

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	3BEZ
Title	:	Crystal structure of Escherichia coli Signal peptide peptidase (SppA), SeMet
		crystals
Authors	:	Paetzel, M.
Deposited on	:	2007-11-20
Resolution	:	2.76 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.76 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1235(2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 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% 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 cl	nain		
1	А	593	% 57%	20%		20%
1	В	593	55%	20%		20%
1	С	593	% 55%	22%	·	20%
1	D	593	2% 5 9%	20%	•	19%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14989 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	472	Total	С	Ν	Ο	Se	0	0	0
	A	475	473 3576 2257 610 701 8	0	0	U				
1	р	472	Total	С	Ν	Ο	Se	0	0	0
	D	475	3572	2254	609	701	8	0	0	0
1	C	476	Total	С	Ν	Ο	Se	0	0	0
		470	3597	2269	616	704	8	0		
1	П	D 470	Total	С	Ν	Ο	Se	0	0	0
	479	3617	2279	619	711	8	0	0	0	

• Molecule 1 is a protein called Protease 4.

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	26	MSE	-	EXPRESSION TAG	UNP P08395
А	27	GLY	-	EXPRESSION TAG	UNP P08395
А	28	SER	-	EXPRESSION TAG	UNP P08395
А	29	SER	-	EXPRESSION TAG	UNP P08395
А	30	HIS	-	EXPRESSION TAG	UNP P08395
A	31	HIS	-	EXPRESSION TAG	UNP P08395
А	32	HIS	-	EXPRESSION TAG	UNP P08395
A	33	HIS	-	EXPRESSION TAG	UNP P08395
A	34	HIS	-	EXPRESSION TAG	UNP P08395
А	35	HIS	-	EXPRESSION TAG	UNP P08395
A	36	SER	-	EXPRESSION TAG	UNP P08395
А	37	SER	-	EXPRESSION TAG	UNP P08395
A	38	GLY	-	EXPRESSION TAG	UNP P08395
А	39	LEU	-	EXPRESSION TAG	UNP P08395
А	40	VAL	-	EXPRESSION TAG	UNP P08395
A	41	PRO	-	EXPRESSION TAG	UNP P08395
A	42	ARG	-	EXPRESSION TAG	UNP P08395
A	43	GLY	-	EXPRESSION TAG	UNP P08395
A	44	SER	-	EXPRESSION TAG	UNP P08395
А	45	HIS	-	EXPRESSION TAG	UNP P08395
А	46	MSE	-	EXPRESSION TAG	UNP P08395



Chain	Residue	Modelled	Actual	Comment	Reference
В	26	MSE	-	EXPRESSION TAG	UNP P08395
В	27	GLY	-	EXPRESSION TAG	UNP P08395
В	28	SER	_	EXPRESSION TAG	UNP P08395
В	29	SER	-	EXPRESSION TAG	UNP P08395
В	30	HIS	-	EXPRESSION TAG	UNP P08395
В	31	HIS	-	EXPRESSION TAG	UNP P08395
В	32	HIS	-	EXPRESSION TAG	UNP P08395
В	33	HIS	-	EXPRESSION TAG	UNP P08395
В	34	HIS	-	EXPRESSION TAG	UNP P08395
В	35	HIS	-	EXPRESSION TAG	UNP P08395
В	36	SER	-	EXPRESSION TAG	UNP P08395
В	37	SER	-	EXPRESSION TAG	UNP P08395
В	38	GLY	-	EXPRESSION TAG	UNP P08395
В	39	LEU	-	EXPRESSION TAG	UNP P08395
В	40	VAL	-	EXPRESSION TAG	UNP P08395
В	41	PRO	-	EXPRESSION TAG	UNP P08395
В	42	ARG	-	EXPRESSION TAG	UNP P08395
В	43	GLY	-	EXPRESSION TAG	UNP P08395
В	44	SER	-	EXPRESSION TAG	UNP P08395
В	45	HIS	-	EXPRESSION TAG	UNP P08395
В	46	MSE	-	EXPRESSION TAG	UNP P08395
С	26	MSE	_	EXPRESSION TAG	UNP P08395
С	27	GLY	_	EXPRESSION TAG	UNP P08395
С	28	SER	_	EXPRESSION TAG	UNP P08395
С	29	SER	_	EXPRESSION TAG	UNP P08395
С	30	HIS	_	EXPRESSION TAG	UNP P08395
С	31	HIS	-	EXPRESSION TAG	UNP P08395
С	32	HIS	-	EXPRESSION TAG	UNP P08395
С	33	HIS	-	EXPRESSION TAG	UNP P08395
С	34	HIS	-	EXPRESSION TAG	UNP P08395
С	35	HIS	-	EXPRESSION TAG	UNP P08395
С	36	SER	-	EXPRESSION TAG	UNP P08395
С	37	SER	-	EXPRESSION TAG	UNP P08395
С	38	GLY	-	EXPRESSION TAG	UNP P08395
С	39	LEU	-	EXPRESSION TAG	UNP P08395
C	40	VAL	-	EXPRESSION TAG	UNP P08395
C	41	PRO	-	EXPRESSION TAG	UNP P08395
C	42	ARG	-	EXPRESSION TAG	UNP P08395
C	43	GLY	_	EXPRESSION TAG	UNP P08395
C	44	SER	-	EXPRESSION TAG	UNP P08395
C	45	HIS	-	EXPRESSION TAG	UNP P08395
С	46	MSE	_	EXPRESSION TAG	UNP P08395



Chain	Residue	Modelled	Actual	Comment	Reference
D	26	MSE	-	EXPRESSION TAG	UNP P08395
D	27	GLY	-	EXPRESSION TAG	UNP P08395
D	28	SER	-	EXPRESSION TAG	UNP P08395
D	29	SER	-	EXPRESSION TAG	UNP P08395
D	30	HIS	-	EXPRESSION TAG	UNP P08395
D	31	HIS	-	EXPRESSION TAG	UNP P08395
D	32	HIS	-	EXPRESSION TAG	UNP P08395
D	33	HIS	-	EXPRESSION TAG	UNP P08395
D	34	HIS	-	EXPRESSION TAG	UNP P08395
D	35	HIS	-	EXPRESSION TAG	UNP P08395
D	36	SER	-	EXPRESSION TAG	UNP P08395
D	37	SER	-	EXPRESSION TAG	UNP P08395
D	38	GLY	-	EXPRESSION TAG	UNP P08395
D	39	LEU	-	EXPRESSION TAG	UNP P08395
D	40	VAL	-	EXPRESSION TAG	UNP P08395
D	41	PRO	-	EXPRESSION TAG	UNP P08395
D	42	ARG	-	EXPRESSION TAG	UNP P08395
D	43	GLY	-	EXPRESSION TAG	UNP P08395
D	44	SER	-	EXPRESSION TAG	UNP P08395
D	45	HIS	-	EXPRESSION TAG	UNP P08395
D	46	MSE	-	EXPRESSION TAG	UNP P08395

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	149	Total O 149 149	0	0
2	В	166	Total O 166 166	0	0
2	С	139	Total O 139 139	0	0
2	D	173	Total O 173 173	0	0



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 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: Protease 4





GLN 7466 R357 MAIA R467 R357 MAIA R467 R360 MAIA R487 R360 MAIA R451 R361 MAIA M410 R363 MAIA M510 M367 MAIA M510 M367 MAIA M540 M416 MAIA M540 M416 MAIA M540 M416 MAIA M540 M416 <



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	93.02Å 153.04 Å 100.21 Å	Depositor
a, b, c, α , β , γ	90.00° 104.17° 90.00°	Depositor
Bosolution (Å)	46.63 - 2.76	Depositor
	46.85 - 2.76	EDS
$\% { m Data \ completeness}$	$100.0 \ (46.63-2.76)$	Depositor
(in resolution range)	98.6(46.85 - 2.76)	EDS
R_{merge}	0.18	Depositor
R _{sym}	0.18	Depositor
$< I/\sigma(I) > 1$	$2.84 (at 2.77 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
B B.	0.200 , 0.259	Depositor
n, n_{free}	0.200 , 0.269	DCC
R_{free} test set	3501 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	29.4	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.37 , 47.5	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14989	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 3.78% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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).

Mal	Chain	Bo	nd lengths	Bond angles		
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.80	1/3635~(0.0%)	0.85	5/4922~(0.1%)	
1	В	0.81	1/3631~(0.0%)	0.87	1/4918~(0.0%)	
1	С	0.81	0/3656	0.88	2/4950~(0.0%)	
1	D	0.80	2/3676~(0.1%)	0.86	2/4977~(0.0%)	
All	All	0.80	4/14598~(0.0%)	0.86	10/19767~(0.1%)	

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
1	А	0	2
1	В	0	2
1	С	0	2
1	D	0	1
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	В	542	VAL	CA-CB	6.76	1.69	1.54
1	А	542	VAL	CA-CB	6.10	1.67	1.54
1	D	542	VAL	CA-CB	5.75	1.66	1.54
1	D	545	TRP	CE3-CZ3	5.07	1.47	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	350	ASP	CB-CG-OD1	6.16	123.84	118.30
1	А	547	LEU	CA-CB-CG	5.94	128.96	115.30
1	А	219	ASP	CB-CG-OD1	5.83	123.55	118.30
1	С	542	VAL	N-CA-C	5.72	126.43	111.00



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	178	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	С	138	LEU	CA-CB-CG	5.30	127.48	115.30
1	А	138	LEU	CA-CB-CG	5.21	127.29	115.30
1	А	496	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	D	309	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	В	479	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below	N:
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Mol	Chain	\mathbf{Res}	Type	Group
1	А	541	LYS	Peptide
1	А	544	GLN	Peptide
1	В	340	GLY	Peptide
1	В	541	LYS	Peptide
1	С	541	LYS	Peptide
1	С	70	LYS	Peptide
1	D	541	LYS	Peptide

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	А	3576	0	3537	106	0
1	В	3572	0	3526	110	0
1	С	3597	0	3554	127	0
1	D	3617	0	3571	93	0
2	А	149	0	0	0	0
2	В	166	0	0	6	0
2	С	139	0	0	5	0
2	D	173	0	0	2	0
All	All	14989	0	14188	409	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 14.

All (409) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:B:123:PHE:CZ	1:B:131:MSE:HE2	1.73	1.21
1:A:403:MSE:HE2	1:A:423:ALA:HB2	1.27	1.17
1:C:403:MSE:HE2	1:C:423:ALA:HB2	1.28	1.15
1:A:541:LYS:HD3	1:A:542:VAL:HG23	1.24	1.14
1:D:121:LYS:HE2	2:D:691:HOH:O	1.55	1.05
1:D:403:MSE:HE2	1:D:423:ALA:HB2	1.42	1.02
1:D:424:ASN:HD22	1:D:426:SER:H	1.03	1.01
1:A:424:ASN:HD22	1:A:426:SER:H	1.01	1.00
1:B:123:PHE:HZ	1:B:131:MSE:HE2	1.10	0.99
1:D:148:VAL:H	1:D:167:ASN:HD22	1.06	0.98
1:B:424:ASN:ND2	1:B:426:SER:H	1.62	0.97
1:C:424:ASN:HD22	1:C:426:SER:H	0.99	0.96
1:A:148:VAL:H	1:A:167:ASN:HD22	1.06	0.96
1:C:148:VAL:H	1:C:167:ASN:HD22	1.08	0.95
1:A:148:VAL:H	1:A:167:ASN:ND2	1.62	0.95
1:B:148:VAL:H	1:B:167:ASN:HD22	0.97	0.94
1:C:148:VAL:H	1:C:167:ASN:ND2	1.65	0.94
1:B:202:VAL:HG21	1:B:216:ILE:HG21	1.48	0.93
1:A:184:THR:HG22	1:C:455:VAL:H	1.32	0.92
1:C:268:THR:CG2	1:C:271:ASP:HB3	1.99	0.92
1:C:424:ASN:ND2	1:C:426:SER:H	1.67	0.91
1:D:157:GLN:HE22	1:D:181:GLY:H	1.19	0.91
1:B:148:VAL:H	1:B:167:ASN:ND2	1.69	0.90
1:D:157:GLN:NE2	1:D:180:HIS:H	1.68	0.90
1:C:541:LYS:HB3	1:C:542:VAL:HG22	1.51	0.90
1:B:157:GLN:HE22	1:B:181:GLY:H	1.13	0.89
1:A:116:ILE:HB	1:A:148:VAL:HG22	1.53	0.88
1:B:540:ALA:O	1:B:541:LYS:HG3	1.75	0.87
1:A:545:TRP:CZ3	1:A:547:LEU:HD23	2.09	0.87
1:B:424:ASN:HD22	1:B:426:SER:H	0.90	0.86
1:B:123:PHE:CZ	1:B:131:MSE:CE	2.59	0.86
1:B:157:GLN:NE2	1:B:180:HIS:H	1.75	0.85
1:A:399:VAL:H	1:A:419:ASN:ND2	1.75	0.83
1:B:118:MSE:HE1	1:B:162:LEU:HD22	1.60	0.83
1:B:424:ASN:HD22	1:B:426:SER:N	1.74	0.83
1:C:424:ASN:HD22	1:C:426:SER:N	1.76	0.82
1:A:171:LEU:O	1:A:285:LEU:HA	1.79	0.82
1:C:184:THR:HG22	1:D:455:VAL:H	1.45	0.82
1:A:403:MSE:HE2	1:A:423:ALA:CB	2.10	0.81
1:B:123:PHE:CE2	1:B:131:MSE:HE2	2.16	0.81
1:D:403:MSE:HE2	1:D:423:ALA:CB	2.10	0.81
1:D:403:MSE:HE1	1:D:429:THR:HG21	1.62	0.80



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:104:ILE:HD13	1:B:138:LEU:HD13	1.65	0.79
1:B:202:VAL:HG21	1:B:216:ILE:CG2	2.12	0.79
1:A:184:THR:CG2	1:C:455:VAL:H	1.96	0.78
1:C:168:LYS:HE2	1:C:170:TRP:CZ2	2.18	0.78
1:D:399:VAL:H	1:D:419:ASN:HD22	1.32	0.78
1:B:123:PHE:HZ	1:B:131:MSE:CE	1.95	0.78
1:B:287:SER:HB3	1:B:290:GLU:HG3	1.66	0.77
1:D:424:ASN:ND2	1:D:426:SER:H	1.81	0.77
1:C:403:MSE:HE2	1:C:423:ALA:CB	2.13	0.76
1:A:545:TRP:HZ3	1:A:547:LEU:HD23	1.47	0.76
1:B:287:SER:HB3	1:B:290:GLU:CG	2.16	0.76
1:A:370:LEU:HD22	1:A:389:LEU:HD21	1.67	0.74
1:C:157:GLN:NE2	1:C:180:HIS:H	1.85	0.74
1:A:131:MSE:HE2	1:A:162:LEU:HG	1.69	0.74
1:B:156:SER:H	1:B:159:GLN:NE2	1.86	0.74
1:D:403:MSE:HE3	1:D:427:THR:HG21	1.71	0.72
1:A:157:GLN:HE22	1:A:181:GLY:H	1.37	0.72
1:B:148:VAL:N	1:B:167:ASN:HD22	1.82	0.72
1:C:268:THR:HG22	1:C:271:ASP:HB3	1.70	0.72
1:A:123:PHE:CZ	1:A:131:MSE:HE3	2.25	0.72
1:A:360:ARG:HD3	1:A:392:ALA:HA	1.71	0.72
1:B:502:GLN:HG3	2:B:717:HOH:O	1.89	0.72
1:B:356:ILE:HD13	1:B:389:LEU:HD13	1.72	0.72
1:D:292:GLU:O	1:D:296:THR:HG22	1.90	0.72
1:B:399:VAL:H	1:B:419:ASN:ND2	1.87	0.71
1:C:157:GLN:HE22	1:C:181:GLY:H	1.39	0.70
1:A:403:MSE:CE	1:A:423:ALA:HB2	2.17	0.69
1:B:56:ARG:CB	2:B:655:HOH:O	2.41	0.69
1:C:111:ARG:HH11	1:C:111:ARG:HB3	1.57	0.69
1:C:157:GLN:HE22	1:C:180:HIS:H	1.37	0.69
1:D:148:VAL:H	1:D:167:ASN:ND2	1.86	0.69
1:A:157:GLN:NE2	1:A:180:HIS:H	1.91	0.68
1:C:156:SER:H	1:C:159:GLN:NE2	1.92	0.68
1:C:148:VAL:N	1:C:167:ASN:HD22	1.88	0.68
1:A:542:VAL:HG12	1:A:543:LYS:H	1.58	0.68
1:D:420:TYR:HA	1:D:524:ASP:OD2	1.94	0.68
1:A:370:LEU:HD21	1:A:414:ILE:HD12	1.76	0.67
1:B:277:LEU:HD13	1:B:285:LEU:HG	1.77	0.67
1:A:424:ASN:HD22	1:A:426:SER:N	1.84	0.67
1:B:455:VAL:H	1:D:184:THR:HG22	1.59	0.67
1:B:118:MSE:CE	1:B:162:LEU:HD22	2.25	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:213:GLU:N	1:B:214:PRO:HD2	2.11	0.66
1:C:96:SER:HB3	1:C:99:ASP:HB2	1.77	0.66
1:C:268:THR:HG21	1:C:271:ASP:O	1.96	0.66
1:A:446:ASP:OD1	1:A:451:HIS:HE1	1.79	0.65
1:C:540:ALA:O	1:C:541:LYS:HG3	1.95	0.65
1:A:292:GLU:O	1:A:296:THR:HG23	1.97	0.65
1:D:399:VAL:H	1:D:419:ASN:ND2	1.93	0.65
1:A:455:VAL:H	1:B:184:THR:HG22	1.61	0.65
1:C:399:VAL:H	1:C:419:ASN:HD22	1.42	0.65
1:A:148:VAL:N	1:A:167:ASN:HD22	1.89	0.65
1:C:185:ASN:HD21	1:D:452:THR:HB	1.61	0.65
1:D:200:THR:HG21	1:D:215:PHE:HB3	1.78	0.65
1:B:499:THR:OG1	1:B:502:GLN:HG2	1.96	0.64
1:B:326:ASP:H	1:B:545:TRP:HE1	1.45	0.64
1:D:157:GLN:HE22	1:D:180:HIS:H	1.42	0.64
1:A:399:VAL:H	1:A:419:ASN:HD22	1.44	0.63
1:B:337:ILE:HG12	1:B:376:GLY:O	1.99	0.63
1:D:373:ASN:HA	1:D:406:MSE:O	1.99	0.63
1:C:177:VAL:HG12	1:C:179:LEU:HD13	1.81	0.63
1:C:225:ARG:NH2	2:C:673:HOH:O	2.28	0.63
1:A:424:ASN:ND2	1:A:426:SER:H	1.85	0.63
1:C:398:PRO:HG2	1:C:539:LEU:O	1.98	0.63
1:B:200:THR:HG23	1:B:439:THR:HG22	1.81	0.62
1:C:111:ARG:HB3	1:C:111:ARG:NH1	2.15	0.62
1:A:487:ARG:HD3	1:B:174:GLN:HG3	1.82	0.62
1:C:373:ASN:HA	1:C:406:MSE:O	2.00	0.61
1:A:123:PHE:HZ	1:A:131:MSE:HE3	1.63	0.61
1:D:156:SER:H	1:D:159:GLN:NE2	1.98	0.61
1:B:126:GLY:N	1:B:131:MSE:HE3	2.15	0.61
1:C:403:MSE:HE3	1:C:427:THR:HG21	1.82	0.61
1:C:483:ASN:O	1:C:487:ARG:HG3	2.01	0.61
1:D:434:ILE:HG23	1:D:481:ILE:HG23	1.81	0.61
1:D:370:LEU:HD22	1:D:389:LEU:HD21	1.83	0.60
1:B:296:THR:HG22	1:B:308:TYR:HB3	1.84	0.60
1:C:292:GLU:CD	1:D:357:ARG:HH21	2.04	0.60
1:D:424:ASN:HD22	1:D:426:SER:N	1.86	0.60
1:B:213:GLU:N	1:B:214:PRO:CD	2.64	0.60
1:A:157:GLN:HE22	1:A:180:HIS:H	1.48	0.59
1:B:343:THR:O	1:B:344:GLN:HB2	2.01	0.59
1:B:273:ALA:HB1	1:B:285:LEU:HD22	1.83	0.59
1:C:268:THR:HG21	1:C:271:ASP:HB3	1.84	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:452:THR:OG1	1:D:467:ARG:HD2	2.02	0.59
1:B:268:THR:HG22	1:B:271:ASP:HB3	1.85	0.59
1:A:174:GLN:OE1	1:C:487:ARG:HD2	2.02	0.59
1:B:309:ARG:O	1:B:310:ALA:HB2	2.02	0.59
1:B:66:VAL:HG22	1:B:93:GLN:O	2.03	0.59
1:B:520:ASN:HD22	1:B:520:ASN:C	2.07	0.58
1:C:148:VAL:N	1:C:167:ASN:ND2	2.46	0.58
1:A:184:THR:CG2	1:A:184:THR:O	2.51	0.58
1:A:360:ARG:HD3	1:A:392:ALA:CA	2.33	0.58
1:A:542:VAL:CG1	1:A:543:LYS:N	2.67	0.57
1:B:399:VAL:H	1:B:419:ASN:HD22	1.52	0.57
1:A:184:THR:O	1:A:184:THR:HG22	2.04	0.57
1:C:328:ILE:HD11	1:C:537:ALA:HB2	1.86	0.57
1:B:268:THR:HG22	1:B:268:THR:O	2.04	0.57
1:B:393:ARG:HD2	1:B:419:ASN:ND2	2.20	0.57
1:C:410:GLY:O	1:C:413:TRP:HB3	2.05	0.57
1:D:268:THR:HG23	1:D:271:ASP:H	1.70	0.57
1:D:228:ASP:HA	1:D:231:TRP:NE1	2.19	0.57
1:A:168:LYS:HE2	1:A:170:TRP:CZ2	2.39	0.57
1:A:545:TRP:CH2	1:A:547:LEU:HD23	2.39	0.57
1:A:184:THR:HG22	1:C:455:VAL:N	2.10	0.57
1:A:454:GLY:HA3	1:B:184:THR:O	2.05	0.56
1:B:123:PHE:CE2	1:B:131:MSE:CE	2.88	0.56
1:A:481:ILE:C	1:A:483:ASN:H	2.08	0.56
1:D:103:THR:HG23	1:D:316:TYR:CD2	2.41	0.56
1:C:403:MSE:CE	1:C:423:ALA:HB2	2.19	0.56
1:D:148:VAL:N	1:D:167:ASN:HD22	1.90	0.56
1:D:292:GLU:O	1:D:296:THR:CG2	2.54	0.55
1:B:171:LEU:O	1:B:285:LEU:HA	2.07	0.55
1:B:452:THR:HB	1:D:185:ASN:ND2	2.21	0.55
1:A:228:ASP:HA	1:A:231:TRP:NE1	2.22	0.55
1:A:236:TRP:CB	1:C:457:THR:HG21	2.36	0.55
1:B:212:VAL:HG23	1:B:435:PHE:CD2	2.42	0.55
1:A:157:GLN:HE21	1:A:179:LEU:HA	1.71	0.55
1:D:369:VAL:HA	1:D:400:VAL:O	2.07	0.55
1:A:292:GLU:O	1:A:296:THR:CG2	2.56	0.54
1:C:399:VAL:H	1:C:419:ASN:ND2	2.04	0.54
1:D:370:LEU:HB3	1:D:401:VAL:HG22	1.89	0.54
1:B:116:ILE:HB	1:B:148:VAL:HG22	1.88	0.54
1:B:151:VAL:HG12	1:B:170:TRP:HB2	1.89	0.54
1:D:420:TYR:CD2	1:D:535:LYS:HG2	2.43	0.54



	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:116:ILE:HB	1:D:148:VAL:HG22	1.90	0.54
1:B:148:VAL:N	1:B:167:ASN:ND2	2.48	0.54
1:B:373:ASN:HA	1:B:406:MSE:O	2.08	0.54
1:A:373:ASN:HA	1:A:406:MSE:O	2.08	0.54
1:C:232:ILE:HG21	1:D:455:VAL:HG23	1.89	0.54
1:A:520:ASN:HD22	1:A:520:ASN:C	2.12	0.53
1:C:222:PRO:O	1:C:226:GLU:HG2	2.07	0.53
1:C:106:GLN:NE2	1:C:316:TYR:CE2	2.76	0.53
1:A:370:LEU:HD22	1:A:389:LEU:CD2	2.37	0.53
1:B:184:THR:O	1:B:184:THR:HG22	2.08	0.53
1:C:67:ILE:HG12	1:C:123:PHE:HE1	1.73	0.53
1:A:542:VAL:HG12	1:A:543:LYS:N	2.24	0.52
1:B:454:GLY:HA3	1:D:184:THR:O	2.09	0.52
1:C:153:GLU:O	1:C:172:SER:HB3	2.09	0.52
1:D:252:GLU:HB3	2:D:718:HOH:O	2.09	0.52
1:C:228:ASP:HA	1:C:231:TRP:NE1	2.25	0.52
1:C:268:THR:HG22	1:C:268:THR:O	2.07	0.52
1:B:352:THR:O	1:B:356:ILE:HG13	2.09	0.52
1:C:501:GLU:CD	1:C:501:GLU:H	2.13	0.52
1:C:113:ILE:CD1	1:C:316:TYR:HE1	2.23	0.52
1:B:309:ARG:NH2	2:B:784:HOH:O	2.43	0.52
1:D:93:GLN:HG2	1:D:94:GLU:N	2.25	0.52
1:D:268:THR:HG21	1:D:271:ASP:O	2.09	0.52
1:C:547:LEU:HD23	2:C:688:HOH:O	2.10	0.51
1:C:205:VAL:HG23	1:C:481:ILE:HG22	1.92	0.51
1:C:297:LYS:O	1:C:297:LYS:HG2	2.10	0.51
1:A:131:MSE:HE2	1:A:162:LEU:CG	2.40	0.51
1:A:431:SER:HA	1:A:509:GLY:O	2.11	0.51
1:C:268:THR:HG23	1:C:274:LYS:CD	2.40	0.51
1:B:452:THR:HB	1:D:185:ASN:HD21	1.75	0.51
1:C:518:LYS:HG2	1:C:526:LEU:HG	1.92	0.51
1:B:421:ILE:N	1:B:524:ASP:OD2	2.35	0.51
1:C:200:THR:HG23	1:C:439:THR:HG22	1.93	0.51
1:C:217:ARG:HD2	2:C:677:HOH:O	2.09	0.51
1:A:163:ALA:C	1:A:165:PHE:H	2.13	0.50
1:A:236:TRP:HB2	1:C:457:THR:HG21	1.93	0.50
1:D:213:GLU:N	1:D:214:PRO:CD	2.74	0.50
1:A:103:THR:HG23	1:A:316:TYR:CD2	2.47	0.50
1:C:268:THR:HG23	1:C:274:LYS:HD3	1.93	0.50
1:B:249:ILE:HD11	1:B:254:VAL:HG22	1.91	0.50
1:B:545:TRP:HZ2	2:B:689:HOH:O	1.94	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:184:THR:HG22	1:D:455:VAL:N	2.20	0.50
1:B:416:THR:N	1:B:417:PRO:CD	2.75	0.50
1:D:95:ASN:ND2	1:D:95:ASN:N	2.59	0.50
1:A:446:ASP:OD1	1:A:451:HIS:CE1	2.61	0.50
1:C:105:ARG:O	1:C:108:LYS:HB3	2.11	0.50
1:D:487:ARG:HG2	1:D:487:ARG:HH11	1.76	0.50
1:B:125:GLY:HA2	1:B:131:MSE:CE	2.42	0.50
1:D:100:ILE:HG21	1:D:134:ILE:HD13	1.94	0.50
1:A:225:ARG:NH2	1:C:454:GLY:O	2.44	0.50
1:D:67:ILE:HG12	1:D:123:PHE:HE1	1.77	0.50
1:B:327:SER:HB3	1:B:545:TRP:CE2	2.47	0.50
1:C:200:THR:CG2	1:C:439:THR:HG22	2.42	0.50
1:B:177:VAL:HG12	1:B:179:LEU:HD13	1.93	0.49
1:C:451:HIS:HA	2:C:654:HOH:O	2.11	0.49
1:D:403:MSE:HE3	1:D:427:THR:CG2	2.42	0.49
1:A:164:SER:O	1:A:246:ASN:HB3	2.12	0.49
1:D:328:ILE:HD13	1:D:367:ALA:HB3	1.93	0.49
1:A:403:MSE:HE3	1:A:427:THR:HG21	1.95	0.49
1:B:161:TYR:HB2	1:B:239:TYR:CE2	2.47	0.49
1:B:324:THR:HB	1:B:545:TRP:CD1	2.48	0.49
1:C:164:SER:HA	1:C:169:ILE:HD11	1.95	0.49
1:C:168:LYS:CE	1:C:170:TRP:CZ2	2.94	0.49
1:C:296:THR:HG21	1:C:301:TRP:HE3	1.77	0.49
1:D:540:ALA:O	1:D:541:LYS:HG3	2.12	0.49
1:A:268:THR:HG21	1:A:271:ASP:O	2.13	0.49
1:A:432:ILE:HB	1:A:507:ALA:HB1	1.94	0.49
1:C:118:MSE:HE1	1:C:162:LEU:HB3	1.95	0.49
1:C:430:GLY:O	1:C:431:SER:CB	2.61	0.49
1:C:97:LEU:HD22	1:C:130:SER:OG	2.13	0.49
1:B:452:THR:HG21	1:B:466:THR:OG1	2.12	0.49
1:A:337:ILE:HA	1:A:347:VAL:HG12	1.95	0.48
1:C:520:ASN:HD22	1:C:520:ASN:C	2.16	0.48
1:D:403:MSE:HE1	1:D:429:THR:CG2	2.36	0.48
1:C:359:ALA:HB1	1:C:365:VAL:HG11	1.94	0.48
1:C:430:GLY:O	1:C:431:SER:HB3	2.14	0.48
1:D:362:ASP:O	1:D:397:LYS:NZ	2.46	0.48
1:D:421:ILE:HD12	1:D:496:ARG:NH1	2.28	0.48
1:B:153:GLU:O	1:B:175:GLY:HA3	2.13	0.48
1:C:168:LYS:HE2	1:C:170:TRP:CH2	2.49	0.48
1:A:231:TRP:O	1:A:235:LEU:HD13	2.13	0.48
1:A:232:ILE:HG21	1:C:455:VAL:HG23	1.95	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:545:TRP:CZ2	2:B:689:HOH:O	2.55	0.48
1:C:164:SER:O	1:C:246:ASN:HB3	2.13	0.48
1:A:383:GLU:HA	1:A:383:GLU:OE1	2.14	0.47
1:C:113:ILE:CD1	1:C:316:TYR:CE1	2.96	0.47
1:D:141:PHE:CE1	1:D:146:LYS:HB2	2.49	0.47
1:B:184:THR:CG2	1:B:184:THR:O	2.61	0.47
1:A:153:GLU:HA	1:A:172:SER:HB3	1.96	0.47
1:B:424:ASN:ND2	1:B:426:SER:N	2.46	0.47
1:C:157:GLN:HE21	1:C:179:LEU:HA	1.80	0.47
1:A:210:SER:O	1:A:213:GLU:HB2	2.15	0.47
1:A:103:THR:HG23	1:A:316:TYR:HD2	1.80	0.47
1:C:403:MSE:HE1	1:C:429:THR:HG21	1.97	0.47
1:B:118:MSE:HE3	1:B:138:LEU:HD21	1.97	0.47
1:B:421:ILE:CG2	1:B:523:VAL:HG22	2.45	0.47
1:A:292:GLU:OE1	1:C:357:ARG:NE	2.35	0.47
1:A:424:ASN:ND2	1:A:425:PRO:HD2	2.30	0.47
1:A:163:ALA:C	1:A:165:PHE:N	2.68	0.47
1:D:168:LYS:HD3	1:D:170:TRP:CH2	2.50	0.46
1:C:113:ILE:HD13	1:C:316:TYR:CE1	2.50	0.46
1:C:213:GLU:N	1:C:214:PRO:HD2	2.30	0.46
1:C:501:GLU:N	1:C:501:GLU:CD	2.69	0.46
1:A:185:ASN:HD21	1:C:452:THR:HB	1.81	0.46
1:C:268:THR:HG22	1:C:271:ASP:CB	2.42	0.46
1:A:545:TRP:HZ3	1:A:547:LEU:CD2	2.22	0.46
1:B:118:MSE:CE	1:B:138:LEU:HD21	2.46	0.46
1:A:131:MSE:HE2	1:A:162:LEU:HB2	1.98	0.46
1:A:154:ASN:OD1	1:A:175:GLY:HA2	2.16	0.46
1:B:472:GLU:O	1:B:476:MSE:HG2	2.16	0.46
1:D:228:ASP:HA	1:D:231:TRP:CD1	2.49	0.46
1:D:360:ARG:HD3	1:D:392:ALA:HA	1.98	0.46
1:C:296:THR:CG2	1:C:301:TRP:HE3	2.29	0.46
1:C:348:GLY:O	1:C:349:GLY:C	2.54	0.46
1:A:324:THR:C	1:A:545:TRP:HE1	2.20	0.45
1:C:116:ILE:HB	1:C:148:VAL:HG22	1.97	0.45
1:D:256:PRO:HB2	1:D:260:GLY:HA3	1.98	0.45
1:B:268:THR:CG2	1:B:274:LYS:HB3	2.46	0.45
1:B:467:ARG:NH2	2:B:720:HOH:O	2.46	0.45
1:A:189:TYR:O	1:A:190:LYS:C	2.54	0.45
1:A:360:ARG:O	1:A:360:ARG:HG3	2.17	0.45
1:B:204:ARG:HD3	1:B:212:VAL:HG11	1.98	0.45
1:C:62:ASP:O	1:C:314:TYR:HE2	2.00	0.45



Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlap (Å)		
1.B.327.SEB.HB3	1.B.545.TRP.NE1	2.31	0.45		
1:D:157:GLN:HE21	1:D:179:LEU:HA	1.81	0.45		
1:A:101:VAL:HG21	1:A:133:TYB:CE2	2.52	0.45		
1:C:213:GLU:N	1:C:214:PRO:CD	2.80	0.45		
1:C:56:ARG:H	1:C:112:ASN:HB3	1.82	0.45		
1:C:296:THR:HG21	1:C:301:TRP:CE3	2.51	0.45		
1:C:393:ARG:HA	1:C:397:LYS:O	2.17	0.45		
1:A:341:GLU:O	1:A:342:GLU:C	2.55	0.45		
1:C:413:TRP:O	1:C:416:THR:HB	2.17	0.45		
1:A:479:LEU:O	1:A:483:ASN:HB2	2.17	0.44		
1:B:113:ILE:HD13	1:B:316:TYR:CE1	2.52	0.44		
1:A:227:ALA:O	1:A:231:TRP:HD1	2.00	0.44		
1:B:203:PHE:O	1:B:435:PHE:HA	2.17	0.44		
1:C:187:LEU:HD23	1:D:452:THR:HG22	1.99	0.44		
1:D:330:VAL:HB	1:D:548:GLU:HG3	2.00	0.44		
1:D:415:SER:C	1:D:417:PRO:HD2	2.38	0.44		
1:A:118:MSE:CE	1:A:166:ALA:HB2	2.47	0.44		
1:A:324:THR:HG22	1:A:325:GLY:H	1.82	0.44		
1:C:520:ASN:ND2	1:C:522:LEU:HG	2.33	0.44		
1:A:228:ASP:HA	1:A:231:TRP:CD1	2.53	0.44		
1:B:388:GLU:O	1:B:391:ALA:HB3	2.17	0.44		
1:C:539:LEU:O	1:C:540:ALA:HB2	2.18	0.44		
1:D:268:THR:HG23	1:D:271:ASP:N	2.31	0.44		
1:B:249:ILE:HB	1:B:250:PRO:HD2	1.98	0.44		
1:B:279:ASN:O	1:B:280:LYS:HB2	2.16	0.44		
1:D:168:LYS:HE2	1:D:170:TRP:CZ2	2.53	0.44		
1:D:236:TRP:O	1:D:239:TYR:HB3	2.18	0.44		
1:D:240:LEU:HD23	1:D:240:LEU:HA	1.67	0.44		
1:A:60:LEU:HB3	1:A:312:SER:HA	1.99	0.44		
1:D:157:GLN:HE21	1:D:180:HIS:H	1.57	0.44		
1:A:369:VAL:HA	1:A:400:VAL:O	2.18	0.44		
1:B:170:TRP:CD1	1:B:284:ALA:HB3	2.52	0.44		
1:B:424:ASN:CG	1:B:425:PRO:HD2	2.37	0.44		
1:C:103:THR:OG1	1:C:318:LEU:HD23	2.17	0.43		
1:C:106:GLN:HE21	1:C:316:TYR:HE2	1.66	0.43		
1:A:420:TYR:CD2	1:A:535:LYS:HG2	2.53	0.43		
1:C:434:ILE:HG23	1:C:481:ILE:HG23	2.01	0.43		
1:B:104:ILE:HD13	1:B:138:LEU:CD1	2.42	0.43		
1:B:64:SER:HA	1:B:122:ASN:O	2.19	0.43		
1:C:120:LEU:HD23	1:C:120:LEU:HA	1.75	0.43		
1:C:189:TYR:O	1:C:190:LYS:C	2.57	0.43		



Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlan (Å)		
1:A:107:ALA:HB1	1:A:113:ILE:HG21	2.01	0.43		
1:A:208:TYR:HB2	1:A:510:HIS:N	2.34	0.43		
1:C:70:LYS:HB2	1:C:334:ASN:HD22	1.84	0.43		
1:A:200:THB:HG21	1:A:215:PHE:HB3	2.01	0.43		
1:A:337:ILE:HD13	1:A:347:VAL:HG11	2.01	0.43		
1:B:111:ARG:HH11	1:B:111:ARG:HB3	1.84	0.43		
1:B:320:THR:HA	1:B:321:PRO:HD3	1.86	0.43		
1:A:67:ILE:HG12	1:A:123:PHE:HE1	1.84	0.42		
1:C:70:LYS:HB2	1:C:334:ASN:ND2	2.34	0.42		
1:C:389:LEU:HD12	1:C:389:LEU:HA	1.88	0.42		
1:C:445:LEU:HB3	1:C:450:VAL:HB	2.00	0.42		
1:D:104:ILE:HD13	1:D:138:LEU:HD13	2.00	0.42		
1:D:338:MSE:HE2	1:D:338:MSE:HA	2.01	0.42		
1:C:185:ASN:ND2	1:D:452:THR:HB	2.33	0.42		
1:B:289:ALA:HA	1:B:292:GLU:HB2	1.99	0.42		
1:B:337:ILE:HA	1:B:347:VAL:HB	2.01	0.42		
1:C:118:MSE:HE2	1:C:120:LEU:HD11	2.01	0.42		
1:A:428:LEU:HA	1:A:428:LEU:HD12	1.81	0.42		
1:D:491:LEU:HD23	1:D:491:LEU:HA	1.76	0.42		
1:D:118:MSE:CE	1:D:166:ALA:HB2	2.50	0.42		
1:A:366:LYS:O	1:A:398:PRO:HD2	2.19	0.42		
1:A:481:ILE:C	1:A:483:ASN:N	2.72	0.42		
1:C:421:ILE:HG22	1:C:523:VAL:HG22	2.02	0.42		
1:B:157:GLN:HE21	1:B:179:LEU:HA	1.85	0.42		
1:B:189:TYR:O	1:B:190:LYS:C	2.57	0.42		
1:C:357:ARG:O	1:C:360:ARG:HB3	2.19	0.42		
1:C:403:MSE:HE1	1:C:429:THR:CB	2.50	0.42		
1:D:403:MSE:CE	1:D:423:ALA:HB2	2.30	0.42		
1:D:67:ILE:HG12	1:D:123:PHE:CE1	2.54	0.42		
1:D:155:TYR:HA	1:D:159:GLN:HE21	1.84	0.42		
1:C:171:LEU:HB2	1:C:282:VAL:HG21	2.02	0.42		
1:C:236:TRP:CB	1:D:457:THR:HG21	2.49	0.42		
1:D:467:ARG:HE	1:D:467:ARG:HB3	1.66	0.42		
1:B:188:TYR:CD1	1:B:188:TYR:N	2.87	0.42		
1:C:476:MSE:HB3	1:C:476:MSE:HE3	1.93	0.42		
1:C:401:VAL:HG21	1:C:415:SER:HA	2.01	0.41		
1:A:231:TRP:CE3	1:A:428:LEU:HD21	2.55	0.41		
1:A:382:SER:HB3	1:A:413:TRP:CD1	2.55	0.41		
1:B:338:MSE:HA	1:B:338:MSE:HE2	2.03	0.41		
1:D:542:VAL:HB	1:D:543:LYS:H	1.65	0.41		
1:A:114:THR:O	1:A:147:PRO:HD2	2.19	0.41		



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:199:SER:O	1:C:439:THR:HA	2.21	0.41
1:B:455:VAL:N	1:D:184:THR:HG22	2.31	0.41
1:D:210:SER:C	1:D:212:VAL:H	2.24	0.41
1:A:266:THR:C	1:A:268:THR:H	2.23	0.41
1:D:148:VAL:O	1:D:167:ASN:N	2.46	0.41
1:A:209:LYS:NZ	1:A:409:SER:HB2	2.35	0.41
1:B:128:GLN:HB3	1:B:129:PRO:HD3	2.03	0.41
1:B:348:GLY:O	1:B:349:GLY:C	2.59	0.41
1:C:70:LYS:HE3	1:C:334:ASN:HB3	2.02	0.41
1:D:452:THR:HG21	1:D:466:THR:OG1	2.20	0.41
1:D:518:LYS:O	1:D:519:ALA:C	2.57	0.41
1:B:147:PRO:HA	1:B:167:ASN:ND2	2.36	0.41
1:D:172:SER:HA	1:D:286:ALA:O	2.20	0.41
1:B:249:ILE:HB	1:B:250:PRO:CD	2.51	0.41
1:D:181:GLY:HA2	1:D:236:TRP:CZ2	2.56	0.41
1:B:157:GLN:HE21	1:B:180:HIS:H	1.62	0.41
1:C:292:GLU:OE1	1:D:357:ARG:NH2	2.44	0.41
1:C:435:PHE:C	1:C:435:PHE:CD2	2.93	0.41
1:B:157:GLN:HE22	1:B:180:HIS:H	1.60	0.41
1:B:540:ALA:O	1:B:541:LYS:CG	2.59	0.41
1:C:111:ARG:HG2	1:C:112:ASN:N	2.36	0.41
1:C:209:LYS:NZ	1:C:409:SER:OG	2.53	0.41
1:D:337:ILE:O	1:D:338:MSE:HE3	2.20	0.41
1:D:434:ILE:HD13	1:D:481:ILE:HD12	2.03	0.41
1:A:259:GLN:HA	1:A:259:GLN:HE21	1.86	0.41
1:A:397:LYS:HA	1:A:398:PRO:HD3	1.87	0.41
1:C:113:ILE:HD11	1:C:316:TYR:CE1	2.56	0.41
1:D:118:MSE:HE3	1:D:150:ALA:HB2	2.03	0.40
1:C:268:THR:CG2	1:C:268:THR:O	2.69	0.40
1:D:171:LEU:O	1:D:285:LEU:HA	2.21	0.40
1:A:249:ILE:HD11	1:A:254:VAL:HG22	2.03	0.40
1:A:302:SER:C	1:A:304:THR:N	2.73	0.40
1:B:266:THR:C	1:B:268:THR:H	2.24	0.40
1:A:413:TRP:O	1:A:416:THR:HB	2.21	0.40
1:B:542:VAL:CG1	1:B:543:LYS:N	2.84	0.40
1:C:153:GLU:HG2	2:C:635:HOH:O	2.21	0.40
1:D:247:ARG:O	1:D:248:GLN:HB2	2.22	0.40
1:C:296:THR:O	1:C:300:GLY:HA2	2.22	0.40
1:C:113:ILE:HD11	1:C:316:TYR:HE1	1.86	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	Percenti	les
1	А	469/593~(79%)	426 (91%)	39 (8%)	4 (1%)	17 31	1
1	В	469/593~(79%)	428 (91%)	32~(7%)	9(2%)	8 14	
1	С	472/593~(80%)	433~(92%)	33~(7%)	6 (1%)	12 21	1
1	D	475/593~(80%)	437~(92%)	37~(8%)	1 (0%)	47 69	9
All	All	1885/2372~(80%)	1724 (92%)	141 (8%)	20 (1%)	14 25	5

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	542	VAL
1	В	326	ASP
1	В	344	GLN
1	В	542	VAL
1	С	326	ASP
1	С	540	ALA
1	D	542	VAL
1	А	324	THR
1	А	340	GLY
1	С	349	GLY
1	С	542	VAL
1	В	267	LYS
1	В	297	LYS
1	С	70	LYS
1	А	342	GLU
1	В	317	ALA
1	С	324	THR
1	В	310	ALA
1	В	172	SER
1	В	349	GLY



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	А	373/460~(81%)	340 (91%)	33~(9%)	10 17
1	В	372/460~(81%)	328 (88%)	44 (12%)	5 8
1	С	374/460~(81%)	333 (89%)	41 (11%)	6 10
1	D	377/460~(82%)	339~(90%)	38 (10%)	7 12
All	All	1496/1840~(81%)	1340~(90%)	156~(10%)	7 11

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	60	LEU
1	А	93	GLN
1	А	121	LYS
1	А	138	LEU
1	А	162	LEU
1	А	172	SER
1	А	179	LEU
1	А	184	THR
1	А	189	TYR
1	А	212	VAL
1	А	219	ASP
1	А	220	MSE
1	А	262	LEU
1	А	265	LEU
1	А	268	THR
1	А	281	LEU
1	А	296	THR
1	А	320	THR
1	А	324	THR
1	А	338	MSE
1	A	344	GLN
1	A	416	THR
1	A	422	VAL
1	A	428	LEU



Mol	Chain	Res	Type
1	А	460	LEU
1	А	479	LEU
1	А	488	PHE
1	А	520	ASN
1	А	525	SER
1	А	541	LYS
1	А	542	VAL
1	А	543	LYS
1	А	547	LEU
1	В	64	SER
1	В	111	ARG
1	В	138	LEU
1	B	168	LYS
1	В	184	THR
1	B	185	ASN
1	B	189	TYR
1	B	200	THR
1	В	202	VAL
1	В	212	VAL
1	В	249	ILE
1	В	262	LEU
1	В	265	LEU
1	В	266	THR
1	В	277	LEU
1	В	278	GLU
1	В	280	LYS
1	В	282	VAL
1	В	290	GLU
1	В	293	LYS
1	В	297	LYS
1	В	303	LYS
1	В	304	THR
1	В	309	ARG
1	В	320	THR
1	В	339	ASP
1	В	344	GLN
1	В	364	LYS
1	В	388	GLU
1	В	416	THR
1	В	422	VAL
1	В	428	LEU
1	В	460	LEU



Mol	Chain	Res	Type
1	В	464	SER
1	В	475	LEU
1	В	481	ILE
1	В	488	PHE
1	В	511	VAL
1	В	520	ASN
1	В	525	SER
1	В	541	LYS
1	В	542	VAL
1	В	543	LYS
1	В	544	GLN
1	С	64	SER
1	С	93	GLN
1	С	111	ARG
1	С	113	ILE
1	С	138	LEU
1	С	170	TRP
1	С	172	SER
1	С	184	THR
1	С	200	THR
1	С	212	VAL
1	С	252	GLU
1	С	265	LEU
1	С	280	LYS
1	С	282	VAL
1	С	287	SER
1	С	304	THR
1	С	309	ARG
1	С	318	LEU
1	С	326	ASP
1	C	339	ASP
1	C	358	ASP
1	C	364	LYS
1	С	378	SER
1	C	388	GLU
1	С	416	THR
1	C	422	VAL
1	С	424	ASN
1	С	434	ILE
1	С	446	ASP
1	C	460	LEU
1	C	471	PRO



Mol	Chain	Res	Type
1	С	478	GLN
1	С	480	SER
1	С	488	PHE
1	С	501	GLU
1	С	511	VAL
1	С	518	LYS
1	С	520	ASN
1	С	525	SER
1	С	542	VAL
1	С	543	LYS
1	D	95	ASN
1	D	111	ARG
1	D	138	LEU
1	D	179	LEU
1	D	184	THR
1	D	191	SER
1	D	207	THR
1	D	230	ARG
1	D	252	GLU
1	D	262	LEU
1	D	265	LEU
1	D	268	THR
1	D	280	LYS
1	D	287	SER
1	D	296	THR
1	D	304	THR
1	D	319	LYS
1	D	326	ASP
1	D	328	ILE
1	D	338	MSE
1	D	344	GLN
1	D	364	LYS
1	D	388	GLU
1	D	416	THR
1	D	422	VAL
1	D	434	ILE
1	D	446	ASP
1	D	460	LEU
1	D	462	ASP
1	D	480	SER
1	D	487	ARG
1	D	488	PHE



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Mol	Chain	Res	Type
1	D	511	VAL
1	D	520	ASN
1	D	523	VAL
1	D	525	SER
1	D	545	TRP
1	D	548	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	157	GLN
1	А	159	GLN
1	А	167	ASN
1	А	185	ASN
1	А	237	GLN
1	А	238	ASN
1	А	241	ASN
1	А	259	GLN
1	А	419	ASN
1	А	424	ASN
1	А	451	HIS
1	А	478	GLN
1	А	520	ASN
1	В	128	GLN
1	В	157	GLN
1	В	159	GLN
1	В	167	ASN
1	В	185	ASN
1	В	238	ASN
1	В	241	ASN
1	В	259	GLN
1	В	344	GLN
1	В	346	ASN
1	В	419	ASN
1	В	424	ASN
1	В	483	ASN
1	В	520	ASN
1	С	128	GLN
1	C	157	GLN
1	С	159	GLN
1	С	167	ASN
1	С	174	GLN



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Mol	Chain	Res	Type
1	С	185	ASN
1	С	238	ASN
1	С	241	ASN
1	С	334	ASN
1	С	344	GLN
1	С	346	ASN
1	С	419	ASN
1	С	424	ASN
1	С	474	GLN
1	С	478	GLN
1	С	520	ASN
1	D	157	GLN
1	D	159	GLN
1	D	167	ASN
1	D	180	HIS
1	D	185	ASN
1	D	238	ASN
1	D	241	ASN
1	D	346	ASN
1	D	419	ASN
1	D	424	ASN
1	D	451	HIS
1	D	520	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)

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, 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	А	465/593~(78%)	-0.38	6 (1%) 77 84	9, 25, 46, 60	0
1	В	465/593~(78%)	-0.33	8 (1%) 70 78	11, 23, 50, 62	0
1	С	468/593~(78%)	-0.38	8 (1%) 70 78	9, 21, 43, 60	0
1	D	471/593~(79%)	-0.35	9 (1%) 66 75	10, 23, 44, 55	0
All	All	1869/2372~(78%)	-0.36	31 (1%) 70 78	9, 23, 47, 62	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	322	ALA	4.2
1	С	324	THR	4.2
1	D	551	VAL	4.0
1	С	325	GLY	3.4
1	D	54	ALA	3.4
1	С	545	TRP	3.1
1	С	551	VAL	3.0
1	А	546	HIS	3.0
1	В	303	LYS	3.0
1	В	317	ALA	2.9
1	D	73	SER	2.8
1	А	322	ALA	2.8
1	А	545	TRP	2.8
1	D	545	TRP	2.7
1	В	289	ALA	2.5
1	D	322	ALA	2.5
1	D	324	THR	2.3
1	D	321	PRO	2.3
1	В	323	ASP	2.3
1	В	324	THR	2.3
1	А	317	ALA	2.3



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Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	546	HIS	2.2
1	С	262	LEU	2.2
1	В	320	THR	2.2
1	А	321	PRO	2.2
1	В	326	ASP	2.2
1	А	323	ASP	2.1
1	В	288	SER	2.1
1	D	111	ARG	2.1
1	D	344	GLN	2.0
1	С	55	SER	2.0

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

