Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:26 PM GMT

PDB ID	:	1K9O
Title	:	CRYSTAL STRUCTURE OF MICHAELIS SERPIN-TRYPSIN COMPLEX
Authors	:	Ye, S.; Cech, A.L.; Belmares, R.; Bergstrom, R.C.; Tong, Y.; Corey, D.R.; Kanost, M.R.; Goldsmith, E.J.
Deposited on	:	2001-10-29
Resolution	:	2.30 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 ①) were used in the production of this report:

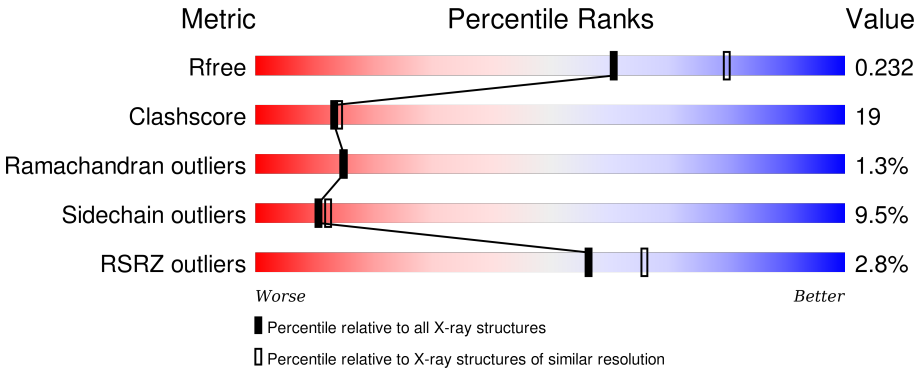
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	I	378	4% 57% 34% 7%
2	E	223	70% 27%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4786 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 ALASERPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	376	Total	C	N	O	S	0	0	0
			2939	1867	492	571	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	280	THR	TYR	SEE REMARK 999	UNP P14754
I	323	THR	TYR	SEE REMARK 999	UNP P14754
I	353	LYS	ALA	ENGINEERED	UNP P14754

- Molecule 2 is a protein called TRYPSIN II ANIONIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	223	Total	C	N	O	S	0	0	0
			1665	1041	285	325	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	195	ALA	SER	ENGINEERED	UNP P00763

- Molecule 3 is water.

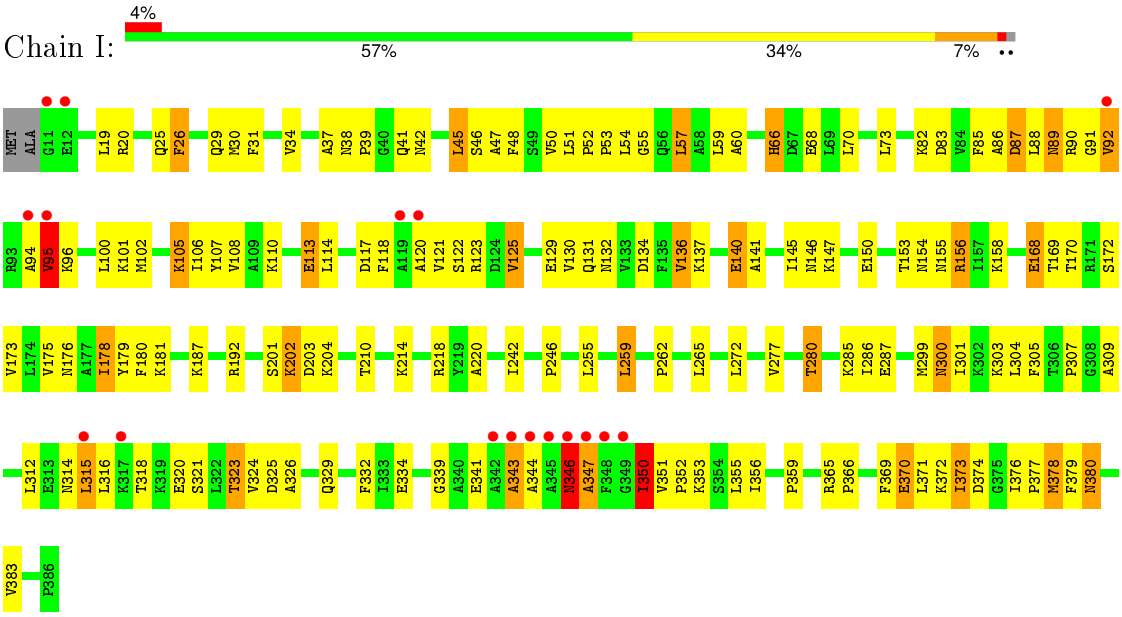
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	83	Total	O	0	0
			83	83		
3	I	99	Total	O	0	0
			99	99		

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.

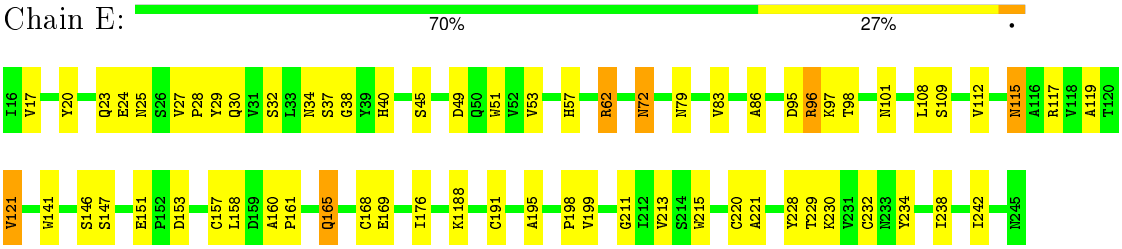
- Molecule 1: ALASERPIN

Chain I:



- Molecule 2: TRYPSIN II ANIONIC

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.57Å 112.57Å 95.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.50 – 2.30	Depositor EDS
% Data completeness (in resolution range)	84.0 (20.00-2.30) 96.3 (19.50-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.30Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.158 , 0.231 0.169 , 0.232	Depositor DCC
R_{free} test set	2880 reflections (10.49%)	DCC
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 19.7	EDS
Estimated twinning fraction	0.457 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Outliers	0 of 30996 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4786	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	I	0.43	0/2985	0.77	4/4035 (0.1%)
2	E	0.40	0/1700	0.69	0/2317
All	All	0.42	0/4685	0.74	4/6352 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	346	ASN	N-CA-C	7.59	131.49	111.00
1	I	350	ILE	N-CA-C	-7.26	91.39	111.00
1	I	169	THR	N-CA-C	-6.43	93.65	111.00
1	I	343	ALA	N-CA-C	5.73	126.47	111.00

There are no chirality outliers.

There are no planarity outliers.

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	I	2939	0	2986	130	0
2	E	1665	0	1603	46	0
3	E	83	0	0	0	0
3	I	99	0	0	1	0
All	All	4786	0	4589	173	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 19.

All (173) 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:I:136:VAL:HG22	1:I:168:GLU:HG3	1.38	1.01
1:I:347:ALA:HB3	1:I:351:VAL:HG13	1.46	0.97
1:I:34:VAL:HG21	1:I:45:LEU:HD22	1.50	0.94
2:E:115:ASN:H	2:E:115:ASN:HD22	1.18	0.87
2:E:115:ASN:N	2:E:115:ASN:HD22	1.73	0.87
2:E:29:TYR:HB2	2:E:121:VAL:HG22	1.57	0.86
1:I:202:LYS:HD3	1:I:202:LYS:H	1.40	0.85
1:I:60:ALA:HA	1:I:314:ASN:HB2	1.64	0.80
2:E:30:GLN:HE22	2:E:198:PRO:HD2	1.46	0.78
2:E:34:ASN:ND2	2:E:38:GLY:H	1.82	0.78
1:I:346:ASN:HD22	1:I:346:ASN:H	1.32	0.78
2:E:158:LEU:HD11	2:E:1188:LYS:HB3	1.67	0.77
1:I:323:THR:HG23	3:I:478:HOH:O	1.84	0.77
1:I:187:LYS:NZ	1:I:343:ALA:HA	2.00	0.76
1:I:372:LYS:HE2	1:I:377:PRO:HD3	1.68	0.75
2:E:45:SER:OG	2:E:198:PRO:HG3	1.87	0.74
1:I:120:ALA:HA	1:I:123:ARG:HG2	1.67	0.73
1:I:344:ALA:HB1	2:E:147:SER:HA	1.71	0.72
2:E:29:TYR:CB	2:E:121:VAL:HG22	2.19	0.72
1:I:307:PRO:HA	1:I:323:THR:HG21	1.71	0.71
1:I:220:ALA:HB2	1:I:272:LEU:HA	1.71	0.71
1:I:277:VAL:HG13	1:I:359:PRO:O	1.93	0.69
1:I:346:ASN:HD22	1:I:346:ASN:N	1.89	0.68
2:E:32:SER:OG	2:E:40:HIS:HD2	1.78	0.67
1:I:108:VAL:O	1:I:132:ASN:HA	1.95	0.67
2:E:115:ASN:N	2:E:115:ASN:ND2	2.43	0.66
2:E:28:PRO:HB2	2:E:119:ALA:HB3	1.77	0.65
1:I:136:VAL:HG22	1:I:168:GLU:CG	2.21	0.65
1:I:25:GLN:NE2	1:I:262:PRO:HG2	2.11	0.65
1:I:320:GLU:HG2	1:I:321:SER:H	1.62	0.64
1:I:134:ASP:O	1:I:141:ALA:HB2	1.99	0.63
1:I:105:LYS:HD2	1:I:129:GLU:O	1.99	0.62
1:I:373:ILE:O	1:I:373:ILE:HG22	1.99	0.62
1:I:86:ALA:O	1:I:90:ARG:HG2	1.99	0.62
1:I:255:LEU:HG	1:I:259:LEU:HD22	1.82	0.61
1:I:202:LYS:CD	1:I:202:LYS:H	2.12	0.61
1:I:89:ASN:HB3	1:I:90:ARG:NH1	2.15	0.61
1:I:55:GLY:O	1:I:59:LEU:HD13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:114:LEU:HA	1:I:316:LEU:HA	1.83	0.59
1:I:102:MET:HE1	1:I:378:MET:HG2	1.84	0.59
2:E:83:VAL:HG11	2:E:108:LEU:HB3	1.83	0.59
2:E:25:ASN:OD1	2:E:117:ARG:HG2	2.01	0.59
2:E:30:GLN:NE2	2:E:198:PRO:HD2	2.17	0.59
1:I:353:LYS:C	2:E:195:ALA:HB2	2.22	0.59
1:I:320:GLU:HG2	1:I:321:SER:N	2.18	0.59
1:I:59:LEU:HD21	1:I:82:LYS:HG3	1.84	0.59
2:E:101:ASN:HA	2:E:234:TYR:OH	2.02	0.59
1:I:370:GLU:HB2	1:I:380:ASN:HB3	1.85	0.59
1:I:146:ASN:O	1:I:150:GLU:HB2	2.03	0.59
1:I:187:LYS:HZ2	1:I:343:ALA:HA	1.68	0.58
2:E:115:ASN:HB2	2:E:117:ARG:H	1.69	0.57
1:I:85:PHE:O	1:I:89:ASN:HB2	2.06	0.56
1:I:30:MET:O	1:I:34:VAL:HG13	2.05	0.56
1:I:102:MET:CE	1:I:378:MET:HG2	2.36	0.56
1:I:150:GLU:HG2	1:I:155:ASN:HA	1.88	0.55
1:I:95:VAL:HG22	1:I:96:LYS:H	1.71	0.55
1:I:176:ASN:ND2	1:I:329:GLN:HE21	2.04	0.55
1:I:30:MET:HE3	1:I:47:ALA:HA	1.87	0.55
1:I:202:LYS:HD3	1:I:202:LYS:N	2.17	0.55
1:I:346:ASN:ND2	1:I:346:ASN:N	2.55	0.55
1:I:218:ARG:HB3	1:I:272:LEU:HG	1.88	0.55
1:I:66:HIS:CD2	1:I:70:LEU:HD22	2.41	0.55
1:I:34:VAL:HG21	1:I:45:LEU:CD2	2.32	0.54
1:I:83:ASP:O	1:I:87:ASP:HB2	2.07	0.54
1:I:346:ASN:ND2	1:I:346:ASN:H	2.04	0.54
1:I:307:PRO:CA	1:I:323:THR:HG21	2.38	0.54
1:I:114:LEU:HD13	1:I:315:LEU:HD22	1.89	0.53
2:E:57:HIS:HB2	2:E:96:ARG:NH2	2.24	0.53
1:I:242:ILE:O	1:I:369:PHE:HA	2.08	0.53
1:I:26:PHE:CD2	1:I:51:LEU:HD21	2.44	0.53
1:I:94:ALA:O	1:I:95:VAL:HG12	2.09	0.53
2:E:17:VAL:O	2:E:1188:LYS:HA	2.09	0.53
1:I:307:PRO:HA	1:I:323:THR:CG2	2.39	0.52
1:I:285:LYS:HG2	1:I:334:GLU:HG3	1.91	0.52
2:E:230:LYS:HE3	2:E:232:CYS:SG	2.48	0.52
2:E:165:GLN:O	2:E:169:GLU:HG3	2.09	0.52
1:I:350:ILE:O	1:I:352:PRO:HD3	2.09	0.52
1:I:19:LEU:HD21	1:I:88:LEU:HD13	1.91	0.52
2:E:146:SER:HB3	2:E:221:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:PHE:CD2	1:I:378:MET:HG3	2.45	0.51
1:I:176:ASN:HD21	1:I:329:GLN:HE21	1.57	0.51
1:I:170:THR:HG23	1:I:325:ASP:HB2	1.93	0.51
1:I:187:LYS:HZ1	1:I:343:ALA:HA	1.72	0.51
1:I:101:LYS:HB2	1:I:179:TYR:HB3	1.93	0.51
1:I:110:LYS:HA	1:I:132:ASN:HB3	1.93	0.50
1:I:154:ASN:HD22	1:I:154:ASN:N	2.09	0.50
1:I:46:SER:HB3	1:I:178:ILE:HG21	1.93	0.50
1:I:29:GLN:OE1	1:I:299:MET:HE3	2.11	0.50
1:I:30:MET:CE	1:I:47:ALA:HA	2.42	0.49
1:I:210:THR:CG2	1:I:280:THR:HG22	2.42	0.49
1:I:153:THR:O	1:I:156:ARG:HB2	2.13	0.49
2:E:17:VAL:HG23	2:E:191:CYS:HB2	1.95	0.49
1:I:108:VAL:HG21	1:I:114:LEU:HD11	1.94	0.49
2:E:72:ASN:C	2:E:72:ASN:HD22	2.16	0.49
1:I:92:VAL:HG13	1:I:92:VAL:O	2.12	0.49
1:I:265:LEU:HD21	1:I:370:GLU:OE2	2.13	0.49
1:I:66:HIS:NE2	1:I:70:LEU:HD22	2.28	0.49
2:E:24:GLU:O	2:E:25:ASN:HB2	2.12	0.48
1:I:121:VAL:O	1:I:125:VAL:HB	2.13	0.48
1:I:50:VAL:HG22	1:I:176:ASN:ND2	2.29	0.48
1:I:134:ASP:OD1	1:I:136:VAL:HG23	2.13	0.48
1:I:136:VAL:CG2	1:I:168:GLU:HG3	2.27	0.48
1:I:353:LYS:HD2	2:E:215:TRP:HA	1.95	0.48
2:E:34:ASN:HD21	2:E:38:GLY:H	1.62	0.48
1:I:299:MET:O	1:I:300:ASN:HB2	2.14	0.48
1:I:31:PHE:HD1	1:I:380:ASN:ND2	2.12	0.47
1:I:113:GLU:OE2	1:I:318:THR:HG21	2.15	0.47
1:I:286:ILE:HD11	1:I:383:VAL:HG22	1.97	0.47
1:I:246:PRO:O	1:I:365:ARG:HD2	2.15	0.46
2:E:86:ALA:HB2	2:E:109:SER:HA	1.98	0.46
2:E:199:VAL:HG21	2:E:228:TYR:CD2	2.50	0.46
2:E:213:VAL:HA	2:E:228:TYR:CD2	2.51	0.46
1:I:54:LEU:HB2	1:I:73:LEU:HD21	1.98	0.46
1:I:37:ALA:C	1:I:39:PRO:HD3	2.36	0.46
1:I:366:PRO:HA	1:I:383:VAL:O	2.16	0.46
1:I:107:TYR:HA	1:I:131:GLN:O	2.16	0.45
1:I:117:ASP:O	1:I:120:ALA:HB3	2.16	0.45
1:I:371:LEU:HD22	1:I:379:PHE:CZ	2.51	0.45
1:I:101:LYS:O	1:I:178:ILE:HA	2.16	0.45
1:I:95:VAL:HG13	1:I:96:LYS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:213:VAL:HG22	2:E:228:TYR:HE2	1.82	0.45
1:I:52:PRO:HB2	1:I:53:PRO:HD3	1.99	0.45
1:I:136:VAL:HA	1:I:168:GLU:HB2	1.98	0.45
1:I:118:PHE:C	1:I:120:ALA:H	2.20	0.45
1:I:316:LEU:CD1	1:I:320:GLU:HB3	2.47	0.45
1:I:155:ASN:HB3	1:I:158:LYS:NZ	2.31	0.44
1:I:41:GLN:HG2	1:I:42:ASN:N	2.32	0.44
1:I:218:ARG:CZ	1:I:272:LEU:HD23	2.47	0.44
1:I:130:VAL:HG11	1:I:315:LEU:HD21	1.98	0.44
1:I:187:LYS:HB3	1:I:339:GLY:HA3	1.98	0.44
1:I:145:ILE:CG2	1:I:175:VAL:HG11	2.47	0.44
1:I:214:LYS:HD3	1:I:214:LYS:N	2.32	0.44
2:E:72:ASN:HA	2:E:153:ASP:O	2.18	0.44
1:I:26:PHE:CG	1:I:51:LEU:HD21	2.53	0.44
2:E:51:TRP:CD2	2:E:242:ILE:HG12	2.53	0.43
1:I:180:PHE:CZ	1:I:371:LEU:HD13	2.54	0.43
1:I:373:ILE:CG2	1:I:373:ILE:O	2.65	0.43
1:I:137:LYS:HB3	1:I:140:GLU:HB3	2.00	0.43
1:I:371:LEU:HD22	1:I:379:PHE:CE2	2.53	0.43
1:I:68:GLU:HG2	1:I:300:ASN:O	2.18	0.43
1:I:89:ASN:HB3	1:I:90:ARG:HH11	1.84	0.42
1:I:172:SER:OG	1:I:324:VAL:HA	2.19	0.42
2:E:160:ALA:HA	2:E:161:PRO:HD3	1.74	0.42
1:I:31:PHE:O	1:I:34:VAL:HG22	2.20	0.42
1:I:181:LYS:HG3	1:I:334:GLU:HB3	2.02	0.42
2:E:168:CYS:SG	2:E:176:ILE:HD12	2.60	0.42
1:I:170:THR:HA	1:I:325:ASP:OD1	2.19	0.41
1:I:57:LEU:HG	1:I:304:LEU:HD11	2.01	0.41
1:I:105:LYS:HG3	1:I:106:ILE:N	2.34	0.41
1:I:210:THR:HG21	1:I:280:THR:HG22	2.01	0.41
1:I:145:ILE:HG21	1:I:175:VAL:HG11	2.02	0.41
2:E:95:ASP:HB3	2:E:98:THR:OG1	2.20	0.41
1:I:356:ILE:N	1:I:356:ILE:HD12	2.35	0.41
2:E:27:VAL:HG13	2:E:29:TYR:CZ	2.56	0.41
1:I:201:SER:OG	1:I:204:LYS:HB2	2.20	0.41
1:I:173:VAL:HG22	1:I:326:ALA:HB3	2.02	0.41
2:E:37:SER:HA	2:E:62:ARG:NH1	2.35	0.41
1:I:59:LEU:HD21	1:I:82:LYS:CG	2.49	0.41
2:E:20:TYR:CE2	2:E:157:CYS:HB2	2.56	0.41
2:E:146:SER:HB2	2:E:220:CYS:O	2.21	0.41
2:E:83:VAL:HG21	2:E:112:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:154:ASN:N	1:I:154:ASN:ND2	2.69	0.41
2:E:234:TYR:O	2:E:238:ILE:HG13	2.21	0.41
1:I:38:ASN:N	1:I:39:PRO:HD3	2.36	0.41
1:I:45:LEU:O	1:I:379:PHE:HB2	2.21	0.41
1:I:373:ILE:HB	1:I:378:MET:SD	2.61	0.41
2:E:40:HIS:CE1	2:E:141:TRP:HB2	2.56	0.40
2:E:97:LYS:HA	2:E:97:LYS:HD3	1.80	0.40
1:I:303:LYS:HG2	1:I:309:ALA:HB1	2.03	0.40
1:I:107:TYR:O	1:I:172:SER:HA	2.22	0.40
1:I:287:GLU:HB3	1:I:332:PHE:HD1	1.87	0.40
1:I:114:LEU:HD22	1:I:316:LEU:HD23	2.04	0.40
2:E:211:GLY:HA2	2:E:229:THR:O	2.20	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	I	374/378 (99%)	338 (90%)	29 (8%)	7 (2%)	10 8
2	E	221/223 (99%)	207 (94%)	13 (6%)	1 (0%)	34 41
All	All	595/601 (99%)	545 (92%)	42 (7%)	8 (1%)	15 15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	95	VAL
1	I	346	ASN
1	I	347	ALA
2	E	49	ASP
1	I	91	GLY
1	I	300	ASN

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Mol	Chain	Res	Type
1	I	125	VAL
1	I	301	ILE

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	I	323/324 (100%)	285 (88%)	38 (12%)	6 7
2	E	184/184 (100%)	174 (95%)	10 (5%)	27 36
All	All	507/508 (100%)	459 (90%)	48 (10%)	11 12

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	20	ARG
1	I	26	PHE
1	I	45	LEU
1	I	57	LEU
1	I	66	HIS
1	I	87	ASP
1	I	89	ASN
1	I	92	VAL
1	I	95	VAL
1	I	100	LEU
1	I	105	LYS
1	I	113	GLU
1	I	122	SER
1	I	136	VAL
1	I	140	GLU
1	I	147	LYS
1	I	156	ARG
1	I	168	GLU
1	I	178	ILE
1	I	192	ARG
1	I	202	LYS

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Mol	Chain	Res	Type
1	I	203	ASP
1	I	259	LEU
1	I	280	THR
1	I	305	PHE
1	I	312	LEU
1	I	315	LEU
1	I	323	THR
1	I	341	GLU
1	I	346	ASN
1	I	350	ILE
1	I	355	LEU
1	I	370	GLU
1	I	373	ILE
1	I	374	ASP
1	I	376	ILE
1	I	378	MET
1	I	380	ASN
2	E	23	GLN
2	E	53	VAL
2	E	62	ARG
2	E	72	ASN
2	E	79	ASN
2	E	96	ARG
2	E	115	ASN
2	E	121	VAL
2	E	151	GLU
2	E	165	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	25	GLN
1	I	41	GLN
1	I	56	GLN
1	I	115	ASN
1	I	155	ASN
1	I	176	ASN
1	I	199	HIS
1	I	257	GLN
1	I	346	ASN
2	E	30	GLN
2	E	34	ASN

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Mol	Chain	Res	Type
2	E	40	HIS
2	E	50	GLN
2	E	72	ASN
2	E	79	ASN
2	E	84	ASN
2	E	101	ASN
2	E	115	ASN
2	E	165	GLN

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 carbohydrates 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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	I	376/378 (99%)	-0.24	17 (4%) 37 46	7, 30, 60, 72	0
2	E	223/223 (100%)	-0.73	0 100 100	3, 15, 27, 31	0
All	All	599/601 (99%)	-0.42	17 (2%) 56 66	3, 22, 57, 72	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	347	ALA	5.2
1	I	345	ALA	4.7
1	I	348	PHE	4.3
1	I	315	LEU	4.1
1	I	119	ALA	4.0
1	I	120	ALA	3.5
1	I	349	GLY	3.4
1	I	346	ASN	3.3
1	I	11	GLY	3.2
1	I	94	ALA	3.0
1	I	92	VAL	2.9
1	I	343	ALA	2.4
1	I	95	VAL	2.3
1	I	12	GLU	2.3
1	I	342	ALA	2.2
1	I	317	LYS	2.1
1	I	344	ALA	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.