Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2017 – 02:51 PM EDT

PDB ID	:	3EQ9
Title	:	Prolyl oligopeptidase complexed with R-Pro-(decarboxy-Pro)-Type inhibitors
Authors	:	Kanai, K.; Aranyi, P.; Bocskei, Z.; Ferenczy, G.; Harmat, V.; Simon, K.; Naray-Szabo, G.; Hermecz, I.
Deposited on	:	unknown
Resolution	:	2.47 Å(reported)

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

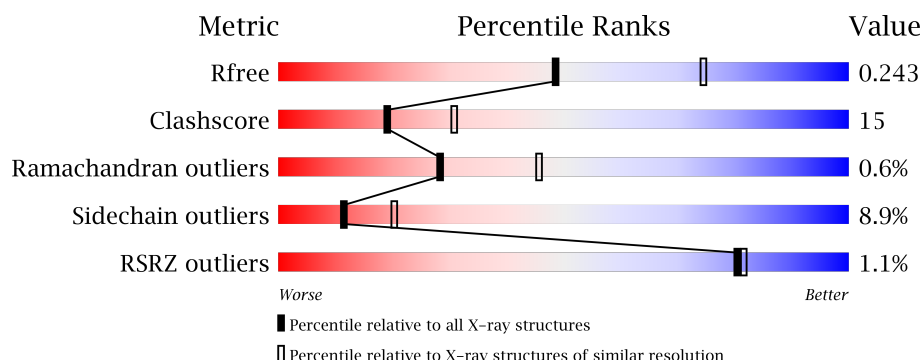|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 2.47 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	Percentile Ranks	Value
Rfree		0.243
Clashscore		15
Ramachandran outliers		0.6%
Sidechain outliers		8.9%
RSRZ outliers		1.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4719 (2.50-2.46)
Clashscore	112137	5483 (2.50-2.46)
Ramachandran outliers	110173	5388 (2.50-2.46)
Sidechain outliers	110143	5390 (2.50-2.46)
RSRZ outliers	101464	4754 (2.50-2.46)

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	A	710	.% 69% 26% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5843 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 Prolyl endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	5	0
			5675	3647	942	1059	27			

- Molecule 2 is 3-{4-oxo-4-[(2S)-2-(pyrrolidin-1-ylcarbonyl)pyrrolidin-1-yl]butyl}-5,5-diphenyl imidazolidine-2,4-dione (three-letter code: X97) (formula: $C_{28}H_{32}N_4O_4$).
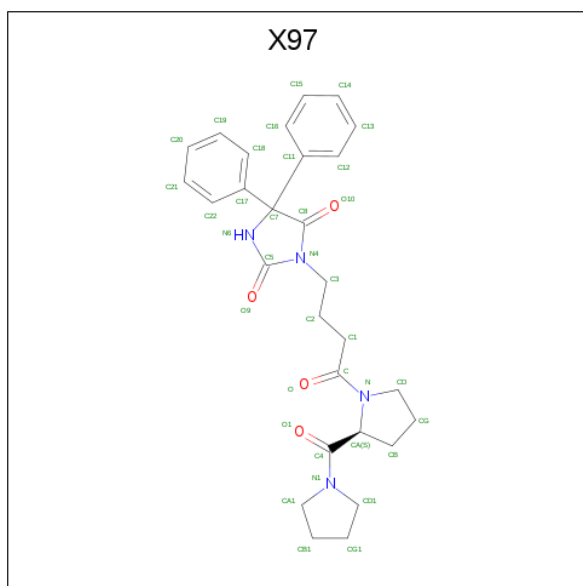
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	28	4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	0
			132	132		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Prolyl endopeptidase
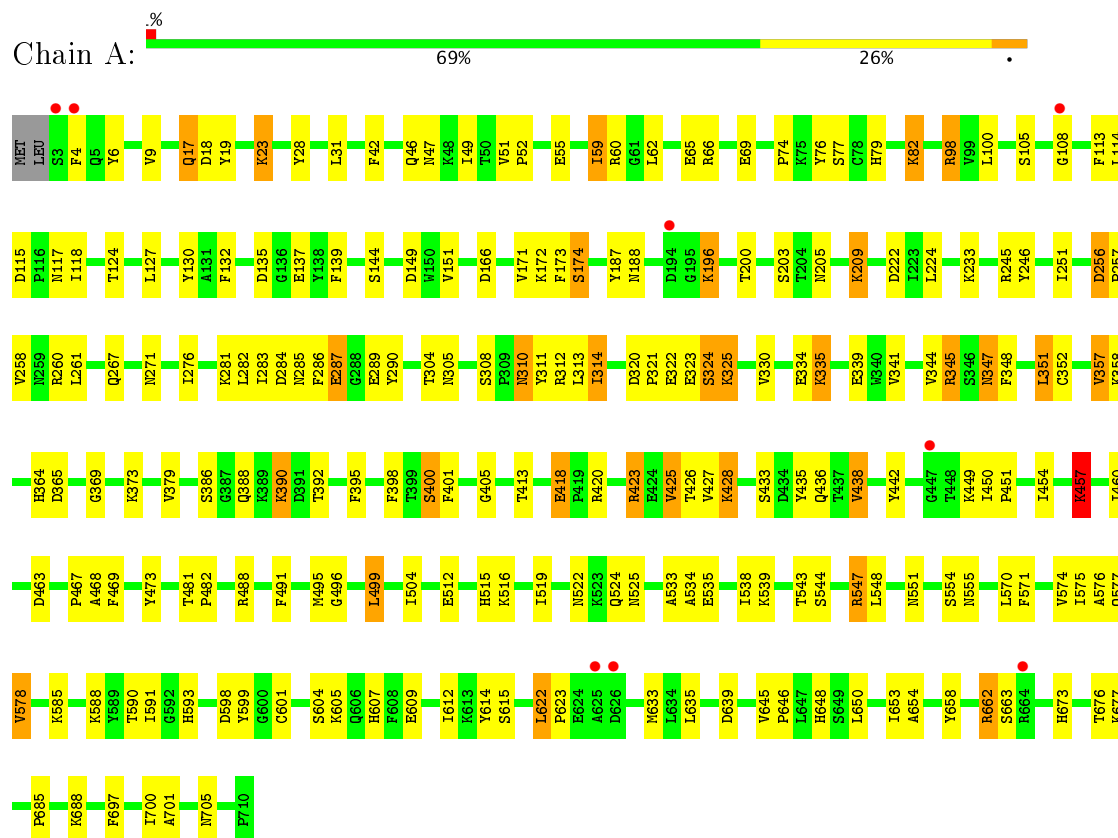
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.55Å 101.46Å 112.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.50 – 2.47 34.52 – 2.47	Depositor EDS
% Data completeness (in resolution range)	(Not available) (34.50-2.47) 93.2 (34.52-2.47)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.84 (at 2.48Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.174 , 0.244 0.174 , 0.243	Depositor DCC
R_{free} test set	2819 reflections (9.94%)	DCC
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 46.3	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5843	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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: X97

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	A	2.15	2/5858 (0.0%)	0.73	4/7943 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457[A]	LYS	CD-CE	114.69	4.38	1.51
1	A	457[B]	LYS	CD-CE	114.69	4.38	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457[A]	LYS	CG-CD-CE	-23.21	42.28	111.90
1	A	457[B]	LYS	CG-CD-CE	-23.21	42.28	111.90
1	A	457[A]	LYS	CD-CE-NZ	-15.17	76.80	111.70
1	A	457[B]	LYS	CD-CE-NZ	-15.17	76.80	111.70

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	A	5675	0	5478	164	0
2	A	36	0	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	132	0	0	3	0
All	All	5843	0	5510	164	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 15.

All (164) 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:A:428:LYS:H	1:A:428:LYS:HD3	1.03	1.07
1:A:390:LYS:HE2	1:A:390:LYS:H	1.29	0.94
1:A:51:VAL:HB	1:A:52:PRO:HD3	1.53	0.88
1:A:388:GLN:HB3	1:A:390:LYS:HE3	1.57	0.87
1:A:428:LYS:H	1:A:428:LYS:CD	1.88	0.86
1:A:428:LYS:N	1:A:428:LYS:HD3	1.86	0.86
1:A:390:LYS:HE2	1:A:390:LYS:N	1.97	0.80
1:A:251:ILE:HB	1:A:260:ARG:HB2	1.67	0.74
1:A:544:SER:HB2	1:A:547:ARG:HD2	1.70	0.73
1:A:495:MET:CE	1:A:701:ALA:HB2	2.19	0.73
1:A:438:VAL:HG22	1:A:454:ILE:HB	1.73	0.71
1:A:245:ARG:HG2	1:A:246:TYR:CD1	2.26	0.70
1:A:436:GLN:HE21	1:A:438:VAL:CG1	2.05	0.69
1:A:17:GLN:HG2	1:A:19:TYR:CE1	2.28	0.69
1:A:495:MET:HE3	1:A:701:ALA:HB2	1.73	0.68
1:A:100:LEU:HD23	1:A:113:PHE:HD2	1.58	0.68
1:A:345:ARG:HH21	1:A:347:ASN:HD21	1.43	0.66
1:A:320:ASP:OD1	1:A:325:LYS:HD2	1.95	0.66
1:A:313:LEU:HD12	1:A:330:VAL:CG2	2.24	0.66
1:A:622:LEU:HD22	1:A:623:PRO:HD2	1.78	0.65
1:A:435:TYR:HE1	1:A:457[A]:LYS:HD2	1.61	0.65
1:A:344:VAL:O	1:A:348:PHE:HB2	1.97	0.65
1:A:358:LYS:HD3	1:A:379:VAL:HG22	1.79	0.64
1:A:622:LEU:HD11	1:A:663:SER:CB	2.28	0.64
1:A:398:PHE:O	1:A:405:GLY:HA2	1.99	0.62
1:A:310:ASN:N	1:A:310:ASN:HD22	1.98	0.62
1:A:358:LYS:CD	1:A:379:VAL:HG22	2.31	0.61
1:A:322:GLU:HB2	1:A:325:LYS:HG3	1.83	0.61
1:A:100:LEU:CD2	1:A:113:PHE:HD2	2.14	0.60
1:A:313:LEU:HD21	1:A:341:VAL:HG21	1.83	0.60
1:A:257:PRO:O	1:A:289:GLU:HB2	2.01	0.60
1:A:261:LEU:HD12	1:A:282:LEU:HD23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ASP:HB3	1:A:258:VAL:HG22	1.84	0.60
1:A:46:GLN:O	1:A:49:ILE:HG12	2.01	0.59
1:A:245:ARG:HG2	1:A:246:TYR:CE1	2.38	0.58
1:A:341:VAL:HG13	1:A:351:LEU:HD22	1.87	0.57
1:A:554:SER:HA	1:A:578:VAL:O	2.04	0.57
1:A:65:GLU:O	1:A:69:GLU:HG3	2.05	0.57
1:A:51:VAL:HB	1:A:52:PRO:CD	2.29	0.56
1:A:522:ASN:O	1:A:525:ASN:HB2	2.05	0.56
1:A:174:SER:HB2	1:A:188:ASN:HB2	1.87	0.56
1:A:18:ASP:OD2	1:A:23:LYS:HE3	2.05	0.56
1:A:196:LYS:HE3	1:A:200:THR:OG1	2.04	0.56
1:A:673:HIS:HD2	3:A:836:HOH:O	1.87	0.56
1:A:305:ASN:HB3	1:A:311:TYR:CE2	2.40	0.56
1:A:622:LEU:CD2	1:A:623:PRO:HD2	2.35	0.56
1:A:697:PHE:HA	1:A:700:ILE:HD12	1.88	0.56
1:A:435:TYR:CE1	1:A:457[A]:LYS:HD2	2.40	0.56
1:A:4:PHE:HE1	1:A:6:TYR:CE2	2.24	0.56
1:A:676:THR:O	1:A:677:LYS:HB2	2.06	0.55
1:A:17:GLN:HG3	1:A:18:ASP:N	2.22	0.55
1:A:320:ASP:N	1:A:321:PRO:HD3	2.21	0.55
1:A:308:SER:OG	1:A:312:ARG:HD3	2.07	0.55
1:A:28:TYR:HB3	1:A:31:LEU:HD12	1.89	0.54
1:A:392:THR:HB	1:A:413:THR:HG22	1.88	0.54
1:A:59:ILE:HD13	1:A:701:ALA:HB1	1.90	0.54
1:A:390:LYS:H	1:A:390:LYS:CE	2.12	0.54
1:A:488:ARG:HD2	1:A:499:LEU:HD21	1.89	0.54
1:A:551:ASN:ND2	1:A:575:ILE:O	2.39	0.54
1:A:345:ARG:HG2	1:A:392:THR:HA	1.90	0.54
1:A:622:LEU:HD11	1:A:663:SER:HB2	1.88	0.54
1:A:673:HIS:CD2	3:A:836:HOH:O	2.60	0.53
1:A:534:ALA:O	1:A:538:ILE:HD12	2.08	0.53
1:A:400:SER:OG	1:A:401:PHE:N	2.41	0.53
1:A:100:LEU:HD23	1:A:113:PHE:CD2	2.43	0.53
1:A:51:VAL:O	1:A:55:GLU:HG3	2.09	0.53
1:A:281:LYS:HD2	1:A:284:ASP:OD1	2.09	0.52
1:A:76:TYR:CD1	1:A:423:ARG:HD2	2.45	0.52
1:A:260:ARG:NH1	1:A:286:PHE:CE1	2.78	0.52
1:A:653:ILE:HG23	1:A:654:ALA:N	2.25	0.52
1:A:460:ILE:O	1:A:460:ILE:HG13	2.08	0.52
1:A:578:VAL:O	1:A:578:VAL:HG23	2.10	0.52
1:A:577:GLN:O	1:A:578:VAL:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ALA:HB2	1:A:543:THR:HB	1.93	0.50
1:A:650:LEU:O	1:A:653:ILE:HG22	2.11	0.50
1:A:130:TYR:HB2	1:A:139:PHE:CE1	2.47	0.50
1:A:436:GLN:HE21	1:A:438:VAL:HG12	1.77	0.50
1:A:313:LEU:HD12	1:A:330:VAL:HG21	1.94	0.49
1:A:98:ARG:HG2	3:A:753:HOH:O	2.13	0.49
1:A:171:VAL:HG13	1:A:188:ASN:O	2.13	0.48
1:A:9:VAL:HG21	1:A:42:PHE:HE1	1.77	0.48
1:A:555:ASN:ND2	1:A:599:TYR:OH	2.45	0.48
1:A:323:GLU:C	1:A:325:LYS:H	2.16	0.48
1:A:205:ASN:O	1:A:593:HIS:HE1	1.96	0.48
1:A:405:GLY:O	1:A:425:VAL:HG23	2.13	0.48
1:A:522:ASN:HB3	1:A:525:ASN:HD22	1.77	0.48
1:A:74:PRO:O	1:A:425:VAL:HG11	2.14	0.47
1:A:339:GLU:HB2	1:A:352:CYS:O	2.15	0.47
1:A:82:LYS:HG3	1:A:132:PHE:CG	2.49	0.47
1:A:66:ARG:HD2	1:A:66:ARG:HA	1.72	0.47
1:A:516:LYS:HA	1:A:519:ILE:HG12	1.97	0.46
1:A:245:ARG:CZ	1:A:267:GLN:OE1	2.63	0.46
1:A:82:LYS:HA	1:A:82:LYS:HD3	1.73	0.46
1:A:614:TYR:O	1:A:615:SER:C	2.53	0.46
1:A:304:THR:CG2	1:A:314:ILE:HG12	2.46	0.46
1:A:522:ASN:HB3	1:A:525:ASN:ND2	2.31	0.46
1:A:427:VAL:HG12	1:A:427:VAL:O	2.15	0.46
1:A:386:SER:OG	1:A:395:PHE:HB2	2.16	0.45
1:A:548:LEU:HD23	1:A:570:LEU:O	2.16	0.45
1:A:335:LYS:HD2	1:A:335:LYS:HA	1.48	0.45
1:A:442:TYR:OH	1:A:533:ALA:HB2	2.17	0.45
1:A:124:THR:OG1	1:A:677:LYS:HE2	2.16	0.45
1:A:18:ASP:OD2	1:A:23:LYS:CE	2.63	0.45
1:A:365:ASP:O	1:A:369:GLY:N	2.47	0.45
1:A:473:TYR:CZ	1:A:555:ASN:HB3	2.51	0.45
1:A:285:ASN:OD1	1:A:287:GLU:HB2	2.16	0.45
1:A:645:VAL:HG23	1:A:648:HIS:CD2	2.51	0.45
1:A:304:THR:HG21	1:A:314:ILE:HG12	1.99	0.45
1:A:469:PHE:HB2	1:A:491:PHE:CE2	2.51	0.45
1:A:639:ASP:OD2	1:A:676:THR:HG22	2.18	0.44
1:A:82:LYS:HG3	1:A:132:PHE:CD1	2.53	0.44
1:A:576:ALA:HB3	1:A:635:LEU:HD23	2.00	0.44
1:A:467:PRO:HD2	1:A:496:GLY:O	2.17	0.44
1:A:365:ASP:O	1:A:369:GLY:HA2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASP:HB2	1:A:172:LYS:HE2	2.00	0.43
1:A:47:ASN:O	1:A:51:VAL:HG23	2.18	0.43
1:A:283:ILE:HG21	1:A:290:TYR:CE1	2.52	0.43
1:A:187:TYR:OH	1:A:222:ASP:OD2	2.18	0.43
1:A:436:GLN:HE21	1:A:438:VAL:HG11	1.80	0.43
1:A:653:ILE:CG2	1:A:654:ALA:N	2.81	0.43
1:A:105:SER:HB3	1:A:108:GLY:H	1.84	0.43
1:A:351:LEU:N	1:A:351:LEU:HD23	2.33	0.43
1:A:135:ASP:OD1	1:A:137:GLU:HB2	2.18	0.43
1:A:149:ASP:O	1:A:151:VAL:HG23	2.19	0.42
1:A:554:SER:OG	1:A:555:ASN:N	2.53	0.42
1:A:442:TYR:CZ	1:A:533:ALA:HB2	2.54	0.42
1:A:605:LYS:O	1:A:609:GLU:HG2	2.19	0.42
1:A:428:LYS:CD	1:A:428:LYS:N	2.61	0.42
1:A:601:CYS:O	1:A:607:HIS:HB2	2.19	0.42
1:A:74:PRO:HB2	1:A:76:TYR:CE1	2.54	0.42
1:A:463:ASP:OD1	1:A:463:ASP:N	2.53	0.42
1:A:653:ILE:HA	1:A:653:ILE:HD12	1.86	0.42
1:A:260:ARG:HG3	1:A:286:PHE:CE2	2.54	0.42
1:A:345:ARG:NH2	1:A:347:ASN:HD21	2.13	0.42
1:A:351:LEU:HG	1:A:364:HIS:CD2	2.54	0.42
1:A:115:ASP:OD1	1:A:117:ASN:HB2	2.20	0.41
1:A:345:ARG:HE	1:A:345:ARG:HB3	1.49	0.41
1:A:685:PRO:HG2	1:A:688:LYS:HG3	2.01	0.41
1:A:585:LYS:HB3	1:A:588:LYS:HD2	2.02	0.41
1:A:209:LYS:HB3	1:A:224:LEU:HD11	2.02	0.41
1:A:535:GLU:HG2	1:A:570:LEU:HD21	2.02	0.41
1:A:574:VAL:HB	1:A:633:MET:HG2	2.03	0.41
1:A:450:ILE:HA	1:A:451:PRO:HD3	1.95	0.41
1:A:172:LYS:O	1:A:173:PHE:C	2.60	0.41
1:A:512:GLU:OE1	1:A:512:GLU:HA	2.21	0.41
1:A:62:LEU:HA	1:A:62:LEU:HD23	1.73	0.41
1:A:645:VAL:HA	1:A:646:PRO:HD3	1.83	0.41
1:A:256:ASP:HA	1:A:257:PRO:HD3	1.90	0.41
1:A:323:GLU:C	1:A:325:LYS:N	2.74	0.41
1:A:76:TYR:CE1	1:A:423:ARG:HD2	2.56	0.41
1:A:524:GLN:O	1:A:524:GLN:HG3	2.21	0.40
1:A:512:GLU:O	1:A:515:HIS:HB3	2.21	0.40
1:A:481:THR:HB	1:A:482:PRO:CD	2.52	0.40
1:A:591:ILE:HG13	1:A:591:ILE:O	2.22	0.40
1:A:9:VAL:HG21	1:A:42:PHE:CE1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ARG:O	1:A:245:ARG:HG3	2.21	0.40
1:A:357:VAL:HG12	1:A:357:VAL:O	2.21	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	A	711/710 (100%)	672 (94%)	35 (5%)	4 (1%)	28 46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	VAL
1	A	324	SER
1	A	590	THR
1	A	357	VAL

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	A	611/617 (99%)	554 (91%)	57 (9%)	10 18

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	23	LYS
1	A	59	ILE
1	A	60	ARG
1	A	77	SER
1	A	79	HIS
1	A	82	LYS
1	A	98	ARG
1	A	114	LEU
1	A	118	ILE
1	A	127	LEU
1	A	144	SER
1	A	166	ASP
1	A	174	SER
1	A	196	LYS
1	A	203	SER
1	A	209	LYS
1	A	233	LYS
1	A	256	ASP
1	A	271	ASN
1	A	276	ILE
1	A	287	GLU
1	A	310	ASN
1	A	314	ILE
1	A	324	SER
1	A	325	LYS
1	A	334	GLU
1	A	335	LYS
1	A	345	ARG
1	A	347	ASN
1	A	351	LEU
1	A	373	LYS
1	A	390	LYS
1	A	400	SER
1	A	418[A]	GLU
1	A	418[B]	GLU
1	A	423	ARG
1	A	425	VAL
1	A	426	THR
1	A	428	LYS
1	A	433	SER
1	A	438	VAL
1	A	449	LYS

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Mol	Chain	Res	Type
1	A	457[A]	LYS
1	A	457[B]	LYS
1	A	499	LEU
1	A	504	ILE
1	A	539	LYS
1	A	547	ARG
1	A	571	PHE
1	A	598	ASP
1	A	604	SER
1	A	612	ILE
1	A	622	LEU
1	A	662[A]	ARG
1	A	662[B]	ARG
1	A	705	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	ASN
1	A	315	ASN
1	A	347	ASN
1	A	436	GLN
1	A	555	ASN
1	A	593	HIS
1	A	606	GLN
1	A	673	HIS
1	A	705	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 carbohydrates 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	#$|Z| > 2$
2	X97	A	711	-	40,40,40	1.05	3 (7%)	55,57,57	0.92	3 (5%)

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	X97	A	711	-	-	0/30/66/66	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	711	X97	C3-N4	-2.09	1.42	1.47
2	A	711	X97	C7-C8	2.15	1.59	1.55
2	A	711	X97	C5-N6	3.54	1.41	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	711	X97	O10-C8-C7	2.50	128.28	124.14
2	A	711	X97	C8-C7-N6	2.77	101.28	99.21
2	A	711	X97	N6-C5-N4	2.86	108.96	107.25

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)

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	A	708/710 (99%)	-0.38	8 (1%)	80	81	6, 23, 51, 85	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	ASP	3.4
1	A	4	PHE	3.2
1	A	664	ARG	2.9
1	A	626	ASP	2.8
1	A	625	ALA	2.5
1	A	3	SER	2.4
1	A	108	GLY	2.4
1	A	447	GLY	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	X97	A	711	36/36	0.94	0.15	1.02	9,39,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.