Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:51 AM GMT

PDB ID	:	3CDD
Title	:	Crystal structure of prophage MuSo2, 43 kDa tail protein from Shewanella oneidensis
Authors	:	Chang, C.; Evdokimova, E.; Kudritska, M.; Savchenko, A.; Edwards, A.M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2008-02-26
Resolution	:	2.10 Å(reported)

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

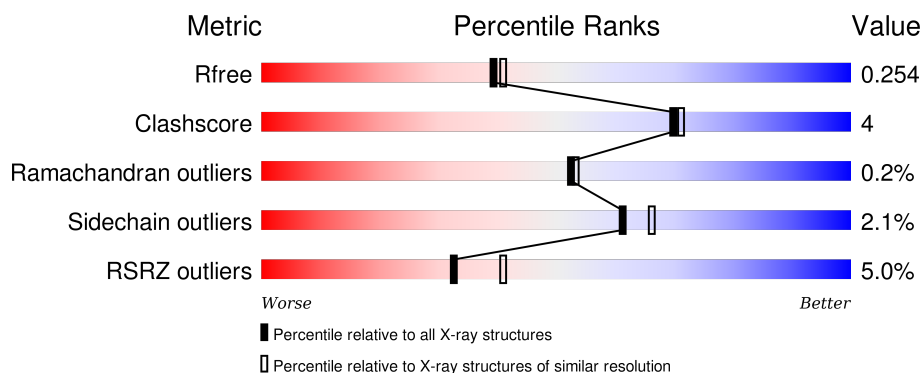|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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		0.254
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		2.1%
RSRZ outliers		5.0%

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$_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	361	6% / 79% / 10% • 9%
1	B	361	2% / 83% / 7% • 10%
1	C	361	2% / 80% / 10% •• 9%
1	D	361	6% / 78% / 12% • 8%
1	E	361	4% / 83% / 6% 11%

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Mol	Chain	Length	Quality of chain
1	F	361	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16250 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 Prophage MuSo2, 43 kDa tail protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	Se	1	8	0
			2539	1606	431	492	3	7			
1	B	326	Total	C	N	O	S	Se	0	5	0
			2517	1590	431	487	3	6			
1	C	328	Total	C	N	O	S	Se	2	6	0
			2546	1609	435	490	3	9			
1	D	331	Total	C	N	O	S	Se	1	4	0
			2540	1604	439	486	3	8			
1	E	322	Total	C	N	O	S	Se	1	8	0
			2508	1581	428	489	3	7			
1	F	325	Total	C	N	O	S	Se	0	4	0
			2510	1588	432	481	3	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	EXPRESSION TAG	UNP Q8EDP4
A	0	GLY	-	EXPRESSION TAG	UNP Q8EDP4
A	1	HIS	-	EXPRESSION TAG	UNP Q8EDP4
B	-1	GLN	-	EXPRESSION TAG	UNP Q8EDP4
B	0	GLY	-	EXPRESSION TAG	UNP Q8EDP4
B	1	HIS	-	EXPRESSION TAG	UNP Q8EDP4
C	-1	GLN	-	EXPRESSION TAG	UNP Q8EDP4
C	0	GLY	-	EXPRESSION TAG	UNP Q8EDP4
C	1	HIS	-	EXPRESSION TAG	UNP Q8EDP4
D	-1	GLN	-	EXPRESSION TAG	UNP Q8EDP4
D	0	GLY	-	EXPRESSION TAG	UNP Q8EDP4
D	1	HIS	-	EXPRESSION TAG	UNP Q8EDP4
E	-1	GLN	-	EXPRESSION TAG	UNP Q8EDP4
E	0	GLY	-	EXPRESSION TAG	UNP Q8EDP4
E	1	HIS	-	EXPRESSION TAG	UNP Q8EDP4
F	-1	GLN	-	EXPRESSION TAG	UNP Q8EDP4
F	0	GLY	-	EXPRESSION TAG	UNP Q8EDP4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	HIS	-	EXPRESSION TAG	UNP Q8EDP4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	225	Total 225	O 225	0	0
2	B	166	Total 166	O 166	0	0
2	C	174	Total 174	O 174	0	0
2	D	183	Total 183	O 183	0	0
2	E	199	Total 199	O 199	0	0
2	F	143	Total 143	O 143	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 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: Prophage MuSo2, 43 kDa tail protein

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Chain D:

6%

78% 12% • 8%

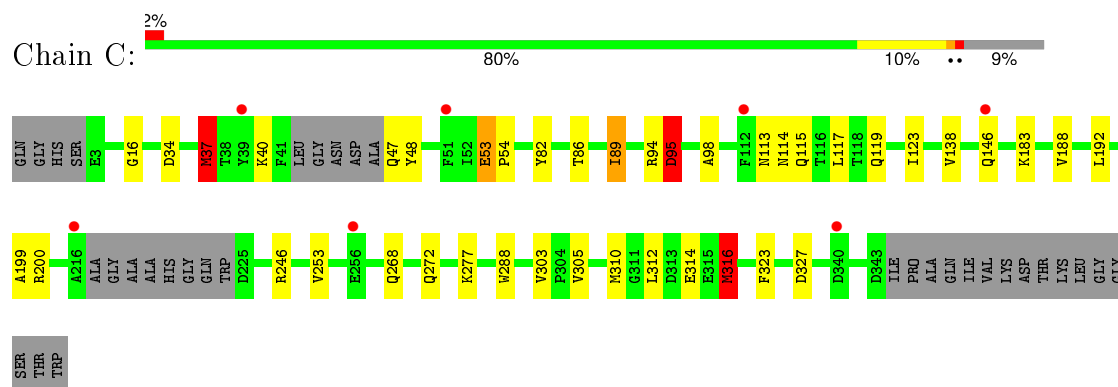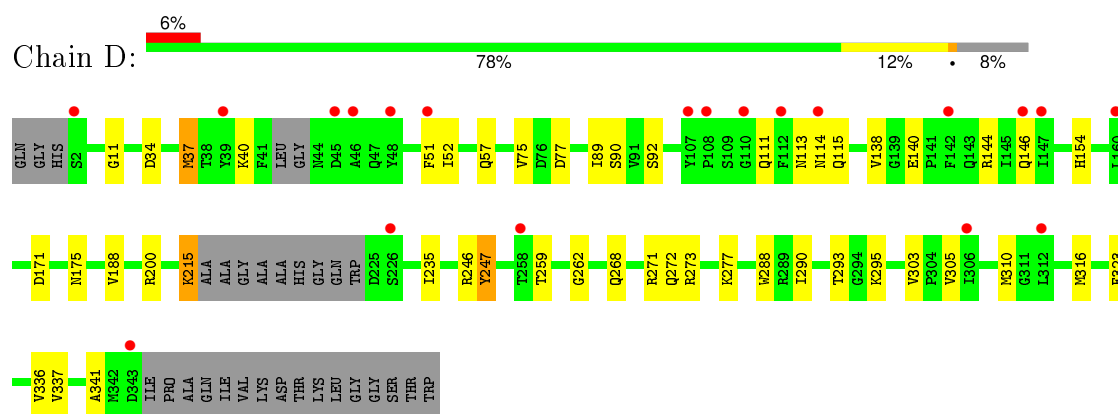GLN GLY HIS S2 G11 D34 M37 T38 Y39 K40 F41 LEU GLY N44 D45 A46 Q47 Y48 F51 I52 Q57 V75 D76 D77 I89 S90 V91 S92 Y107 P108 S109 G110 Q111 F112 N113 N114 Q115 V138 G139 E140 P141 F142 Q143 R144 I145 Q146 I147 H154 L160

D171 M175 V188 R200 K215 ALA ALA GLY ALA HIS GLY GLN TRP D225 S226 I235 R246 Y247 T258 T259 G262 Q268 R271 Q272 R273 K277 W288 R289 I290 T293 G294 K295 V303 P304 V305 I306 M310 G311 L312 M316 F323

V336 V337 A341 M342 D343 ILE PRO ALA GLN ILE VAL LYS ASP THR LYS LEU GLY GLY SER THR TRP

• Molecule 1: Prophage MuSo2, 43 kDa tail protein

Chain E:

4%

83% 6% 11%

GLN G0 H1 G16 D34 M37 K40 D45 K49 C61 T86 D106 P127 E148 K185 I191 S204 I214 K215 ALA ALA GLY ALA ALA HIS GLY GLN TRP ASP SER ALA GLY LEU PRO THR VAL GLY GLY ILE LYS ALA D238 V239 T240

Y247 R248 P249 I252 V253 E256 V257 G262 A263 A264 G267 Q268 W269 E270 S278 I306 E315 M316 A328 D343 ILE PRO ALA GLN ILE VAL LYS ASP THR LYS LEU GLY GLY SER THR TRP

• Molecule 1: Prophage MuSo2, 43 kDa tail protein

Chain F:

7%

79% 11% • 10%

GLN GLY HIS SER E3 E4 I5 V6 L7 I13 Y14 Q15 S30 M37 T38 Y39 K40 F41 LEU GLY N44 I65 V70 D77 W78 V79 S90 R94 D95 A98 Q111 L117 I120 I123 P127 K131 V138 I145 Q146 R206 Q207

I214 K215 A216 A217 GLY ALA ALA HIS GLY GLN TRP ASP SER ALA GLY LEU PRO THR VAL GLY G234 I235 K236 A237 R246 Y247 I252 V253 N254 E255 E256 V257 T258 T259 A260 E261 G262 A263 W269 Q272 R273 W288 M310 E314 R330 V337 M342 D343 I344 P345

ALA GLN ILE VAL LYS ASP THR LYS LEU GLY GLY SER THR TRP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.34Å 82.44Å 151.83Å 90.00° 100.20° 90.00°	Depositor
Resolution (Å)	47.69 – 2.10 47.69 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.6 (47.69-2.10) 96.6 (47.69-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.38 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.257 0.200 , 0.254	Depositor DCC
R_{free} test set	6655 reflections (5.29%)	DCC
Wilson B-factor (Å²)	36.5	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.29 , 36.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.33$	Xtriage
Outliers	0 of 132662 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16250	wwPDB-VP
Average B, all atoms (Å²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.62 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.0621e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.83	6/2590 (0.2%)	0.75	6/3497 (0.2%)
1	B	0.58	1/2564 (0.0%)	0.63	1/3464 (0.0%)
1	C	1.42	9/2585 (0.3%)	1.06	9/3487 (0.3%)
1	D	1.96	8/2576 (0.3%)	0.84	5/3477 (0.1%)
1	E	0.56	1/2555 (0.0%)	0.69	3/3450 (0.1%)
1	F	0.51	0/2553	0.62	1/3444 (0.0%)
All	All	1.12	25/15423 (0.2%)	0.78	25/20819 (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	C	1	1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	37[A]	MSE	SE-CE	53.91	5.13	1.95
1	D	37[B]	MSE	SE-CE	53.91	5.13	1.95
1	D	37[A]	MSE	CG-SE	-38.91	0.63	1.95
1	D	37[B]	MSE	CG-SE	-38.91	0.63	1.95
1	C	37[A]	MSE	CG-SE	-36.08	0.72	1.95
1	C	37[B]	MSE	CG-SE	-36.08	0.72	1.95
1	C	316[A]	MSE	SE-CE	-23.73	0.55	1.95
1	C	316[B]	MSE	SE-CE	-23.73	0.55	1.95
1	A	265	LYS	CE-NZ	21.46	2.02	1.49
1	A	265	LYS	CD-CE	15.85	1.90	1.51
1	C	316[A]	MSE	CG-SE	-12.43	1.53	1.95
1	C	316[B]	MSE	CG-SE	-12.43	1.53	1.95
1	C	37[A]	MSE	SE-CE	12.29	2.67	1.95
1	C	37[B]	MSE	SE-CE	12.29	2.67	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	GLY	N-CA	11.89	1.63	1.46
1	A	316[A]	MSE	CG-SE	-8.49	1.66	1.95
1	A	316[B]	MSE	CG-SE	-8.49	1.66	1.95
1	C	114	ASN	CG-ND2	7.85	1.52	1.32
1	E	61	CYS	CB-SG	-7.70	1.69	1.82
1	D	114	ASN	CG-ND2	6.37	1.48	1.32
1	A	61	CYS	CB-SG	-6.14	1.71	1.82
1	A	265	LYS	CG-CD	5.98	1.72	1.52
1	D	111	GLN	C-O	-5.43	1.13	1.23
1	D	115	GLN	CD-NE2	5.37	1.46	1.32
1	D	115	GLN	CD-OE1	5.12	1.35	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	316[A]	MSE	CG-SE-CE	27.48	159.37	98.90
1	C	316[B]	MSE	CG-SE-CE	27.48	159.37	98.90
1	D	37[A]	MSE	CB-CG-SE	18.60	168.51	112.70
1	D	37[B]	MSE	CB-CG-SE	18.60	168.51	112.70
1	C	37[A]	MSE	CB-CG-SE	17.70	165.79	112.70
1	C	37[B]	MSE	CB-CG-SE	17.70	165.79	112.70
1	D	37[A]	MSE	CG-SE-CE	10.32	121.61	98.90
1	D	37[B]	MSE	CG-SE-CE	10.32	121.61	98.90
1	C	316[A]	MSE	CB-CG-SE	10.19	143.27	112.70
1	C	316[B]	MSE	CB-CG-SE	10.19	143.27	112.70
1	A	316[A]	MSE	CG-SE-CE	10.05	121.01	98.90
1	A	316[B]	MSE	CG-SE-CE	10.05	121.01	98.90
1	E	316[A]	MSE	CG-SE-CE	8.44	117.46	98.90
1	E	316[B]	MSE	CG-SE-CE	8.44	117.46	98.90
1	A	265	LYS	CD-CE-NZ	-8.27	92.69	111.70
1	F	246	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	246	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	D	246	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	C	95	ASP	N-CA-C	6.54	128.64	111.00
1	A	246	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	265	LYS	CG-CD-CE	-6.09	93.63	111.90
1	E	37	MSE	CG-SE-CE	-5.96	85.78	98.90
1	A	345	PRO	N-CA-CB	5.77	110.22	103.30
1	C	37[A]	MSE	CG-SE-CE	5.28	110.51	98.90
1	C	37[B]	MSE	CG-SE-CE	5.28	110.51	98.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	95	ASP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	94	ARG	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	A	2539	0	2527	33	1
1	B	2517	0	2499	18	0
1	C	2546	0	2544	28	0
1	D	2540	0	2526	27	1
1	E	2508	0	2466	14	0
1	F	2510	0	2506	25	0
2	A	225	0	0	2	0
2	B	166	0	0	2	0
2	C	174	0	0	4	0
2	D	183	0	0	5	0
2	E	199	0	0	1	0
2	F	143	0	0	3	0
All	All	16250	0	15068	136	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 4.

All (136) 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:265:LYS:CD	1:A:265:LYS:CE	1.90	1.48
1:A:265:LYS:NZ	1:A:265:LYS:CE	2.02	1.22
1:D:316[B]:MSE:HE2	1:D:336:VAL:HG23	1.43	1.00
1:A:213[A]:THR:HG22	1:A:238:ASP:OD1	1.62	0.98
1:A:293[A]:THR:HG23	1:A:295:LYS:H	1.38	0.87
1:D:259:THR:HG22	1:D:262:GLY:H	1.46	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:THR:HB	1:F:262:GLY:H	1.49	0.76
1:A:265:LYS:CG	1:A:265:LYS:CE	2.65	0.74
1:A:112:PHE:CE1	1:A:147:ILE:HD11	2.21	0.73
1:A:269:TRP:HZ3	1:A:344:ILE:HD13	1.55	0.72
1:B:272:GLN:OE1	1:B:344:ILE:HA	1.89	0.71
1:D:293[A]:THR:HG21	2:D:403:HOH:O	1.91	0.70
1:C:312:LEU:HD13	1:C:316[A]:MSE:HE1	1.71	0.70
1:A:112:PHE:HE1	1:A:147:ILE:HD11	1.56	0.69
1:D:316[A]:MSE:HG3	1:D:337:VAL:O	1.91	0.69
1:A:290:ILE:HB	1:A:293[A]:THR:HG22	1.73	0.69
1:C:268:GLN:O	1:C:272:GLN:HG2	1.92	0.68
1:D:305:VAL:HG21	1:D:316[B]:MSE:HG3	1.76	0.67
1:A:269:TRP:CZ3	1:A:344:ILE:HD13	2.30	0.66
1:A:163:GLN:HA	1:A:347:GLN:H	1.60	0.66
1:C:314[A]:GLU:OE2	2:C:501:HOH:O	2.14	0.66
1:D:34[B]:ASP:OD1	1:D:92:SER:HB3	1.96	0.66
1:F:314:GLU:HG2	2:F:414:HOH:O	1.97	0.65
1:D:293[A]:THR:HG23	1:D:295:LYS:H	1.64	0.63
1:F:3:GLU:OE1	1:F:65:ILE:HG22	1.97	0.63
1:A:51:PHE:HD2	1:A:52:ILE:HG23	1.66	0.61
1:D:154:HIS:HD2	2:D:456:HOH:O	1.84	0.61
1:C:314[B]:GLU:HG2	1:C:316[B]:MSE:SE	2.51	0.60
1:A:290:ILE:HB	1:A:293[A]:THR:CG2	2.31	0.60
1:B:8:LYS:HG2	1:B:13:ILE:HG13	1.84	0.59
1:A:269:TRP:HZ2	1:A:273:ARG:HH21	1.50	0.59
1:A:269:TRP:HE3	1:A:344:ILE:HG21	1.67	0.59
1:A:52:ILE:HD11	1:A:89:ILE:HD13	1.83	0.58
1:F:37:MSE:HG2	2:F:480:HOH:O	2.03	0.58
1:F:3:GLU:HB3	1:F:330:ARG:HH12	1.67	0.58
1:C:200:ARG:C	1:C:310:MSE:HE1	2.25	0.57
1:E:185:LYS:NZ	1:E:315:GLU:OE2	2.37	0.57
1:C:183:LYS:HE2	2:C:545:HOH:O	2.04	0.57
1:F:272:GLN:NE2	2:F:458:HOH:O	2.38	0.57
1:B:302:LEU:HB3	1:B:315:GLU:HG2	1.87	0.56
1:F:5:ILE:HD12	1:F:5:ILE:N	2.20	0.56
1:E:16:GLY:O	1:E:37:MSE:HE1	2.06	0.56
1:C:146:GLN:HB2	2:C:546:HOH:O	2.05	0.56
1:F:6:VAL:HG22	1:F:15:GLN:HG3	1.88	0.56
1:D:305:VAL:CG2	1:D:316[B]:MSE:HG3	2.35	0.56
1:A:293[A]:THR:HG21	2:A:459:HOH:O	2.06	0.56
1:D:144:ARG:HH22	1:D:146:GLN:HB2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206[B]:ARG:NH1	1:F:207:GLN:HE21	2.04	0.55
1:D:268:GLN:OE1	1:D:271:ARG:NH2	2.40	0.54
1:A:316[B]:MSE:HE3	1:A:336:VAL:HG23	1.89	0.54
1:B:149:GLN:HG2	1:C:253:VAL:HG11	1.89	0.54
1:E:45:ASP:OD2	1:E:49:LYS:HE2	2.09	0.53
1:D:290:ILE:HB	1:D:293[A]:THR:HG22	1.90	0.53
1:D:171:ASP:OD2	1:D:175:ASN:HB2	2.09	0.53
1:C:188:VAL:O	1:C:303:VAL:HG23	2.09	0.53
1:F:269:TRP:CH2	1:F:273:ARG:HD2	2.43	0.53
1:B:149:GLN:HE21	1:C:253:VAL:HG21	1.74	0.52
1:C:53:GLU:HG3	1:C:54:PRO:HD2	1.91	0.52
1:C:117:LEU:HB3	1:C:138:VAL:HG13	1.91	0.52
1:B:17:TRP:CE3	1:B:37:MSE:HG3	2.45	0.52
1:F:65:ILE:HD12	1:F:70:VAL:HG11	1.92	0.52
1:D:34[B]:ASP:OD1	1:D:92:SER:CB	2.58	0.51
1:D:268:GLN:O	1:D:272:GLN:HG2	2.11	0.51
1:C:117:LEU:HB3	1:C:138:VAL:CG1	2.41	0.50
1:A:191:ILE:HB	1:A:194[A]:ASP:HB3	1.92	0.50
1:D:247:TYR:CE2	1:F:127:PRO:HB2	2.47	0.50
1:E:252:ILE:HD13	1:E:270:GLU:HG2	1.93	0.50
1:F:79:VAL:HB	1:F:90:SER:HB3	1.94	0.50
1:F:5:ILE:HD11	1:F:288:TRP:CZ3	2.48	0.48
1:D:51:PHE:CD2	1:D:52:ILE:HG12	2.49	0.48
1:D:288:TRP:CE2	1:D:323:PHE:HB3	2.49	0.48
1:C:288:TRP:CE2	1:C:323:PHE:HB3	2.47	0.48
1:F:111:GLN:HG2	1:F:146:GLN:HG3	1.96	0.48
1:C:305:VAL:CG2	1:C:316[A]:MSE:HG3	2.43	0.47
1:B:37:MSE:HG2	2:B:364:HOH:O	2.13	0.47
1:E:252:ILE:CD1	1:E:270:GLU:HG2	2.45	0.47
1:E:191:ILE:HG12	1:E:306:ILE:HD12	1.95	0.47
1:E:16:GLY:O	1:E:37:MSE:CE	2.63	0.47
1:B:82:TYR:CZ	1:C:192:LEU:HD13	2.50	0.47
1:C:119:GLN:O	1:C:123:ILE:HG12	2.15	0.47
1:D:57:GLN:HA	1:D:75:VAL:HG12	1.96	0.47
1:A:312:LEU:HD13	1:A:316[B]:MSE:HE2	1.97	0.46
1:C:253:VAL:HG23	1:C:253:VAL:O	2.16	0.46
1:A:290:ILE:CG2	1:A:293[A]:THR:HG22	2.46	0.46
1:E:1:HIS:CE1	2:E:528:HOH:O	2.68	0.46
1:C:98:ALA:HB3	2:C:570:HOH:O	2.16	0.46
1:A:290:ILE:CB	1:A:293[A]:THR:HG22	2.43	0.46
1:B:82:TYR:CZ	1:C:199:ALA:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLY:O	1:C:37[B]:MSE:SE	2.85	0.45
1:D:113:ASN:HB2	2:D:430:HOH:O	2.17	0.45
1:A:188:VAL:O	1:A:303:VAL:HG23	2.17	0.44
1:A:106:ASP:HB3	2:A:509:HOH:O	2.17	0.44
1:A:191:ILE:HB	1:A:194[B]:ASP:HB2	1.99	0.44
1:C:40:LYS:HG2	1:C:86:THR:HG22	1.99	0.44
1:D:154:HIS:HE1	2:D:516:HOH:O	2.00	0.44
1:E:40:LYS:HE2	1:E:86:THR:HG23	1.99	0.44
1:F:214:ILE:HD13	1:F:252:ILE:HB	2.00	0.44
1:A:199:ALA:HB3	1:C:82:TYR:CZ	2.53	0.44
1:E:204:SER:O	1:E:278[A]:SER:HB3	2.18	0.44
1:B:200:ARG:HE	1:B:282:GLU:CD	2.22	0.44
1:F:30:SER:HB2	1:F:95:ASP:HB2	1.99	0.43
1:F:206[B]:ARG:HG2	1:F:207:GLN:HG3	2.00	0.43
1:B:65:ILE:HD12	1:B:70[B]:VAL:HG11	2.00	0.43
1:B:344:ILE:HA	1:B:345:PRO:HD3	1.82	0.43
1:B:74:TYR:CZ	1:C:246:ARG:HD2	2.54	0.43
1:F:117:LEU:HB3	1:F:138:VAL:HG13	2.00	0.43
1:A:46:ALA:O	1:A:87:ILE:HD11	2.19	0.42
1:F:337:VAL:HG21	1:F:342:MSE:HG2	2.02	0.42
1:D:200:ARG:C	1:D:310:MSE:HE1	2.40	0.42
1:C:47:GLN:HG2	1:C:48:TYR:CD2	2.55	0.42
1:F:39:TYR:HB3	1:F:41:PHE:CZ	2.54	0.42
1:A:288:TRP:CE2	1:A:323:PHE:HB3	2.54	0.42
1:C:113:ASN:O	1:C:115:GLN:HG2	2.20	0.42
1:C:37[A]:MSE:HG3	1:C:37[A]:MSE:O	2.19	0.42
1:A:22:ILE:HD11	1:A:63:VAL:HG11	2.02	0.42
1:E:204:SER:O	1:E:278[B]:SER:HB2	2.19	0.42
1:D:215:LYS:HG2	1:D:235:ILE:O	2.20	0.42
1:D:188:VAL:O	1:D:303:VAL:HG23	2.20	0.41
1:B:15:GLN:O	1:B:37:MSE:HE2	2.20	0.41
1:A:35:LEU:O	1:A:90:SER:HB2	2.21	0.41
1:B:207:GLN:NE2	2:B:514:HOH:O	2.54	0.41
1:D:316[B]:MSE:HE2	1:D:336:VAL:CG2	2.32	0.41
1:E:106:ASP:CG	1:F:247:TYR:HH	2.24	0.41
1:B:320:SER:HB3	1:B:335[A]:SER:HB3	2.03	0.41
1:D:89:ILE:O	1:D:89:ILE:HG13	2.21	0.41
1:A:265:LYS:CD	1:A:265:LYS:NZ	2.84	0.41
1:D:337:VAL:HG12	2:D:537:HOH:O	2.21	0.41
1:F:94:ARG:CZ	1:F:98:ALA:HB1	2.51	0.41
1:C:89:ILE:O	1:C:89:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:TYR:CZ	1:E:249:PRO:HG3	2.56	0.41
1:F:6:VAL:HG13	1:F:13:ILE:HG23	2.02	0.41
1:E:127:PRO:HB2	1:F:247:TYR:CE2	2.57	0.40
1:A:53:GLU:HG3	1:A:54:PRO:HD2	2.04	0.40
1:A:272:GLN:HA	1:A:272:GLN:NE2	2.34	0.40
1:B:70[A]:VAL:HG13	1:B:71:ILE:HG12	2.03	0.40
1:B:77:ASP:OD2	1:B:92:SER:OG	2.39	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)
1:A:327:ASP:OD2	1:D:11:GLY:N[2_746]	2.16	0.04

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	330/361 (91%)	314 (95%)	15 (4%)	1 (0%)	46	45
1	B	327/361 (91%)	314 (96%)	13 (4%)	0	100	100
1	C	328/361 (91%)	311 (95%)	16 (5%)	1 (0%)	46	45
1	D	329/361 (91%)	314 (95%)	13 (4%)	2 (1%)	30	24
1	E	326/361 (90%)	308 (94%)	18 (6%)	0	100	100
1	F	323/361 (90%)	313 (97%)	10 (3%)	0	100	100
All	All	1963/2166 (91%)	1874 (96%)	85 (4%)	4 (0%)	52	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	PRO

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Mol	Chain	Res	Type
1	C	95	ASP
1	D	247	TYR
1	D	341	ALA

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	270/290 (93%)	266 (98%)	4 (2%)	72	78
1	B	267/290 (92%)	263 (98%)	4 (2%)	72	78
1	C	271/290 (93%)	261 (96%)	10 (4%)	41	41
1	D	266/290 (92%)	256 (96%)	10 (4%)	40	40
1	E	266/290 (92%)	262 (98%)	4 (2%)	72	78
1	F	265/290 (91%)	259 (98%)	6 (2%)	58	62
All	All	1605/1740 (92%)	1567 (98%)	38 (2%)	61	61

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASP
1	A	215	LYS
1	A	272	GLN
1	A	344	ILE
1	B	149	GLN
1	B	240[A]	THR
1	B	240[B]	THR
1	B	272	GLN
1	C	34	ASP
1	C	37[A]	MSE
1	C	37[B]	MSE
1	C	53	GLU
1	C	89	ILE
1	C	95	ASP
1	C	277	LYS

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Mol	Chain	Res	Type
1	C	316[A]	MSE
1	C	316[B]	MSE
1	C	327	ASP
1	D	37[A]	MSE
1	D	37[B]	MSE
1	D	40	LYS
1	D	77	ASP
1	D	90	SER
1	D	138	VAL
1	D	140	GLU
1	D	215	LYS
1	D	273	ARG
1	D	277	LYS
1	E	34[A]	ASP
1	E	34[B]	ASP
1	E	148	GLU
1	E	238	ASP
1	F	15	GLN
1	F	77	ASP
1	F	236	LYS
1	F	259	THR
1	F	310	MSE
1	F	343	ASP

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

Mol	Chain	Res	Type
1	A	272	GLN
1	B	47	GLN
1	B	149	GLN
1	D	154	HIS
1	F	207	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 (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	322/361 (89%)	0.58	21 (6%)	22	29	25, 32, 43, 70	0
1	B	320/361 (88%)	0.39	7 (2%)	65	71	25, 34, 42, 55	0
1	C	322/361 (89%)	0.35	7 (2%)	65	71	16, 31, 42, 58	0
1	D	325/361 (90%)	0.57	20 (6%)	24	32	15, 32, 49, 57	0
1	E	316/361 (87%)	0.59	16 (5%)	32	40	26, 32, 51, 61	0
1	F	319/361 (88%)	0.52	25 (7%)	16	22	26, 34, 44, 58	0
All	All	1924/2166 (88%)	0.50	96 (4%)	32	41	15, 33, 46, 70	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	217	ALA	13.5
1	A	348	ILE	6.8
1	A	344	ILE	6.6
1	E	262	GLY	6.0
1	B	258	THR	5.5
1	F	234	GLY	5.4
1	A	345	PRO	5.3
1	E	343	ASP	5.1
1	F	216	ALA	4.8
1	F	263	ALA	4.8
1	E	1	HIS	4.6
1	E	239	VAL	4.5
1	F	235	ILE	4.5
1	E	263	ALA	4.5
1	A	347	GLN	4.4
1	E	0	GLY	4.4
1	E	267	GLY	4.3
1	A	239	VAL	4.2
1	D	51	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	252	ILE	3.8
1	A	341	ALA	3.7
1	D	2	SER	3.7
1	E	269	TRP	3.6
1	E	256	GLU	3.6
1	F	256	GLU	3.6
1	A	149	GLN	3.5
1	A	346	ALA	3.5
1	A	256	GLU	3.5
1	E	214	ILE	3.4
1	D	146	GLN	3.3
1	E	264	ALA	3.3
1	A	257	VAL	3.3
1	A	343	ASP	3.3
1	F	145	ILE	3.2
1	A	253	VAL	3.2
1	D	112	PHE	3.2
1	F	41	PHE	3.2
1	F	260	ALA	3.2
1	A	263	ALA	3.1
1	A	269	TRP	3.1
1	C	51	PHE	3.1
1	A	214	ILE	3.0
1	F	258	THR	2.9
1	F	214	ILE	2.9
1	D	343	ASP	2.9
1	A	237	ALA	2.9
1	E	257	VAL	2.8
1	D	147	ILE	2.8
1	D	160	LEU	2.8
1	C	216	ALA	2.8
1	A	216	ALA	2.7
1	B	259	THR	2.7
1	F	253	VAL	2.7
1	D	107	TYR	2.7
1	D	226	SER	2.7
1	B	234	GLY	2.6
1	F	255	GLU	2.6
1	A	217	ALA	2.6
1	B	253	VAL	2.6
1	C	340	ASP	2.6
1	B	263	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	45	ASP	2.5
1	F	7	LEU	2.5
1	F	131	LYS	2.5
1	F	252	ILE	2.5
1	A	262	GLY	2.5
1	B	257	VAL	2.4
1	D	142	PHE	2.4
1	E	240	THR	2.4
1	F	262	GLY	2.4
1	F	237	ALA	2.4
1	E	253	VAL	2.4
1	F	120	ILE	2.4
1	D	108	PRO	2.3
1	B	143	GLN	2.3
1	D	39	TYR	2.3
1	D	46	ALA	2.3
1	F	344	ILE	2.3
1	D	110	GLY	2.2
1	C	112	PHE	2.2
1	D	114	ASN	2.2
1	C	256	GLU	2.2
1	E	328	ALA	2.2
1	D	306	ILE	2.2
1	F	215	LYS	2.1
1	A	2	SER	2.1
1	A	255	GLU	2.1
1	D	312	LEU	2.1
1	C	39	TYR	2.1
1	D	48	TYR	2.1
1	D	258	THR	2.0
1	F	254	ASN	2.0
1	F	123	ILE	2.0
1	C	146	GLN	2.0
1	F	39	TYR	2.0
1	F	343	ASP	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.