOVO BPN'

Chain E:



• Molecule 2: EGLIN C

Chain I:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	84.90Å 84.90Å 89.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	5.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.159 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2655	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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: CA

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	0.87	0/1976	2.05	58/2697 (2.2%)
2	I	0.85	0/538	2.00	20/735 (2.7%)
All	All	0.86	0/2514	2.04	78/3432 (2.3%)

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	186	ARG	NE-CZ-NH1	-12.52	114.04	120.30
1	E	36	ASP	CB-CG-OD2	11.48	128.63	118.30
1	E	96	LEU	CA-CB-CG	10.30	138.99	115.30
1	E	247	ARG	NE-CZ-NH2	9.46	125.03	120.30
1	E	200	ALA	N-CA-CB	9.39	123.24	110.10
1	E	197	ASP	CB-CG-OD2	-8.90	110.29	118.30
1	E	84	VAL	CG1-CB-CG2	8.66	124.75	110.90
1	E	36	ASP	CB-CG-OD1	-8.43	110.72	118.30
1	E	41	ASP	CB-CG-OD2	7.80	125.32	118.30
1	E	186	ARG	NE-CZ-NH2	7.72	124.16	120.30
2	I	51	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	E	233	LEU	CA-CB-CG	7.53	132.62	115.30
1	E	105	SER	N-CA-CB	7.41	121.62	110.50
1	E	247	ARG	NH1-CZ-NH2	-7.30	111.37	119.40
1	E	165	VAL	CG1-CB-CG2	-7.25	99.31	110.90
1	E	32	ASP	CB-CG-OD1	7.06	124.66	118.30
1	E	227	VAL	CG1-CB-CG2	-6.83	99.97	110.90
1	E	30	VAL	CA-CB-CG1	6.80	121.11	110.90
1	E	60	ASP	CB-CG-OD2	-6.76	112.22	118.30
2	I	46	ASP	CB-CG-OD1	-6.60	112.36	118.30
2	I	48	ARG	N-CA-CB	6.58	122.45	110.60
1	E	247	ARG	NE-CZ-NH1	6.52	123.56	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	212	ASN	CA-CB-CG	6.44	127.57	113.40
1	E	112	GLU	CA-CB-CG	6.43	127.56	113.40
1	E	182	SER	O-C-N	6.42	132.96	122.70
1	E	269	ASN	CA-C-O	-6.36	106.75	120.10
1	E	118	ASN	CA-CB-CG	6.34	127.34	113.40
1	E	40	PRO	C-N-CA	6.23	137.28	121.70
2	I	24	TYR	CB-CG-CD1	6.22	124.73	121.00
1	E	72	VAL	CA-CB-CG2	6.21	120.22	110.90
2	I	51	ARG	NH1-CZ-NH2	6.21	126.23	119.40
1	E	257	LEU	CA-CB-CG	6.15	129.45	115.30
2	I	39	GLU	CA-CB-CG	6.11	126.84	113.40
1	E	60	ASP	CB-CG-OD1	6.07	123.77	118.30
1	E	75	LEU	CA-CB-CG	6.07	129.25	115.30
2	I	51	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	E	77	ASN	CA-CB-CG	6.04	126.69	113.40
1	E	78	SER	N-CA-CB	-6.01	101.48	110.50
1	E	74	ALA	CB-CA-C	6.01	119.12	110.10
2	I	22	ARG	CD-NE-CZ	5.99	131.99	123.60
1	E	165	VAL	CA-CB-CG1	5.98	119.87	110.90
1	E	73	ALA	N-CA-CB	-5.94	101.78	110.10
2	I	49	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	E	45	ALA	CB-CA-C	-5.91	101.23	110.10
1	E	50	MET	CA-CB-CG	-5.87	103.31	113.30
1	E	132	SER	CB-CA-C	-5.86	98.96	110.10
1	E	110	GLY	C-N-CA	5.82	136.24	121.70
2	I	22	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	E	219	GLY	O-C-N	5.73	131.87	122.70
2	I	33	ASP	CB-CA-C	5.69	121.79	110.40
1	E	144	ALA	CB-CA-C	5.62	118.53	110.10
2	I	47	LEU	CA-CB-CG	5.60	128.18	115.30
1	E	92	ALA	CB-CA-C	-5.54	101.78	110.10
1	E	6	TYR	CA-C-N	5.49	127.17	116.20
2	I	12	GLU	CA-CB-CG	5.42	125.31	113.40
1	E	189	PHE	CB-CA-C	5.41	121.21	110.40
1	E	136	LYS	CB-CA-C	-5.37	99.65	110.40
2	I	53	LYS	N-CA-CB	5.34	120.21	110.60
2	I	61	ASN	CA-CB-CG	5.29	125.03	113.40
2	I	24	TYR	CB-CG-CD2	-5.28	117.83	121.00
2	I	9	SER	O-C-N	5.23	131.07	122.70
1	E	163	SER	N-CA-CB	5.23	118.34	110.50
1	E	259	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	E	73	ALA	N-CA-C	5.22	125.09	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	54	VAL	C-N-CA	5.19	134.67	121.70
1	E	31	ILE	CA-C-O	5.18	130.97	120.10
1	E	249	SER	O-C-N	5.17	130.98	122.70
1	E	26	VAL	CB-CA-C	5.15	121.18	111.40
1	E	139	VAL	CA-CB-CG1	5.15	118.62	110.90
1	E	120	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	E	95	VAL	CG1-CB-CG2	5.13	119.11	110.90
1	E	182	SER	CA-C-O	-5.13	109.32	120.10
1	E	185	GLN	CB-CA-C	-5.13	100.14	110.40
1	E	269	ASN	N-CA-C	-5.13	97.16	111.00
1	E	197	ASP	OD1-CG-OD2	5.09	132.97	123.30
2	I	42	PRO	O-C-N	5.08	130.82	122.70
1	E	126	LEU	CB-CG-CD1	5.04	119.58	111.00
2	I	27	LEU	N-CA-CB	-5.02	100.36	110.40

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	1938	0	1898	173	0
2	I	520	0	498	87	0
3	E	2	0	0	0	0
4	E	155	0	0	27	1
4	I	40	0	0	7	0
All	All	2655	0	2396	247	1

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 51.

All (247) 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:242:THR:H	1:E:245:GLN:NE2	1.15	1.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:60:THR:O	2:I:62:VAL:HG12	1.41	1.18
2:I:60:THR:HG22	2:I:62:VAL:CG1	1.76	1.16
1:E:242:THR:N	1:E:245:GLN:HE21	1.48	1.10
1:E:242:THR:N	1:E:245:GLN:NE2	2.00	1.08
1:E:196:LEU:HD13	4:E:342:HOH:O	1.59	1.03
1:E:102:GLY:O	2:I:42:PRO:HD2	1.59	1.02
1:E:196:LEU:HD22	4:E:342:HOH:O	1.61	0.99
1:E:170:LYS:HG3	1:E:195:GLU:HG2	1.48	0.96
2:I:31:GLN:H	2:I:31:GLN:NE2	1.66	0.93
1:E:221:SER:OG	2:I:45:LEU:C	2.10	0.90
1:E:170:LYS:CG	1:E:195:GLU:HG2	2.03	0.88
2:I:22:ARG:HA	2:I:22:ARG:HH11	1.40	0.87
2:I:50:ASN:HD22	2:I:50:ASN:H	1.23	0.86
1:E:108:ILE:HG23	1:E:138:ALA:HB2	1.59	0.85
1:E:49:SER:O	1:E:50:MET:HG2	1.76	0.84
1:E:40:PRO:O	4:E:337:HOH:O	1.94	0.84
2:I:11:PRO:HA	2:I:66:VAL:HG13	1.57	0.84
2:I:31:GLN:H	2:I:31:GLN:HE21	1.26	0.83
2:I:60:THR:HG22	2:I:62:VAL:HG12	1.60	0.83
1:E:165:VAL:O	1:E:170:LYS:HD2	1.79	0.83
2:I:31:GLN:HE21	2:I:31:GLN:N	1.76	0.83
1:E:235:LEU:HD21	1:E:246:VAL:HG21	1.62	0.82
1:E:49:SER:C	1:E:50:MET:HG2	1.97	0.81
1:E:15:ALA:CB	1:E:271:GLN:HG3	2.10	0.81
1:E:11:ILE:O	1:E:12:LYS:HB2	1.81	0.79
1:E:221:SER:OG	2:I:45:LEU:O	2.01	0.78
1:E:206:GLN:OE1	1:E:216:ALA:HB2	1.84	0.78
2:I:64:ASN:H	2:I:64:ASN:HD22	1.32	0.77
1:E:230:ALA:HB1	1:E:270:VAL:HG13	1.65	0.77
1:E:108:ILE:HG23	1:E:138:ALA:CB	2.13	0.77
1:E:196:LEU:CD2	4:E:342:HOH:O	2.26	0.77
2:I:57:ASN:O	2:I:61:ASN:HA	1.84	0.77
1:E:104:TYR:CE1	2:I:42:PRO:HG3	2.20	0.77
1:E:148:VAL:HG22	1:E:243:ASN:HB2	1.68	0.76
1:E:238:HIS:O	1:E:241:TRP:HB2	1.85	0.76
2:I:11:PRO:CA	2:I:66:VAL:HG13	2.14	0.75
1:E:123:ASN:ND2	1:E:224:SER:OG	2.19	0.75
1:E:139:VAL:HA	4:E:412:HOH:O	1.86	0.75
1:E:230:ALA:HB1	1:E:270:VAL:CG1	2.16	0.75
2:I:14:VAL:HG21	2:I:66:VAL:HG22	1.67	0.75
1:E:196:LEU:CD1	4:E:342:HOH:O	2.26	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:20:GLN:HA	4:I:92:HOH:O	1.87	0.73
1:E:200:ALA:HB1	1:E:201:PRO:CD	2.19	0.72
1:E:189:PHE:HA	4:E:315:HOH:O	1.91	0.71
1:E:136:LYS:O	1:E:136:LYS:HG2	1.91	0.70
2:I:11:PRO:HB3	2:I:66:VAL:HG11	1.74	0.70
2:I:60:THR:HG22	2:I:62:VAL:HG13	1.71	0.70
1:E:96:LEU:CD1	2:I:44:THR:HG22	2.20	0.70
1:E:62:ASN:O	1:E:63:SER:HB3	1.91	0.70
2:I:50:ASN:H	2:I:50:ASN:ND2	1.90	0.70
1:E:17:HIS:NE2	1:E:84:VAL:O	2.25	0.69
2:I:64:ASN:HD22	2:I:64:ASN:N	1.89	0.69
2:I:43:VAL:HG11	2:I:53:LYS:HD3	1.75	0.69
1:E:152:ALA:HB3	2:I:45:LEU:HD12	1.75	0.69
1:E:18:SER:HB3	4:E:413:HOH:O	1.93	0.69
2:I:50:ASN:HD22	2:I:50:ASN:N	1.89	0.68
2:I:22:ARG:HD3	2:I:22:ARG:C	2.12	0.68
1:E:242:THR:H	1:E:245:GLN:HE21	0.71	0.67
1:E:243:ASN:HD22	1:E:244:THR:N	1.93	0.67
1:E:10:GLN:HE21	1:E:184:ASN:HD21	1.43	0.67
1:E:108:ILE:HG22	1:E:108:ILE:O	1.94	0.66
1:E:1:ALA:HA	1:E:78:SER:O	1.95	0.66
2:I:11:PRO:HB3	2:I:66:VAL:CG1	2.25	0.66
1:E:36:ASP:C	1:E:36:ASP:OD1	2.32	0.66
1:E:275:GLN:CG	4:E:305:HOH:O	2.44	0.66
1:E:22:THR:HB	1:E:86:PRO:HG2	1.78	0.66
1:E:236:SER:HB2	4:E:410:HOH:O	1.96	0.66
2:I:59:GLY:C	2:I:61:ASN:H	1.98	0.66
1:E:15:ALA:HB3	1:E:271:GLN:HG3	1.78	0.66
1:E:200:ALA:HB1	1:E:201:PRO:HD2	1.79	0.65
2:I:64:ASN:H	2:I:64:ASN:ND2	1.94	0.65
2:I:24:TYR:CE1	2:I:28:HIS:ND1	2.65	0.65
1:E:10:GLN:HE21	1:E:184:ASN:ND2	1.95	0.65
2:I:19:ASP:N	4:I:108:HOH:O	2.29	0.64
1:E:272:ALA:O	1:E:275:GLN:NE2	2.30	0.64
1:E:95:VAL:HG23	1:E:95:VAL:O	1.97	0.64
1:E:142:ALA:O	1:E:147:VAL:HB	1.97	0.64
1:E:275:GLN:HG2	4:E:305:HOH:O	1.97	0.64
1:E:44:VAL:N	4:E:336:HOH:O	2.29	0.63
2:I:60:THR:O	2:I:62:VAL:N	2.32	0.63
2:I:18:VAL:O	2:I:22:ARG:HB2	1.99	0.63
2:I:16:LYS:HB3	2:I:20:GLN:HB2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:10:PHE:CA	2:I:12:GLU:OE1	2.47	0.62
1:E:51:VAL:HG12	1:E:54:GLU:HB2	1.81	0.62
1:E:107:ILE:CD1	1:E:126:LEU:HD13	2.30	0.62
1:E:132:SER:HB2	1:E:135:LEU:H	1.65	0.61
2:I:10:PHE:HA	2:I:12:GLU:OE1	2.00	0.61
1:E:104:TYR:CE1	2:I:42:PRO:CG	2.83	0.61
1:E:170:LYS:NZ	4:E:422:HOH:O	2.13	0.60
1:E:49:SER:N	1:E:57:PRO:HG3	2.16	0.60
2:I:29:TYR:HB3	2:I:32:TYR:HD2	1.67	0.60
2:I:24:TYR:HE1	2:I:28:HIS:ND1	2.00	0.59
1:E:205:ILE:HD12	4:E:429:HOH:O	2.01	0.59
1:E:10:GLN:NE2	1:E:184:ASN:ND2	2.51	0.59
1:E:107:ILE:HD13	1:E:126:LEU:CD1	2.33	0.58
2:I:22:ARG:HD3	2:I:22:ARG:O	2.04	0.58
2:I:64:ASN:ND2	2:I:65:HIS:ND1	2.51	0.58
1:E:43:LYS:NZ	4:E:348:HOH:O	2.36	0.58
1:E:115:ILE:HD11	1:E:142:ALA:HB2	1.86	0.58
1:E:107:ILE:HD13	1:E:126:LEU:HD11	1.85	0.57
1:E:107:ILE:HD11	1:E:126:LEU:HD13	1.86	0.57
1:E:2:GLN:HA	1:E:80:GLY:O	2.05	0.57
1:E:96:LEU:HD21	1:E:126:LEU:HD22	1.87	0.57
1:E:108:ILE:CG2	1:E:138:ALA:HB2	2.34	0.57
1:E:130:SER:HA	1:E:167:TYR:CE1	2.40	0.56
1:E:51:VAL:CG1	1:E:54:GLU:HB2	2.36	0.56
1:E:208:THR:O	1:E:209:LEU:HD23	2.05	0.56
2:I:10:PHE:C	2:I:12:GLU:OE1	2.44	0.56
2:I:60:THR:HG22	2:I:62:VAL:HG11	1.81	0.56
1:E:115:ILE:HD11	1:E:142:ALA:CA	2.36	0.56
1:E:242:THR:H	1:E:245:GLN:HE22	1.39	0.55
1:E:234:ILE:CG2	1:E:241:TRP:CZ3	2.88	0.55
2:I:24:TYR:HE1	2:I:28:HIS:HD1	1.51	0.55
2:I:27:LEU:HD22	2:I:28:HIS:CD2	2.41	0.55
1:E:96:LEU:HD12	2:I:44:THR:HG22	1.87	0.55
2:I:35:TYR:OH	4:I:106:HOH:O	2.18	0.54
1:E:267:LEU:HG	1:E:268:ILE:O	2.07	0.54
1:E:184:ASN:O	1:E:257:LEU:HD13	2.07	0.54
1:E:132:SER:HB2	1:E:135:LEU:CB	2.38	0.53
1:E:176:ALA:O	1:E:197:ASP:HB2	2.09	0.53
1:E:48:ALA:HB2	1:E:113:TRP:NE1	2.23	0.53
1:E:170:LYS:HG2	1:E:195:GLU:HG2	1.88	0.53
1:E:108:ILE:O	1:E:108:ILE:CG2	2.56	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:13:VAL:HG23	2:I:24:TYR:CE2	2.43	0.53
2:I:59:GLY:C	2:I:61:ASN:N	2.63	0.53
2:I:59:GLY:O	2:I:61:ASN:N	2.42	0.52
1:E:111:ILE:HG21	4:E:412:HOH:O	2.10	0.52
1:E:154:GLY:C	1:E:191:SER:OG	2.47	0.52
1:E:141:LYS:HB2	1:E:141:LYS:NZ	2.25	0.51
1:E:7:GLY:CA	1:E:201:PRO:HG2	2.40	0.51
1:E:11:ILE:O	1:E:12:LYS:CB	2.57	0.51
1:E:55:THR:O	1:E:57:PRO:HD3	2.10	0.51
1:E:57:PRO:C	1:E:59:GLN:H	2.13	0.51
1:E:101:SER:OG	2:I:37:LEU:HD22	2.10	0.51
2:I:15:GLY:O	2:I:62:VAL:HG23	2.10	0.51
2:I:31:GLN:NE2	2:I:31:GLN:N	2.39	0.51
1:E:275:GLN:HG3	4:E:305:HOH:O	2.08	0.50
1:E:234:ILE:HG21	1:E:241:TRP:HZ3	1.77	0.50
1:E:62:ASN:ND2	1:E:98:ALA:O	2.34	0.50
1:E:124:MET:CE	1:E:149:VAL:HG13	2.42	0.50
1:E:62:ASN:O	1:E:63:SER:CB	2.59	0.50
1:E:107:ILE:CD1	1:E:126:LEU:CD1	2.90	0.50
1:E:248:SER:O	1:E:252:ASN:HB2	2.12	0.50
1:E:106:TRP:HA	4:E:432:HOH:O	2.11	0.50
1:E:258:GLY:O	1:E:259:ASP:C	2.49	0.49
2:I:22:ARG:HD2	4:I:89:HOH:O	2.12	0.49
1:E:28:VAL:HG22	1:E:121:VAL:HB	1.94	0.49
1:E:96:LEU:CD1	2:I:44:THR:CG2	2.88	0.49
1:E:13:ALA:N	1:E:14:PRO:CD	2.75	0.49
1:E:71:THR:CG2	1:E:225:PRO:HB2	2.43	0.49
1:E:113:TRP:O	1:E:117:ASN:ND2	2.46	0.49
2:I:24:TYR:CD1	2:I:24:TYR:C	2.84	0.49
2:I:17:THR:OG1	4:I:108:HOH:O	2.20	0.48
1:E:55:THR:HG23	4:E:403:HOH:O	2.13	0.48
2:I:34:VAL:HA	2:I:52:VAL:O	2.12	0.48
1:E:10:GLN:NE2	1:E:184:ASN:HD21	2.08	0.48
1:E:115:ILE:CD1	1:E:142:ALA:HA	2.44	0.48
1:E:242:THR:CA	1:E:245:GLN:HE21	2.25	0.48
1:E:104:TYR:CE2	1:E:131:GLY:HA2	2.49	0.48
1:E:234:ILE:HG21	1:E:241:TRP:CZ3	2.49	0.47
1:E:24:SER:O	1:E:25:ASN:HB2	2.12	0.47
1:E:59:GLN:O	1:E:94:LYS:CE	2.62	0.47
1:E:104:TYR:O	1:E:108:ILE:HG13	2.14	0.47
1:E:148:VAL:CG2	1:E:243:ASN:HB2	2.42	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:THR:OG1	4:E:285:HOH:O	2.18	0.47
1:E:16:LEU:HD11	1:E:274:ALA:CB	2.43	0.47
1:E:99:ASP:HB3	4:E:319:HOH:O	2.13	0.47
1:E:102:GLY:O	2:I:42:PRO:CD	2.48	0.47
1:E:155:ASN:ND2	2:I:47:LEU:HD22	2.29	0.47
1:E:15:ALA:HB1	1:E:271:GLN:HG3	1.92	0.46
1:E:209:LEU:HB2	1:E:213:LYS:HB2	1.97	0.46
2:I:11:PRO:CB	2:I:66:VAL:HG13	2.45	0.46
1:E:1:ALA:CA	1:E:78:SER:O	2.62	0.46
2:I:10:PHE:HD1	2:I:67:PRO:O	1.99	0.46
2:I:16:LYS:HB3	2:I:20:GLN:CB	2.44	0.46
2:I:12:GLU:HG2	2:I:24:TYR:CE2	2.51	0.45
1:E:7:GLY:HA2	1:E:201:PRO:HG2	1.97	0.45
2:I:23:GLU:O	2:I:27:LEU:HB2	2.16	0.45
1:E:115:ILE:HD11	1:E:142:ALA:N	2.31	0.45
1:E:48:ALA:HB1	1:E:50:MET:CE	2.47	0.45
1:E:243:ASN:HD22	1:E:243:ASN:C	2.19	0.45
1:E:49:SER:OG	1:E:54:GLU:O	2.25	0.45
1:E:108:ILE:HG23	1:E:138:ALA:HB1	1.98	0.45
2:I:60:THR:O	2:I:62:VAL:CG1	2.35	0.45
1:E:175:ILE:HG12	1:E:247:ARG:NE	2.31	0.44
1:E:25:ASN:HA	4:E:431:HOH:O	2.16	0.44
1:E:103:GLN:HG3	1:E:106:TRP:CE2	2.53	0.44
1:E:227:VAL:HG22	1:E:268:ILE:HD13	1.99	0.44
1:E:275:GLN:OXT	4:E:305:HOH:O	2.21	0.44
2:I:37:LEU:O	2:I:38:PRO:C	2.54	0.44
1:E:230:ALA:HA	1:E:270:VAL:HG11	1.99	0.44
1:E:256:LYS:HE3	4:E:423:HOH:O	2.16	0.44
1:E:49:SER:C	1:E:50:MET:CG	2.76	0.44
2:I:60:THR:C	2:I:62:VAL:H	2.22	0.43
1:E:83:GLY:O	1:E:86:PRO:HD3	2.18	0.43
1:E:12:LYS:HD3	1:E:269:ASN:OD1	2.17	0.43
1:E:260:SER:HB2	4:E:419:HOH:O	2.18	0.43
2:I:13:VAL:HG11	2:I:67:PRO:HG3	2.00	0.43
2:I:37:LEU:O	2:I:55:PHE:HA	2.18	0.43
1:E:119:MET:O	1:E:147:VAL:HG22	2.18	0.43
2:I:36:PHE:C	2:I:37:LEU:HG	2.39	0.43
2:I:38:PRO:HB3	2:I:58:PRO:HG3	2.01	0.43
1:E:180:VAL:HG13	1:E:199:MET:HE2	2.01	0.43
1:E:48:ALA:HB2	1:E:113:TRP:CE2	2.54	0.43
1:E:104:TYR:CD1	2:I:42:PRO:CG	3.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:17:THR:OG1	2:I:20:GLN:HG3	2.19	0.42
1:E:175:ILE:HG21	1:E:175:ILE:HD13	1.65	0.42
1:E:235:LEU:CD2	1:E:246:VAL:HG21	2.40	0.42
1:E:104:TYR:HD1	1:E:107:ILE:HD12	1.84	0.42
1:E:115:ILE:HD11	1:E:142:ALA:CB	2.47	0.42
1:E:79:ILE:HD13	1:E:79:ILE:HG21	1.87	0.42
1:E:130:SER:O	1:E:167:TYR:CE1	2.72	0.42
1:E:230:ALA:HB1	1:E:270:VAL:HG11	2.01	0.42
2:I:13:VAL:HG23	2:I:24:TYR:HE2	1.84	0.42
1:E:108:ILE:O	1:E:112:GLU:HG2	2.19	0.42
2:I:24:TYR:CE1	2:I:28:HIS:CG	3.08	0.42
1:E:115:ILE:CD1	1:E:142:ALA:CA	2.96	0.42
1:E:243:ASN:HD22	1:E:244:THR:H	1.67	0.42
2:I:57:ASN:ND2	2:I:58:PRO:HD2	2.35	0.41
1:E:224:SER:N	1:E:225:PRO:HD2	2.34	0.41
2:I:24:TYR:HE1	2:I:28:HIS:CG	2.37	0.41
1:E:59:GLN:O	1:E:94:LYS:HE3	2.20	0.41
1:E:71:THR:HG22	1:E:225:PRO:HB2	2.00	0.41
1:E:230:ALA:CB	1:E:270:VAL:CG1	2.94	0.41
2:I:50:ASN:ND2	2:I:50:ASN:N	2.54	0.41
1:E:138:ALA:C	4:E:412:HOH:O	2.58	0.41
1:E:184:ASN:HD22	1:E:184:ASN:HA	1.72	0.41
1:E:230:ALA:CA	1:E:270:VAL:HG11	2.51	0.41
1:E:234:ILE:CG2	1:E:241:TRP:HZ3	2.30	0.41
1:E:235:LEU:HD21	1:E:246:VAL:CG2	2.42	0.41
2:I:19:ASP:HA	4:I:109:HOH:O	2.20	0.41
2:I:22:ARG:CD	4:I:89:HOH:O	2.69	0.41
1:E:51:VAL:O	1:E:54:GLU:O	2.39	0.41
1:E:73:ALA:O	1:E:74:ALA:C	2.59	0.41
1:E:122:ILE:HG13	1:E:147:VAL:HG11	2.01	0.41
1:E:193:GLY:N	1:E:261:PHE:O	2.50	0.41
2:I:10:PHE:N	2:I:10:PHE:CD1	2.88	0.41
2:I:66:VAL:HA	2:I:67:PRO:HD2	1.89	0.41
1:E:221:SER:O	1:E:225:PRO:CD	2.69	0.41
2:I:28:HIS:CD2	2:I:28:HIS:N	2.89	0.41
2:I:11:PRO:HB3	2:I:66:VAL:HG13	2.01	0.40
1:E:49:SER:HA	1:E:94:LYS:HB3	2.03	0.40
1:E:167:TYR:HB3	1:E:168:PRO:HA	2.03	0.40
1:E:52:PRO:HA	4:E:347:HOH:O	2.21	0.40
1:E:122:ILE:HD13	1:E:122:ILE:HG21	1.82	0.40
2:I:41:SER:HA	2:I:42:PRO:HD3	1.66	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:365:HOH:O	4:E:365:HOH:O[4_556]	1.85	0.35

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	273/275 (99%)	246 (90%)	25 (9%)	2 (1%)	22 32
2	I	61/70 (87%)	48 (79%)	10 (16%)	3 (5%)	2 1
All	All	334/345 (97%)	294 (88%)	35 (10%)	5 (2%)	10 14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	61	ASN
1	E	63	SER
1	E	259	ASP
2	I	60	THR
2	I	24	TYR

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	205/205 (100%)	177 (86%)	28 (14%)	3 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	I	58/64 (91%)	46 (79%)	12 (21%)	1 1
All	All	263/269 (98%)	223 (85%)	40 (15%)	3 3

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	SER
1	E	5	PRO
1	E	6	TYR
1	E	12	LYS
1	E	16	LEU
1	E	32	ASP
1	E	43	LYS
1	E	56	ASN
1	E	76	ASN
1	E	78	SER
1	E	103	GLN
1	E	118	ASN
1	E	125	SER
1	E	139	VAL
1	E	145	SER
1	E	156	GLU
1	E	159	SER
1	E	162	SER
1	E	212	ASN
1	E	221	SER
1	E	222	MET
1	E	241	TRP
1	E	243	ASN
1	E	244	THR
1	E	249	SER
1	E	270	VAL
1	E	271	GLN
1	E	275	GLN
2	I	8	LYS
2	I	10	PHE
2	I	16	LYS
2	I	22	ARG
2	I	24	TYR
2	I	31	GLN
2	I	39	GLU
2	I	43	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	50	ASN
2	I	57	ASN
2	I	62	VAL
2	I	64	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	56	ASN
1	E	59	GLN
1	E	61	ASN
1	E	76	ASN
1	E	118	ASN
1	E	123	ASN
1	E	184	ASN
1	E	185	GLN
1	E	238	HIS
1	E	243	ASN
1	E	245	GLN
1	E	275	GLN
2	I	31	GLN
2	I	50	ASN
2	I	57	ASN
2	I	64	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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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.