Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:38 PM GMT

PDB ID	:	1BRO
Title	:	BROMOPEROXIDASE A2
Authors	:	Hecht, H.J.; Sobek, H.; Haag, T.; Pfeifer, O.; Van Pee, K.H.
Deposited on	:	1996-06-01
Resolution	:	2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

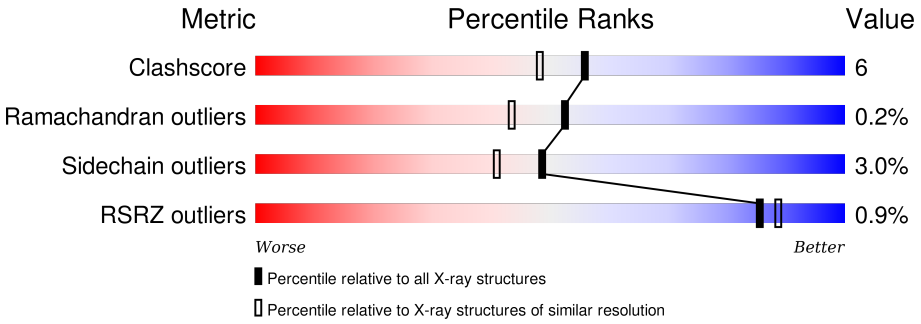
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.05 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))
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	277	2% 64% 29% 8%
1	B	277	62% 35% .

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4529 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 BROMOPEROXIDASE A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2147	1372	356	418	1			
1	B	277	Total	C	N	O	S	0	0	0
			2147	1372	356	418	1			

- Molecule 2 is water.

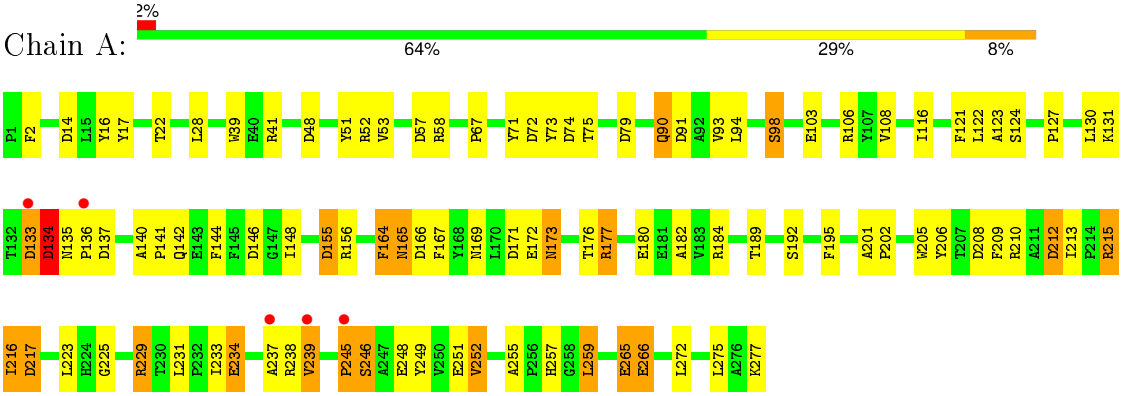
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	141	Total	O	0	0
			141	141		

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.

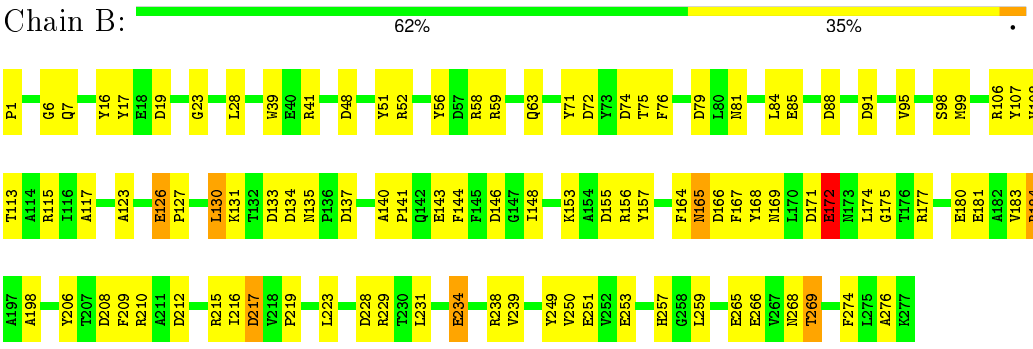
- Molecule 1: BROMOPEROXIDASE A2

Chain A:



- Molecule 1: BROMOPEROXIDASE A2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	126.50Å 126.50Å 126.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.05 44.72 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.2 (10.00-2.05) 97.5 (44.72-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.05Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available) 0.166 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 66.4	EDS
Estimated twinning fraction	0.036 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 41451 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4529	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	1.24	5/2205 (0.2%)	2.42	109/3010 (3.6%)
1	B	1.34	8/2205 (0.4%)	2.58	139/3010 (4.6%)
All	All	1.29	13/4410 (0.3%)	2.50	248/6020 (4.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	ARG	CZ-NH2	7.01	1.42	1.33
1	B	253	GLU	CD-OE2	6.82	1.33	1.25
1	B	184	ARG	CZ-NH1	6.72	1.41	1.33
1	B	180	GLU	CD-OE1	6.48	1.32	1.25
1	A	265	GLU	CD-OE2	6.45	1.32	1.25
1	B	217	ASP	CA-CB	6.26	1.67	1.53
1	B	184	ARG	NE-CZ	6.05	1.41	1.33
1	A	180	GLU	CD-OE1	5.90	1.32	1.25
1	A	215	ARG	CZ-NH2	5.79	1.40	1.33
1	B	215	ARG	CZ-NH2	5.40	1.40	1.33
1	B	16	TYR	CE2-CZ	5.39	1.45	1.38
1	A	41	ARG	NE-CZ	5.32	1.40	1.33
1	A	192	SER	CB-OG	5.25	1.49	1.42

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	184	ARG	NE-CZ-NH1	21.43	131.02	120.30
1	A	177	ARG	NE-CZ-NH1	20.56	130.58	120.30
1	B	215	ARG	NE-CZ-NH1	19.69	130.15	120.30
1	B	115	ARG	NE-CZ-NH1	18.23	129.41	120.30
1	B	184	ARG	NE-CZ-NH2	18.18	129.39	120.30
1	B	177	ARG	NE-CZ-NH1	17.99	129.29	120.30
1	B	210	ARG	NE-CZ-NH1	17.00	128.80	120.30
1	A	184	ARG	NE-CZ-NH2	-16.82	111.89	120.30
1	B	106	ARG	NE-CZ-NH1	16.70	128.65	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	177	ARG	NE-CZ-NH2	-15.95	112.33	120.30
1	A	229	ARG	NE-CZ-NH2	-15.79	112.41	120.30
1	B	166	ASP	CB-CG-OD1	15.08	131.87	118.30
1	A	41	ARG	NE-CZ-NH2	14.83	127.71	120.30
1	B	115	ARG	NE-CZ-NH2	-14.81	112.90	120.30
1	B	134	ASP	CB-CG-OD2	-14.67	105.10	118.30
1	A	229	ARG	NE-CZ-NH1	14.39	127.50	120.30
1	B	266	GLU	OE1-CD-OE2	-14.19	106.28	123.30
1	B	41	ARG	NE-CZ-NH1	14.03	127.31	120.30
1	B	215	ARG	NE-CZ-NH2	-13.93	113.34	120.30
1	B	166	ASP	CB-CG-OD2	-13.79	105.89	118.30
1	A	215	ARG	NE-CZ-NH1	13.58	127.09	120.30
1	B	177	ARG	NE-CZ-NH2	-12.41	114.09	120.30
1	B	41	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	B	133	ASP	CB-CG-OD2	-12.12	107.39	118.30
1	A	52	ARG	NE-CZ-NH2	12.04	126.32	120.30
1	A	184	ARG	CD-NE-CZ	11.73	140.02	123.60
1	A	238	ARG	NE-CZ-NH1	-11.56	114.52	120.30
1	A	41	ARG	NH1-CZ-NH2	-11.43	106.82	119.40
1	B	52	ARG	NE-CZ-NH2	11.40	126.00	120.30
1	B	48	ASP	CB-CG-OD2	-11.34	108.09	118.30
1	B	58	ARG	NE-CZ-NH2	-11.10	114.75	120.30
1	A	249	TYR	CB-CG-CD2	-11.07	114.36	121.00
1	B	155	ASP	CB-CG-OD1	11.04	128.24	118.30
1	B	228	ASP	CB-CG-OD2	11.03	128.22	118.30
1	A	41	ARG	CD-NE-CZ	-10.92	108.31	123.60
1	A	48	ASP	CB-CG-OD2	-10.69	108.68	118.30
1	B	265	GLU	OE1-CD-OE2	-10.61	110.57	123.30
1	B	229	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	A	238	ARG	NE-CZ-NH2	10.39	125.50	120.30
1	B	146	ASP	CB-CG-OD1	10.38	127.64	118.30
1	A	41	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	B	156	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	A	72	ASP	CB-CG-OD1	10.01	127.31	118.30
1	A	165	ASN	OD1-CG-ND2	9.96	144.81	121.90
1	A	14	ASP	CB-CG-OD1	9.83	127.14	118.30
1	A	234	GLU	CG-CD-OE2	9.79	137.89	118.30
1	A	156	ARG	NE-CZ-NH2	-9.75	115.42	120.30
1	A	249	TYR	CB-CG-CD1	9.72	126.83	121.00
1	B	59	ARG	NE-CZ-NH2	9.66	125.13	120.30
1	A	216	ILE	C-N-CA	9.40	145.19	121.70
1	B	134	ASP	CB-CG-OD1	9.19	126.57	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	TYR	CB-CG-CD2	-9.09	115.55	121.00
1	A	134	ASP	CB-CG-OD2	-8.93	110.26	118.30
1	B	16	TYR	CB-CG-CD2	-8.80	115.72	121.00
1	A	91	ASP	CB-CG-OD2	-8.79	110.39	118.30
1	A	248	GLU	OE1-CD-OE2	8.79	133.85	123.30
1	B	184	ARG	CG-CD-NE	8.78	130.25	111.80
1	B	217	ASP	CA-CB-CG	-8.76	94.14	113.40
1	A	106	ARG	CD-NE-CZ	8.73	135.82	123.60
1	A	246	SER	N-CA-CB	-8.71	97.43	110.50
1	B	249	TYR	CB-CG-CD2	8.69	126.21	121.00
1	B	265	GLU	CG-CD-OE1	8.62	135.54	118.30
1	B	133	ASP	OD1-CG-OD2	8.44	139.33	123.30
1	A	234	GLU	CG-CD-OE1	-8.39	101.53	118.30
1	A	71	TYR	CB-CG-CD1	-8.35	115.99	121.00
1	B	196	PHE	CB-CG-CD2	-8.35	114.95	120.80
1	A	52	ARG	NH1-CZ-NH2	-8.18	110.41	119.40
1	B	238	ARG	NE-CZ-NH2	8.04	124.32	120.30
1	A	106	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	58	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	56	TYR	CB-CG-CD1	-8.01	116.19	121.00
1	B	181	GLU	CG-CD-OE1	7.99	134.28	118.30
1	B	106	ARG	NH1-CZ-NH2	-7.96	110.65	119.40
1	B	111	TYR	CB-CG-CD2	-7.87	116.28	121.00
1	A	165	ASN	N-CA-CB	-7.83	96.50	110.60
1	B	217	ASP	N-CA-CB	-7.82	96.52	110.60
1	B	217	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	B	171	ASP	CB-CG-OD1	7.79	125.31	118.30
1	B	107	TYR	CB-CG-CD2	-7.71	116.38	121.00
1	B	165	ASN	OD1-CG-ND2	7.68	139.56	121.90
1	B	99	MET	CG-SD-CE	-7.67	87.92	100.20
1	A	171	ASP	CB-CG-OD2	7.66	125.19	118.30
1	B	167	PHE	CB-CG-CD2	-7.63	115.46	120.80
1	A	210	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	172	GLU	CA-CB-CG	7.40	129.69	113.40
1	B	143	GLU	OE1-CD-OE2	7.37	132.15	123.30
1	A	217	ASP	N-CA-CB	-7.36	97.34	110.60
1	B	165	ASN	CA-CB-CG	-7.31	97.31	113.40
1	A	166	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	A	106	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	B	130	LEU	CB-CG-CD2	-7.25	98.68	111.00
1	B	216	ILE	C-N-CA	7.25	139.81	121.70
1	A	208	ASP	CB-CG-OD2	-7.19	111.83	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	106	ARG	NH1-CZ-NH2	-7.13	111.56	119.40
1	B	174	LEU	CB-CG-CD2	-7.08	98.95	111.00
1	B	72	ASP	CB-CG-OD1	7.07	124.67	118.30
1	B	167	PHE	CB-CG-CD1	7.02	125.71	120.80
1	B	59	ARG	NH1-CZ-NH2	-7.01	111.69	119.40
1	B	175	GLY	O-C-N	-6.97	111.55	122.70
1	B	249	TYR	CB-CG-CD1	-6.96	116.83	121.00
1	B	217	ASP	CB-CA-C	-6.95	96.50	110.40
1	B	239	VAL	CG1-CB-CG2	-6.93	99.81	110.90
1	B	109	SER	N-CA-CB	-6.91	100.14	110.50
1	B	85	GLU	CG-CD-OE2	6.86	132.01	118.30
1	A	215	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	19	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	A	74	ASP	CB-CG-OD1	6.76	124.38	118.30
1	B	229	ARG	CD-NE-CZ	6.71	132.99	123.60
1	B	74	ASP	CB-CG-OD1	6.70	124.33	118.30
1	B	217	ASP	N-CA-C	6.66	128.99	111.00
1	A	266	GLU	OE1-CD-OE2	-6.65	115.32	123.30
1	A	217	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	165	ASN	CB-CG-OD1	-6.63	108.34	121.60
1	B	131	LYS	CA-CB-CG	-6.62	98.83	113.40
1	B	71	TYR	CG-CD2-CE2	-6.61	116.01	121.30
1	B	156	ARG	CD-NE-CZ	6.60	132.85	123.60
1	A	265	GLU	CG-CD-OE2	-6.49	105.31	118.30
1	B	7	GLN	CG-CD-OE1	-6.45	108.69	121.60
1	B	16	TYR	CD1-CE1-CZ	-6.45	114.00	119.80
1	B	276	ALA	N-CA-CB	6.43	119.10	110.10
1	A	137	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	B	210	ARG	NH1-CZ-NH2	-6.42	112.34	119.40
1	B	76	PHE	CG-CD1-CE1	-6.41	113.75	120.80
1	A	90	GLN	O-C-N	6.35	132.86	122.70
1	B	274	PHE	CB-CG-CD1	-6.25	116.43	120.80
1	B	88	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	277	LYS	CB-CG-CD	-6.24	95.38	111.60
1	A	164	PHE	CZ-CE2-CD2	-6.23	112.62	120.10
1	B	106	ARG	CD-NE-CZ	6.22	132.31	123.60
1	A	180	GLU	OE1-CD-OE2	6.21	130.75	123.30
1	B	52	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	B	234	GLU	N-CA-CB	6.18	121.73	110.60
1	B	268	ASN	O-C-N	6.18	132.59	122.70
1	A	127	PRO	N-CD-CG	-6.16	93.96	103.20
1	B	52	ARG	CD-NE-CZ	6.15	132.21	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	58	ARG	CD-NE-CZ	6.12	132.16	123.60
1	B	184	ARG	NH1-CZ-NH2	-6.11	112.67	119.40
1	A	195	PHE	O-C-N	-6.10	112.94	122.70
1	B	196	PHE	CB-CG-CD1	6.10	125.07	120.80
1	A	134	ASP	CB-CA-C	6.10	122.60	110.40
1	B	234	GLU	CB-CA-C	-6.08	98.24	110.40
1	A	57	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	205	TRP	CE3-CZ3-CH2	6.07	127.87	121.20
1	B	6	GLY	O-C-N	6.06	132.39	122.70
1	A	155	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	192	SER	CA-C-N	6.04	128.28	116.20
1	A	91	ASP	N-CA-CB	-6.04	99.73	110.60
1	A	98	SER	CB-CA-C	6.00	121.49	110.10
1	B	166	ASP	CA-CB-CG	-5.99	100.23	113.40
1	A	166	ASP	O-C-N	5.98	132.27	122.70
1	B	172	GLU	CG-CD-OE1	-5.98	106.34	118.30
1	B	183	VAL	O-C-N	-5.98	113.14	122.70
1	B	143	GLU	CG-CD-OE2	-5.97	106.36	118.30
1	B	133	ASP	CB-CA-C	-5.97	98.46	110.40
1	A	137	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	A	53	VAL	CA-CB-CG2	5.94	119.81	110.90
1	A	121	PHE	CB-CG-CD1	-5.93	116.64	120.80
1	A	52	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	137	ASP	OD1-CG-OD2	5.92	134.55	123.30
1	A	239	VAL	CB-CA-C	5.88	122.58	111.40
1	A	17	TYR	CZ-CE2-CD2	-5.85	114.53	119.80
1	B	269	THR	OG1-CB-CG2	-5.83	96.58	110.00
1	B	39	TRP	CA-C-O	-5.83	107.86	120.10
1	B	228	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	A	249	TYR	N-CA-CB	-5.82	100.13	110.60
1	A	252	VAL	CA-C-N	-5.80	104.44	117.20
1	B	168	TYR	CA-C-O	-5.79	107.94	120.10
1	A	22	THR	CA-CB-CG2	5.74	120.44	112.40
1	B	79	ASP	O-C-N	5.72	131.85	122.70
1	B	198	ALA	N-CA-CB	5.70	118.08	110.10
1	B	76	PHE	CD1-CE1-CZ	5.70	126.94	120.10
1	A	142	GLN	CG-CD-NE2	-5.69	103.04	116.70
1	A	156	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	209	PHE	CB-CG-CD1	-5.67	116.83	120.80
1	A	177	ARG	CD-NE-CZ	5.66	131.53	123.60
1	A	182	ALA	N-CA-CB	5.65	118.01	110.10
1	B	76	PHE	CA-CB-CG	5.65	127.46	113.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	157	TYR	CB-CG-CD1	-5.64	117.61	121.00
1	B	59	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	75	THR	CA-CB-OG1	-5.64	97.16	109.00
1	B	181	GLU	CG-CD-OE2	-5.64	107.03	118.30
1	A	131	LYS	CB-CG-CD	-5.62	96.97	111.60
1	B	133	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	B	217	ASP	OD1-CG-OD2	5.60	133.94	123.30
1	B	84	LEU	O-C-N	5.58	131.63	122.70
1	B	180	GLU	N-CA-CB	-5.56	100.59	110.60
1	B	56	TYR	CB-CG-CD2	5.55	124.33	121.00
1	B	74	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	124	SER	CB-CA-C	-5.53	99.59	110.10
1	A	67	PRO	CA-C-O	5.53	133.47	120.20
1	A	103	GLU	N-CA-CB	5.51	120.51	110.60
1	B	153	LYS	O-C-N	5.51	131.51	122.70
1	B	208	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	B	212	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	177	ARG	CA-CB-CG	-5.48	101.34	113.40
1	B	164	PHE	CG-CD2-CE2	-5.46	114.79	120.80
1	B	107	TYR	CB-CG-CD1	5.44	124.27	121.00
1	B	71	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	B	148	ILE	CA-CB-CG1	-5.42	100.69	111.00
1	B	63	GLN	CA-C-O	-5.40	108.76	120.10
1	B	88	ASP	CB-CG-OD1	5.38	123.15	118.30
1	A	75	THR	CA-CB-OG1	-5.35	97.76	109.00
1	B	23	GLY	O-C-N	5.35	131.27	122.70
1	A	165	ASN	CA-CB-CG	-5.33	101.66	113.40
1	A	2	PHE	CB-CG-CD2	-5.32	117.07	120.80
1	A	265	GLU	N-CA-C	5.32	125.37	111.00
1	B	156	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	17	TYR	CG-CD2-CE2	5.30	125.54	121.30
1	A	74	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	91	ASP	CA-CB-CG	-5.29	101.77	113.40
1	A	172	GLU	CB-CG-CD	5.28	128.46	114.20
1	B	172	GLU	CG-CD-OE2	5.27	128.85	118.30
1	A	51	TYR	CG-CD1-CE1	-5.27	117.09	121.30
1	B	51	TYR	CA-CB-CG	-5.27	103.39	113.40
1	A	229	ARG	CA-CB-CG	5.27	124.98	113.40
1	B	165	ASN	CB-CG-ND2	-5.26	104.06	116.70
1	B	135	ASN	CA-C-O	5.25	131.12	120.10
1	B	251	GLU	OE1-CD-OE2	-5.25	117.01	123.30
1	A	2	PHE	CB-CA-C	-5.24	99.92	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	52	ARG	CB-CG-CD	-5.24	97.98	111.60
1	B	111	TYR	CZ-CE2-CD2	-5.24	115.08	119.80
1	A	265	GLU	CB-CA-C	-5.23	99.93	110.40
1	A	173	ASN	N-CA-C	5.23	125.12	111.00
1	A	71	TYR	CA-CB-CG	-5.22	103.47	113.40
1	B	17	TYR	CZ-CE2-CD2	-5.22	115.10	119.80
1	B	155	ASP	OD1-CG-OD2	-5.22	113.39	123.30
1	B	238	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	B	23	GLY	N-CA-C	-5.21	100.07	113.10
1	A	73	TYR	CA-CB-CG	-5.21	103.51	113.40
1	A	251	GLU	N-CA-CB	5.20	119.96	110.60
1	A	245	PRO	CA-C-N	-5.17	105.82	117.20
1	A	133	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	B	109	SER	O-C-N	-5.16	114.45	122.70
1	A	79	ASP	CA-CB-CG	5.16	124.74	113.40
1	A	91	ASP	OD1-CG-OD2	5.15	133.09	123.30
1	A	251	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	A	146	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	259	LEU	CA-CB-CG	5.13	127.09	115.30
1	B	157	TYR	CD1-CE1-CZ	-5.13	115.19	119.80
1	A	272	LEU	CB-CA-C	5.12	119.92	110.20
1	A	217	ASP	N-CA-C	5.09	124.76	111.00
1	A	259	LEU	CB-CA-C	5.09	119.88	110.20
1	B	192	SER	O-C-N	-5.08	114.56	123.20
1	A	212	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	137	ASP	O-C-N	5.07	131.81	123.20
1	A	16	TYR	CZ-CE2-CD2	-5.04	115.26	119.80
1	B	126	GLU	CG-CD-OE1	5.04	128.37	118.30
1	B	58	ARG	NH1-CZ-NH2	5.03	124.93	119.40

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	2147	0	2033	34	0
1	B	2147	0	2033	18	0
2	A	94	0	0	1	0
2	B	141	0	0	3	0
All	All	4529	0	4066	52	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 6.

All (52) 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:231:LEU:HD12	1:B:257:HIS:HE1	1.49	0.77
1:A:252:VAL:HG12	1:A:255:ALA:HB2	1.69	0.75
1:A:176:THR:HG22	1:A:177:ARG:HG3	1.71	0.72
1:B:28:LEU:HD23	1:B:95:VAL:HB	1.74	0.69
1:A:201:ALA:HB3	1:A:202:PRO:HD3	1.76	0.67
1:B:140:ALA:HB1	1:B:141:PRO:HD2	1.78	0.64
1:A:130:LEU:O	1:A:135:ASN:ND2	2.31	0.62
1:A:212:ASP:O	1:A:215:ARG:HB2	2.02	0.59
1:A:93:VAL:HG11	1:A:275:LEU:HD21	1.85	0.58
1:B:126:GLU:HB3	1:B:127:PRO:HA	1.87	0.57
1:A:122:LEU:CD2	1:A:223:LEU:HB3	2.34	0.57
1:B:108:VAL:HG22	1:B:113:THR:HG22	1.86	0.57
1:B:1:PRO:N	2:B:374:HOH:O	2.31	0.57
1:A:231:LEU:HD12	1:A:257:HIS:HE1	1.69	0.56
1:B:130:LEU:HB2	1:B:206:TYR:HB2	1.88	0.55
1:A:134:ASP:C	1:A:136:PRO:HD3	2.27	0.54
1:B:231:LEU:HD12	1:B:257:HIS:CE1	2.37	0.54
1:A:94:LEU:HG	1:A:116:ILE:HD12	1.89	0.54
1:A:130:LEU:HB2	1:A:206:TYR:HB2	1.90	0.53
1:A:122:LEU:HD23	1:A:223:LEU:HB3	1.91	0.51
1:A:245:PRO:HG2	1:A:246:SER:H	1.75	0.51
1:A:141:PRO:O	1:A:144:PHE:HB3	2.10	0.50
1:A:164:PHE:HA	1:A:167:PHE:HB3	1.93	0.50
1:A:173:ASN:ND2	1:A:177:ARG:HD2	2.28	0.49
1:A:189:THR:HG21	2:A:284:HOH:O	2.11	0.49
1:B:169:ASN:HB3	1:B:172:GLU:HG3	1.93	0.49
1:A:209:PHE:O	1:A:213:ILE:HG13	2.12	0.48
1:A:169:ASN:HA	1:A:229:ARG:NH1	2.27	0.48
1:A:144:PHE:CZ	1:A:148:ILE:HD11	2.48	0.48
1:B:223:LEU:HA	1:B:250:VAL:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLN:NE2	1:A:90:GLN:HA	2.29	0.47
1:B:98:SER:HA	1:B:123:ALA:O	2.15	0.47
1:A:130:LEU:HA	1:A:130:LEU:HD12	1.82	0.46
1:A:108:VAL:HG11	1:A:216:ILE:HG12	1.97	0.46
1:B:169:ASN:HB3	1:B:172:GLU:CG	2.45	0.45
1:B:81:ASN:ND2	2:B:386:HOH:O	2.46	0.45
1:A:265:GLU:HB2	1:A:266:GLU:OE1	2.17	0.45
1:A:233:ILE:HG13	1:A:237:ALA:HB3	1.99	0.44
1:A:98:SER:HA	1:A:123:ALA:O	2.18	0.44
1:A:225:GLY:HA2	1:A:255:ALA:HB3	2.00	0.43
1:B:126:GLU:CB	1:B:127:PRO:HA	2.47	0.43
1:A:93:VAL:HG11	1:A:275:LEU:CD2	2.48	0.43
1:A:134:ASP:O	1:A:136:PRO:HD3	2.19	0.43
1:A:201:ALA:N	1:A:202:PRO:CD	2.82	0.42
1:A:140:ALA:HB1	1:A:141:PRO:HD2	2.01	0.42
1:B:269:THR:HG21	2:B:373:HOH:O	2.21	0.41
1:B:141:PRO:O	1:B:144:PHE:HB3	2.20	0.41
1:B:117:ALA:O	1:B:219:PRO:HD2	2.21	0.41
1:A:135:ASN:N	1:A:136:PRO:HD3	2.36	0.40
1:B:231:LEU:CD1	1:B:257:HIS:HE1	2.25	0.40
1:A:225:GLY:CA	1:A:255:ALA:HB3	2.51	0.40
1:A:28:LEU:HB3	1:A:39:TRP:CE2	2.56	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	275/277 (99%)	262 (95%)	12 (4%)	1 (0%)	39 28
1	B	275/277 (99%)	266 (97%)	9 (3%)	0	100 100
All	All	550/554 (99%)	528 (96%)	21 (4%)	1 (0%)	52 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ASP

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	219/219 (100%)	212 (97%)	7 (3%)	46 38
1	B	219/219 (100%)	213 (97%)	6 (3%)	52 45
All	All	438/438 (100%)	425 (97%)	13 (3%)	48 41

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ASP
1	A	134	ASP
1	A	165	ASN
1	A	217	ASP
1	A	234	GLU
1	A	239	VAL
1	A	259	LEU
1	B	165	ASN
1	B	172	GLU
1	B	184	ARG
1	B	217	ASP
1	B	234	GLU
1	B	259	LEU

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	90	GLN
1	A	173	ASN
1	A	188	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	81	ASN
1	B	188	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	277/277 (100%)	-0.17	5 (1%) 71 76	19, 29, 49, 68	0
1	B	277/277 (100%)	-0.69	0 100 100	16, 21, 33, 55	0
All	All	554/554 (100%)	-0.43	5 (0%) 85 89	16, 24, 46, 68	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	PRO	2.5
1	A	136	PRO	2.3
1	A	133	ASP	2.1
1	A	237	ALA	2.1
1	A	239	VAL	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.