



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:10 am GMT

PDB ID : 2DB0  
Title : Crystal structure of PH0542  
Authors : Nishino, A.; Handa, N.; Kishishita, S.; Murayama, K.; Shirouzu, M.; RIKEN  
Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-12-14  
Resolution : 2.20 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](mailto: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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

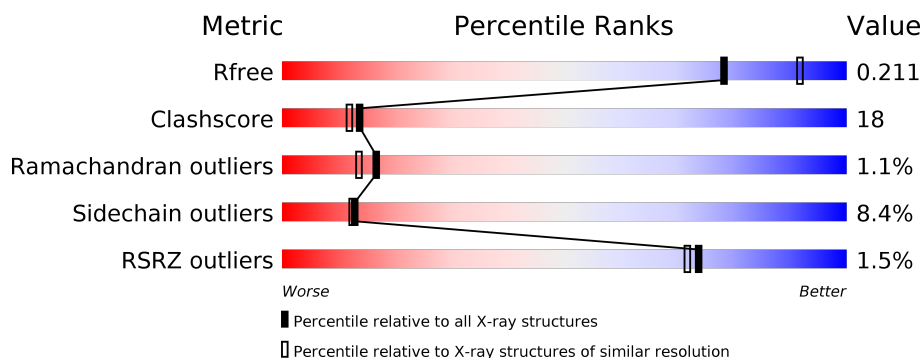
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	253	<div> <div> <div></div> <div>47%</div> <div>38%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	253	<div> <div> <div></div> <div>40%</div> <div>43%</div> <div>10%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3908 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 253aa long hypothetical protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1899	1221	316	352	10			
1	B	240	Total	C	N	O	S	0	0	0
			1908	1226	317	355	10			

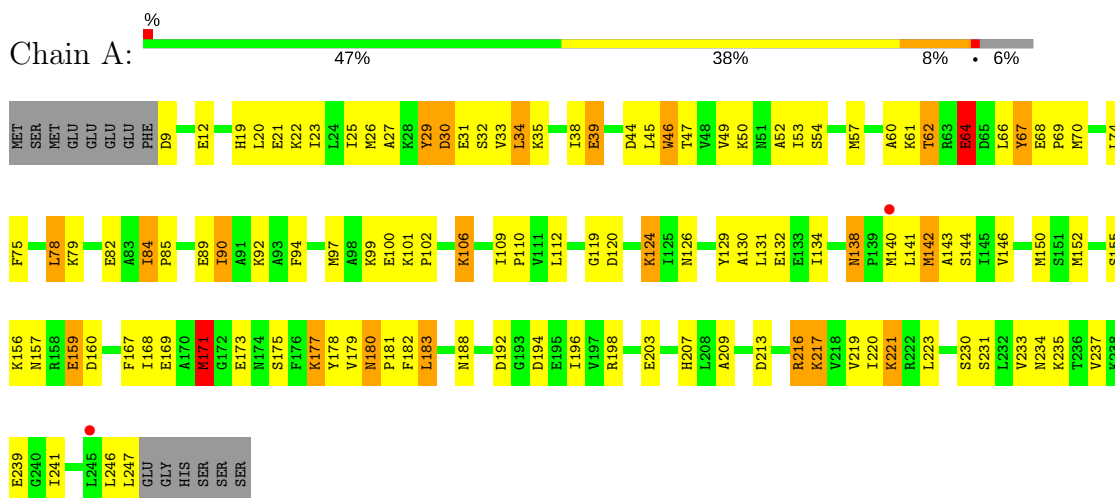
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	43	Total	O	0	0
			43	43		

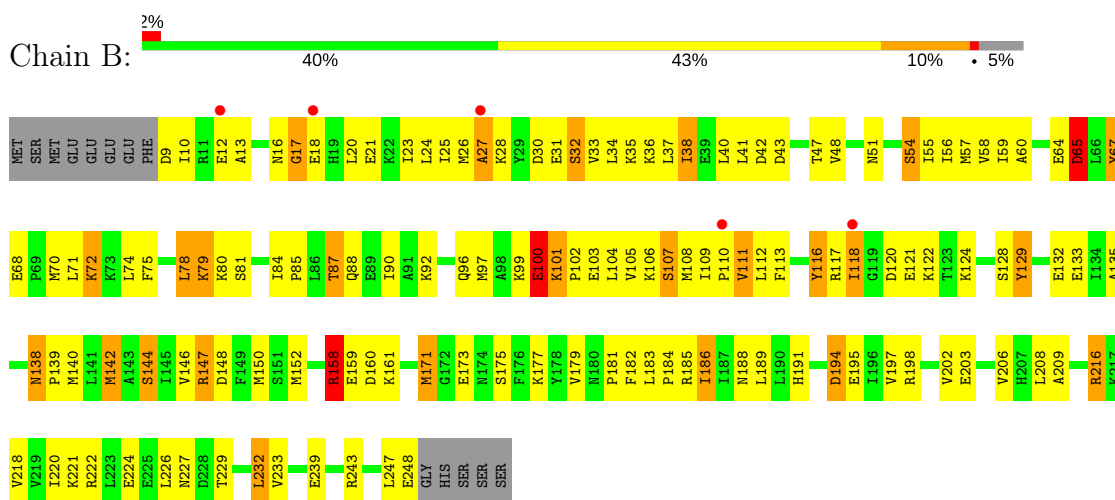
### 3 Residue-property plots

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: 253aa long hypothetical protein



- Molecule 1: 253aa long hypothetical protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.80Å 90.78Å 66.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 66.45 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.20) 98.9 (66.45-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.73 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.205 , 0.268 0.214 , 0.211	Depositor DCC
$R_{free}$ test set	1237 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3908	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 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	A	2.04	52/1922 (2.7%)	1.46	20/2586 (0.8%)
1	B	2.01	50/1931 (2.6%)	1.58	27/2598 (1.0%)
All	All	2.03	102/3853 (2.6%)	1.52	47/5184 (0.9%)

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	MET	SD-CE	-10.09	1.21	1.77
1	A	46	TRP	CB-CG	-9.34	1.33	1.50
1	B	121	GLU	CD-OE1	9.19	1.35	1.25
1	A	124	LYS	CE-NZ	9.15	1.72	1.49
1	B	103	GLU	CD-OE1	-8.73	1.16	1.25
1	B	129	TYR	CD2-CE2	8.69	1.52	1.39
1	B	48	VAL	CB-CG1	8.52	1.70	1.52
1	A	39	GLU	CD-OE1	8.44	1.34	1.25
1	B	100	GLU	CD-OE2	-8.39	1.16	1.25
1	A	64	GLU	CD-OE1	8.36	1.34	1.25
1	B	188	ASN	CG-ND2	7.94	1.52	1.32
1	B	111	VAL	CB-CG2	7.62	1.68	1.52
1	B	122	LYS	CD-CE	7.62	1.70	1.51
1	B	218	VAL	CB-CG1	7.56	1.68	1.52
1	A	167	PHE	CD2-CE2	-7.55	1.24	1.39
1	A	130	ALA	C-O	-7.48	1.09	1.23
1	A	89	GLU	CD-OE2	7.33	1.33	1.25
1	A	64	GLU	CD-OE2	7.30	1.33	1.25
1	B	38	ILE	CB-CG2	7.14	1.75	1.52
1	A	52	ALA	CA-CB	7.09	1.67	1.52
1	A	49	VAL	CB-CG1	7.01	1.67	1.52
1	A	92	LYS	CE-NZ	6.94	1.66	1.49
1	A	169	GLU	C-O	-6.87	1.10	1.23
1	B	116	TYR	CE2-CZ	6.84	1.47	1.38
1	A	97	MET	SD-CE	-6.74	1.40	1.77
1	B	27	ALA	CA-CB	6.68	1.66	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	ALA	CA-CB	6.49	1.66	1.52
1	B	133	GLU	CD-OE1	6.49	1.32	1.25
1	A	106	LYS	CE-NZ	-6.49	1.32	1.49
1	A	50	LYS	CB-CG	6.44	1.70	1.52
1	A	29	TYR	CD2-CE2	6.40	1.49	1.39
1	B	96	GLN	C-O	6.33	1.35	1.23
1	A	92	LYS	CD-CE	6.29	1.67	1.51
1	A	142	MET	CB-CG	6.28	1.71	1.51
1	A	54	SER	CA-CB	6.28	1.62	1.52
1	A	84	ILE	CB-CG2	6.25	1.72	1.52
1	A	173	GLU	CG-CD	6.22	1.61	1.51
1	B	233	VAL	CB-CG2	-6.22	1.39	1.52
1	A	156	LYS	CD-CE	6.19	1.66	1.51
1	A	35	LYS	CB-CG	6.18	1.69	1.52
1	A	21	GLU	CG-CD	6.17	1.61	1.51
1	B	209	ALA	CA-CB	-6.16	1.39	1.52
1	A	142	MET	SD-CE	-6.13	1.43	1.77
1	A	120	ASP	C-O	6.12	1.34	1.23
1	B	161	LYS	CD-CE	-6.07	1.36	1.51
1	B	147	ARG	CG-CD	6.07	1.67	1.51
1	B	181	PRO	CG-CD	6.04	1.70	1.50
1	A	78	LEU	CG-CD2	-6.01	1.29	1.51
1	B	160	ASP	CB-CG	6.00	1.64	1.51
1	A	167	PHE	CE2-CZ	5.96	1.48	1.37
1	A	134	ILE	CA-CB	-5.93	1.41	1.54
1	A	82	GLU	CD-OE1	-5.92	1.19	1.25
1	A	35	LYS	CD-CE	5.88	1.66	1.51
1	A	82	GLU	CA-CB	5.87	1.66	1.53
1	A	23	ILE	CA-CB	-5.86	1.41	1.54
1	A	61	LYS	CD-CE	5.80	1.65	1.51
1	B	79	LYS	CE-NZ	5.79	1.63	1.49
1	B	173	GLU	CD-OE2	5.79	1.32	1.25
1	A	90	ILE	CA-CB	-5.78	1.41	1.54
1	A	171	MET	CG-SD	-5.74	1.66	1.81
1	B	78	LEU	C-O	5.74	1.34	1.23
1	B	159	GLU	CD-OE1	5.74	1.31	1.25
1	B	92	LYS	CD-CE	5.71	1.65	1.51
1	A	179	VAL	CB-CG1	-5.69	1.41	1.52
1	B	68	GLU	CG-CD	5.69	1.60	1.51
1	B	80	LYS	CD-CE	5.68	1.65	1.51
1	A	49	VAL	CA-CB	-5.67	1.42	1.54
1	A	159	GLU	CD-OE2	5.67	1.31	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	GLU	CD-OE1	5.67	1.31	1.25
1	A	57	MET	CB-CG	5.67	1.69	1.51
1	A	67	TYR	CG-CD2	5.60	1.46	1.39
1	B	135	ALA	CA-CB	5.60	1.64	1.52
1	B	221	LYS	CD-CE	5.59	1.65	1.51
1	B	60	ALA	CA-CB	5.58	1.64	1.52
1	B	129	TYR	CE2-CZ	5.57	1.45	1.38
1	A	198	ARG	C-O	-5.56	1.12	1.23
1	B	152	MET	SD-CE	-5.56	1.46	1.77
1	A	196	ILE	C-O	-5.56	1.12	1.23
1	B	54	SER	CB-OG	5.53	1.49	1.42
1	B	186	ILE	CA-CB	-5.50	1.42	1.54
1	B	140	MET	CG-SD	5.49	1.95	1.81
1	A	196	ILE	CA-CB	5.48	1.67	1.54
1	B	146	VAL	CB-CG1	-5.46	1.41	1.52
1	B	239	GLU	CG-CD	5.43	1.60	1.51
1	A	38	ILE	CA-CB	-5.39	1.42	1.54
1	B	28	LYS	CD-CE	5.35	1.64	1.51
1	A	53	ILE	CA-CB	5.34	1.67	1.54
1	B	67	TYR	CZ-OH	5.32	1.46	1.37
1	A	152	MET	CB-CG	5.30	1.68	1.51
1	A	94	PHE	CE2-CZ	5.28	1.47	1.37
1	A	129	TYR	CE2-CZ	-5.26	1.31	1.38
1	B	118	ILE	C-O	5.21	1.33	1.23
1	B	88	GLN	C-O	-5.15	1.13	1.23
1	B	36	LYS	CE-NZ	5.13	1.61	1.49
1	B	129	TYR	CD1-CE1	5.13	1.47	1.39
1	B	203	GLU	C-O	-5.11	1.13	1.23
1	B	229	THR	CB-CG2	5.11	1.69	1.52
1	A	39	GLU	CD-OE2	5.08	1.31	1.25
1	B	191	HIS	CA-CB	5.06	1.65	1.53
1	B	195	GLU	CB-CG	5.06	1.61	1.52
1	B	107	SER	CB-OG	5.05	1.48	1.42
1	A	132	GLU	CD-OE1	-5.03	1.20	1.25

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	ARG	NE-CZ-NH2	-17.58	111.51	120.30
1	B	222	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	B	216	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A	194	ASP	CB-CG-OD1	8.41	125.87	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	ASP	CB-CG-OD2	8.21	125.69	118.30
1	B	222	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	A	192	ASP	CB-CG-OD2	7.83	125.35	118.30
1	B	147	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	42	ASP	CB-CG-OD2	7.68	125.21	118.30
1	A	30	ASP	CB-CG-OD2	7.23	124.81	118.30
1	B	158	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	44	ASP	CB-CG-OD2	7.05	124.65	118.30
1	B	65	ASP	CB-CG-OD2	7.01	124.61	118.30
1	A	194	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	B	42	ASP	CB-CG-OD1	-6.78	112.20	118.30
1	B	117	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	232	LEU	CB-CG-CD2	6.68	122.35	111.00
1	A	92	LYS	CD-CE-NZ	6.67	127.05	111.70
1	A	216	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	229	THR	OG1-CB-CG2	-6.62	94.77	110.00
1	B	226	LEU	CA-CB-CG	6.57	130.42	115.30
1	A	198	ARG	NE-CZ-NH2	6.43	123.51	120.30
1	A	99	LYS	CD-CE-NZ	6.35	126.31	111.70
1	A	246	LEU	CB-CG-CD1	6.29	121.69	111.00
1	A	9	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	9	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	57	MET	CG-SD-CE	-5.90	90.76	100.20
1	A	203	GLU	OE1-CD-OE2	-5.88	116.24	123.30
1	A	9	ASP	OD1-CG-OD2	-5.86	112.18	123.30
1	B	79	LYS	CD-CE-NZ	5.83	125.11	111.70
1	B	152	MET	CA-CB-CG	5.79	123.13	113.30
1	B	177	LYS	CD-CE-NZ	5.74	124.90	111.70
1	A	140	MET	CG-SD-CE	5.68	109.30	100.20
1	A	171	MET	CA-CB-CG	5.59	122.80	113.30
1	B	218	VAL	CA-CB-CG1	5.50	119.15	110.90
1	B	198	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	185	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	120	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	62	THR	CA-CB-CG2	-5.41	104.83	112.40
1	B	26	MET	CA-CB-CG	5.41	122.49	113.30
1	A	34	LEU	CB-CG-CD1	5.38	120.14	111.00
1	B	171	MET	CA-CB-CG	5.32	122.34	113.30
1	B	208	LEU	CB-CG-CD2	-5.25	102.07	111.00
1	B	74	LEU	CB-CG-CD1	5.19	119.82	111.00
1	A	131	LEU	CB-CG-CD1	-5.15	102.24	111.00
1	A	26	MET	CA-CB-CG	5.11	121.98	113.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	197	VAL	CG1-CB-CG2	-5.06	102.80	110.90

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	A	1899	0	2019	59	0
1	B	1908	0	2025	82	0
2	A	58	0	0	1	0
2	B	43	0	0	1	0
All	All	3908	0	4044	140	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 18.

All (140) 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:B:38:ILE:CG2	1:B:38:ILE:CB	1.75	1.63
1:A:124:LYS:CE	1:A:124:LYS:NZ	1.71	1.50
1:B:142:MET:SD	1:B:142:MET:CE	1.21	1.30
1:A:64:GLU:HG3	1:A:101:LYS:NZ	1.53	1.23
1:B:142:MET:HE3	1:B:142:MET:SD	1.78	1.17
1:B:142:MET:SD	1:B:142:MET:HE2	1.78	1.16
1:B:142:MET:SD	1:B:142:MET:HE1	1.78	1.11
1:B:216:ARG:HD2	1:B:248:GLU:OE2	1.59	1.01
1:B:142:MET:CG	1:B:142:MET:CE	2.38	1.00
1:A:217:LYS:O	1:A:221:LYS:HE2	1.64	0.96
1:B:10:ILE:HG23	1:B:23:ILE:HD12	1.46	0.93
1:A:64:GLU:CG	1:A:101:LYS:NZ	2.34	0.90
1:B:30:ASP:OD2	1:B:32:SER:HB2	1.75	0.86
1:B:9:ASP:OD2	1:B:12:GLU:HG3	1.78	0.84
1:A:64:GLU:HG3	1:A:101:LYS:HZ3	1.43	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HG3	1:A:101:LYS:HZ2	1.40	0.83
1:A:177:LYS:H	1:A:177:LYS:HZ3	1.31	0.78
1:A:216:ARG:HD3	2:A:302:HOH:O	1.83	0.77
1:B:106:LYS:HE2	1:B:148:ASP:OD2	1.84	0.76
1:B:10:ILE:HG23	1:B:23:ILE:CD1	2.17	0.74
1:B:81:SER:OG	1:B:87:THR:HG22	1.89	0.72
1:B:21:GLU:O	1:B:25:ILE:HG12	1.90	0.72
1:B:56:ILE:HD13	1:B:70:MET:HE1	1.71	0.71
1:B:56:ILE:HG21	1:B:70:MET:HE3	1.74	0.69
1:A:177:LYS:H	1:A:177:LYS:NZ	1.90	0.69
1:B:13:ALA:HB1	2:B:282:HOH:O	1.94	0.67
1:B:18:GLU:HA	1:B:20:LEU:CD1	2.24	0.67
1:B:158:ARG:HD2	1:B:194:ASP:OD1	1.94	0.67
1:B:38:ILE:CG2	1:B:38:ILE:CG1	2.71	0.66
1:B:38:ILE:O	1:B:41:LEU:HD13	1.96	0.66
1:B:38:ILE:CG2	1:B:38:ILE:CA	2.71	0.65
1:B:41:LEU:HD12	1:B:41:LEU:N	2.11	0.65
1:A:19:HIS:O	1:A:22:LYS:HB3	1.95	0.65
1:A:171:MET:HE2	1:A:171:MET:HA	1.79	0.65
1:B:118:ILE:HD11	1:B:124:LYS:HG3	1.80	0.63
1:B:150:MET:HG3	1:B:182:PHE:CD2	2.34	0.63
1:A:101:LYS:N	1:A:102:PRO:HD3	2.16	0.61
1:A:157:ASN:HD22	1:A:160:ASP:CG	2.02	0.61
1:B:37:LEU:O	1:B:41:LEU:CD1	2.48	0.61
1:B:9:ASP:OD2	1:B:12:GLU:CG	2.50	0.59
1:B:41:LEU:CD1	1:B:41:LEU:H	2.15	0.59
1:A:78:LEU:HD13	1:A:90:ILE:HG21	1.83	0.59
1:A:171:MET:HA	1:A:171:MET:CE	2.32	0.59
1:A:188:ASN:HD21	1:B:102:PRO:HD2	1.66	0.58
1:A:64:GLU:CG	1:A:101:LYS:HZ1	2.14	0.58
1:B:27:ALA:HA	1:B:33:VAL:HG23	1.84	0.58
1:B:78:LEU:HB2	1:B:90:ILE:HG21	1.85	0.57
1:B:64:GLU:OE1	1:B:101:LYS:NZ	2.34	0.57
1:B:183:LEU:HB3	1:B:184:PRO:HD3	1.87	0.57
1:B:109:ILE:HB	1:B:110:PRO:HD3	1.87	0.57
1:B:27:ALA:HA	1:B:33:VAL:CG2	2.35	0.56
1:A:138:ASN:ND2	1:A:141:LEU:H	2.04	0.56
1:B:105:VAL:O	1:B:109:ILE:HG12	2.05	0.56
1:A:27:ALA:HA	1:A:33:VAL:HB	1.88	0.56
1:B:41:LEU:N	1:B:41:LEU:CD1	2.69	0.56
1:B:138:ASN:HD22	1:B:138:ASN:C	2.08	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:HZ3	1:A:177:LYS:N	2.02	0.55
1:B:18:GLU:HA	1:B:20:LEU:HD12	1.89	0.55
1:B:16:ASN:O	1:B:17:GLY:O	2.24	0.55
1:A:142:MET:O	1:A:146:VAL:HG23	2.07	0.54
1:A:138:ASN:HD22	1:A:138:ASN:C	2.11	0.54
1:A:30:ASP:OD2	1:A:32:SER:OG	2.25	0.54
1:B:144:SER:O	1:B:148:ASP:OD2	2.26	0.53
1:B:56:ILE:HG21	1:B:70:MET:CE	2.40	0.52
1:B:16:ASN:O	1:B:17:GLY:C	2.48	0.52
1:B:23:ILE:CG2	1:B:55:ILE:HD13	2.40	0.52
1:A:64:GLU:CA	1:A:64:GLU:OE2	2.58	0.51
1:B:20:LEU:HD23	1:B:55:ILE:HG13	1.93	0.51
1:B:40:LEU:O	1:B:43:ASP:HB2	2.10	0.51
1:B:18:GLU:CG	1:B:20:LEU:HD13	2.41	0.51
1:B:75:PHE:CE2	1:B:79:LYS:HE3	2.46	0.51
1:B:100:GLU:HB3	1:B:101:LYS:HD3	1.92	0.51
1:B:71:LEU:HD23	1:B:108:MET:HG3	1.93	0.50
1:A:171:MET:HE2	1:A:175:SER:OG	2.11	0.50
1:A:235:LYS:O	1:A:239:GLU:HG3	2.12	0.50
1:B:10:ILE:CG2	1:B:23:ILE:HD12	2.31	0.49
1:A:157:ASN:HD21	1:A:159:GLU:HB2	1.77	0.49
1:B:100:GLU:C	1:B:101:LYS:HD3	2.33	0.49
1:B:84:ILE:HB	1:B:85:PRO:HD3	1.95	0.49
1:A:67:TYR:OH	1:A:100:GLU:OE1	2.26	0.49
1:B:109:ILE:CB	1:B:110:PRO:HD3	2.42	0.49
1:B:220:ILE:O	1:B:224:GLU:HG3	2.13	0.49
1:A:34:LEU:HD21	1:A:66:LEU:HD21	1.95	0.49
1:B:41:LEU:HD12	1:B:41:LEU:H	1.76	0.49
1:A:119:GLY:HA2	1:A:124:LYS:HE2	1.95	0.48
1:B:116:TYR:OH	1:B:118:ILE:HD12	2.13	0.48
1:A:64:GLU:HA	1:A:64:GLU:OE2	2.12	0.48
1:A:209:ALA:HB1	1:A:216:ARG:HA	1.95	0.48
1:A:171:MET:O	1:A:207:HIS:HE1	1.97	0.48
1:A:180:ASN:HB3	1:A:181:PRO:HD3	1.96	0.47
1:A:34:LEU:C	1:A:34:LEU:HD23	2.34	0.47
1:B:20:LEU:HD21	1:B:51:ASN:HB3	1.96	0.47
1:B:183:LEU:HA	1:B:186:ILE:HD12	1.95	0.47
1:B:24:LEU:CD1	1:B:59:ILE:HD11	2.45	0.47
1:A:101:LYS:N	1:A:102:PRO:CD	2.77	0.47
1:A:34:LEU:HD11	1:A:66:LEU:HD11	1.97	0.47
1:B:31:GLU:OE1	1:B:35:LYS:NZ	2.47	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:MET:HG3	1:A:182:PHE:CG	2.50	0.46
1:A:30:ASP:OD2	1:A:33:VAL:HG23	2.15	0.46
1:B:71:LEU:HD13	1:B:97:MET:SD	2.56	0.46
1:B:47:THR:HG22	1:B:51:ASN:ND2	2.31	0.46
1:B:128:SER:O	1:B:132:GLU:HG2	2.15	0.45
1:A:230:SER:HB3	1:A:233:VAL:HB	1.99	0.45
1:A:68:GLU:HB3	1:A:69:PRO:HD3	1.98	0.45
1:A:143:ALA:HB2	1:A:178:TYR:CE1	2.51	0.45
1:B:171:MET:HG3	1:B:179:VAL:HG21	1.98	0.45
1:B:71:LEU:HD12	1:B:71:LEU:HA	1.80	0.44
1:B:202:VAL:O	1:B:206:VAL:HG23	2.17	0.44
1:B:72:LYS:HD3	1:B:72:LYS:C	2.38	0.44
1:A:109:ILE:HB	1:A:110:PRO:HD3	2.00	0.44
1:B:142:MET:CE	1:B:142:MET:HG3	2.44	0.44
1:B:64:GLU:O	1:B:65:ASP:C	2.57	0.44
1:B:23:ILE:HG22	1:B:55:ILE:HD13	2.01	0.43
1:A:46:TRP:CZ3	1:A:47:THR:HG22	2.53	0.43
1:A:219:VAL:O	1:A:223:LEU:HG	2.19	0.43
1:B:101:LYS:HB3	1:B:104:LEU:HB3	1.99	0.43
1:A:106:LYS:HE2	1:A:144:SER:OG	2.19	0.42
1:A:75:PHE:CE1	1:A:112:LEU:HB2	2.53	0.42
1:B:64:GLU:CD	1:B:101:LYS:HE3	2.39	0.42
1:B:247:LEU:HD23	1:B:247:LEU:HA	1.64	0.42
1:A:25:ILE:O	1:A:29:TYR:HD1	2.03	0.42
1:B:31:GLU:O	1:B:34:LEU:HB3	2.20	0.42
1:B:101:LYS:N	1:B:101:LYS:CD	2.82	0.42
1:A:106:LYS:CE	1:A:144:SER:OG	2.68	0.42
1:B:118:ILE:HD12	1:B:118:ILE:HA	1.68	0.41
1:A:223:LEU:HB3	1:A:237:VAL:HG13	2.01	0.41
1:B:54:SER:O	1:B:58:VAL:HG23	2.19	0.41
1:A:230:SER:O	1:A:234:ASN:OD1	2.38	0.41
1:A:182:PHE:O	1:A:183:LEU:C	2.57	0.41
1:A:237:VAL:HG12	1:A:241:ILE:HD12	2.03	0.41
1:A:78:LEU:HD12	1:A:126:ASN:HB3	2.02	0.41
1:B:18:GLU:HG3	1:B:20:LEU:HD13	2.02	0.41
1:B:64:GLU:HG2	1:B:67:TYR:CE1	2.56	0.41
1:A:183:LEU:HA	1:A:183:LEU:HD22	1.61	0.40
1:A:84:ILE:CG2	1:A:85:PRO:HD3	2.51	0.40
1:A:168:ILE:HA	1:A:171:MET:HG2	2.02	0.40
1:B:109:ILE:O	1:B:113:PHE:HB2	2.21	0.40
1:B:10:ILE:HD12	1:B:10:ILE:H	1.86	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:MET:O	1:A:74:LEU:HG	2.21	0.40
1:A:216:ARG:O	1:A:220:ILE:HG13	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	237/253 (94%)	226 (95%)	9 (4%)	2 (1%)	22	21
1	B	238/253 (94%)	227 (95%)	8 (3%)	3 (1%)	14	11
All	All	475/506 (94%)	453 (95%)	17 (4%)	5 (1%)	17	13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	B	17	GLY
1	B	65	ASP
1	B	111	VAL
1	A	155	SER

### 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	213/226 (94%)	196 (92%)	17 (8%)	14	14
1	B	214/226 (95%)	195 (91%)	19 (9%)	11	11
All	All	427/452 (94%)	391 (92%)	36 (8%)	13	12

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	20	LEU
1	A	39	GLU
1	A	45	LEU
1	A	62	THR
1	A	64	GLU
1	A	79	LYS
1	A	138	ASN
1	A	171	MET
1	A	177	LYS
1	A	180	ASN
1	A	183	LEU
1	A	213	ASP
1	A	217	LYS
1	A	221	LYS
1	A	231	SER
1	A	247	LEU
1	B	32	SER
1	B	72	LYS
1	B	87	THR
1	B	99	LYS
1	B	100	GLU
1	B	101	LYS
1	B	107	SER
1	B	112	LEU
1	B	129	TYR
1	B	138	ASN
1	B	139	PRO
1	B	144	SER
1	B	147	ARG
1	B	158	ARG
1	B	175	SER
1	B	189	LEU
1	B	227	ASN
1	B	232	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	243	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	157	ASN
1	A	180	ASN
1	A	188	ASN
1	A	207	HIS
1	B	51	ASN
1	B	126	ASN
1	B	138	ASN
1	B	174	ASN
1	B	227	ASN
1	B	234	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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	239/253 (94%)	-0.38	2 (0%) 86 85	16, 34, 62, 70	0
1	B	240/253 (94%)	-0.23	5 (2%) 64 61	21, 39, 61, 74	0
All	All	479/506 (94%)	-0.31	7 (1%) 74 72	16, 37, 61, 74	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	GLU	4.6
1	A	245	LEU	2.7
1	B	110	PRO	2.4
1	B	12	GLU	2.4
1	B	118	ILE	2.3
1	A	140	MET	2.2
1	B	27	ALA	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.