Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:49 AM GMT

PDB ID	:	2EIB
Title	:	Crystal Structure of Galactose Oxidase, W290H mutant
Authors	:	Phillips, S.E.; McPherson, M.J.; Knowles, P.F.; Wilmot, C.
Deposited on	:	2007-03-12
Resolution	:	2.10 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 (i)) were used in the production of this report:

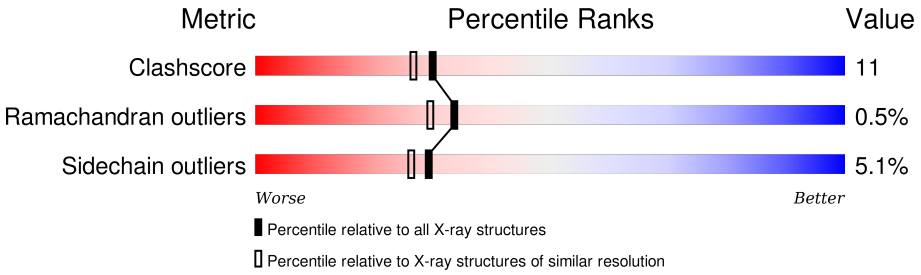
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	639	58% 34% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5171 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 Galactose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			4826	3012	841	954	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	HIS	TRP	ENGINEERED	UNP Q01745

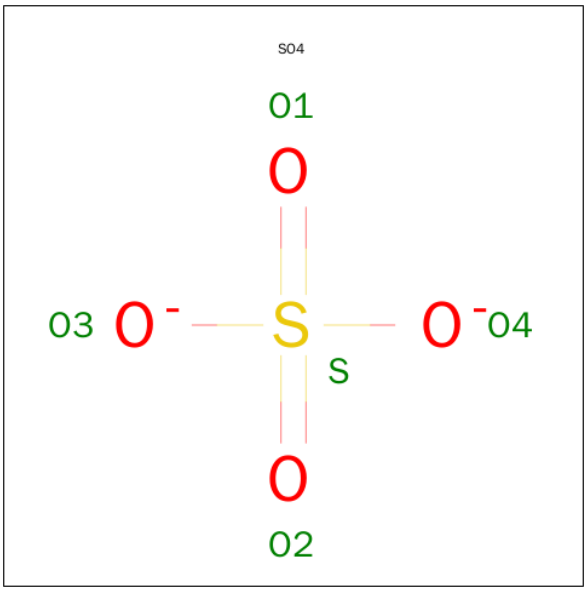
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

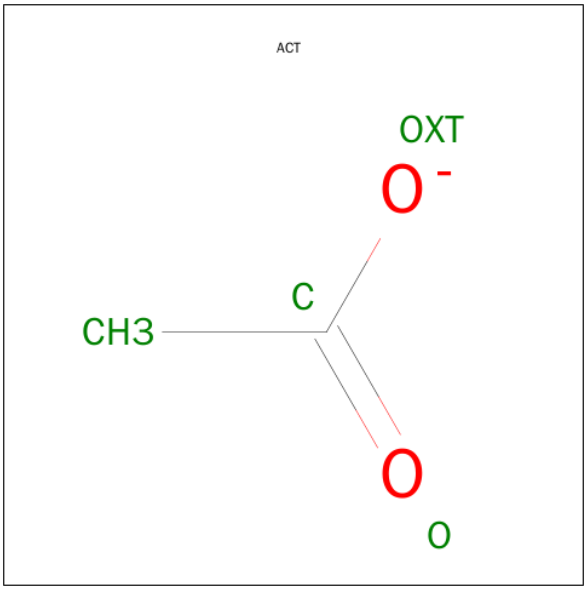
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	326	Total O 326 326	0	0

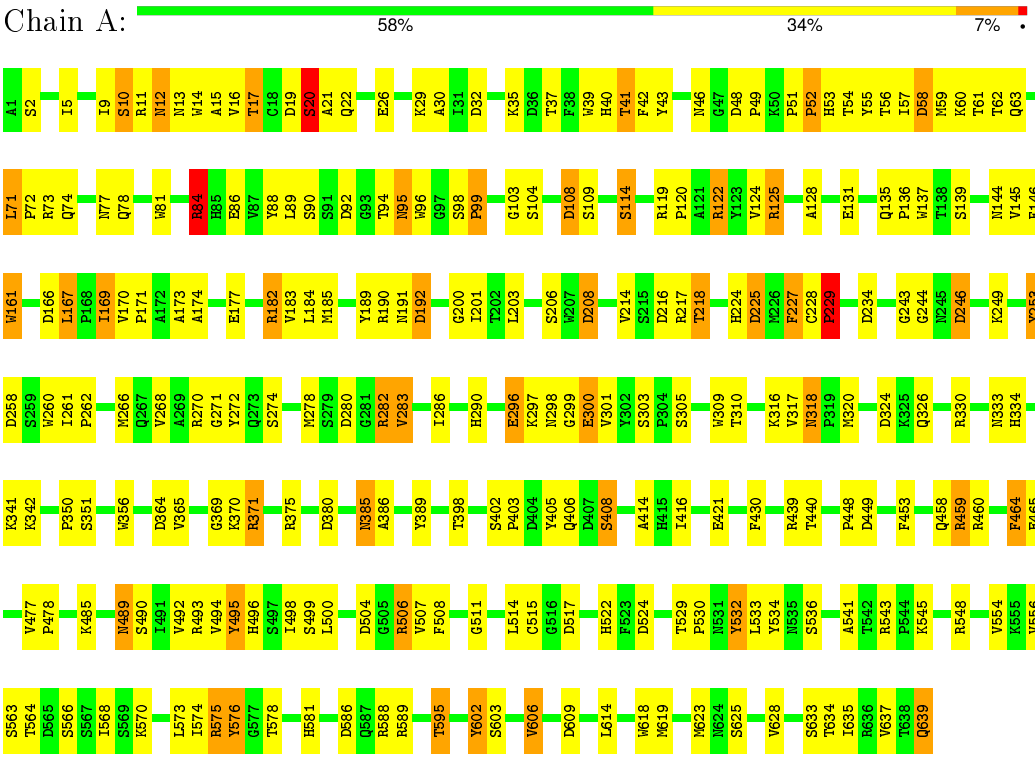
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: Galactose oxidase

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.00Å 89.40Å 86.70Å 90.00° 117.80° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5171	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SO4, CU, ACT

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	1.04	1/4954 (0.0%)	2.27	205/6757 (3.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	GLU	CD-OE2	-5.64	1.19	1.25

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	548	ARG	CD-NE-CZ	31.54	167.76	123.60
1	A	330	ARG	NE-CZ-NH1	21.73	131.16	120.30
1	A	493	ARG	NE-CZ-NH2	-20.24	110.18	120.30
1	A	506	ARG	NE-CZ-NH1	18.37	129.48	120.30
1	A	282	ARG	NE-CZ-NH1	16.71	128.65	120.30
1	A	548	ARG	NE-CZ-NH1	16.17	128.38	120.30
1	A	330	ARG	NE-CZ-NH2	-15.76	112.42	120.30
1	A	192	ASP	CB-CG-OD2	14.26	131.13	118.30
1	A	217	ARG	NE-CZ-NH1	13.38	126.99	120.30
1	A	439	ARG	NE-CZ-NH2	13.13	126.87	120.30
1	A	84	ARG	CD-NE-CZ	12.89	141.65	123.60
1	A	559	ARG	CD-NE-CZ	12.72	141.41	123.60
1	A	602	TYR	CB-CG-CD1	12.70	128.62	121.00
1	A	506	ARG	CD-NE-CZ	11.56	139.79	123.60
1	A	119	ARG	NE-CZ-NH2	-11.29	114.65	120.30
1	A	68	LEU	CA-CB-CG	11.27	141.22	115.30
1	A	602	TYR	CB-CG-CD2	-11.06	114.37	121.00
1	A	69	SER	CB-CA-C	10.77	130.56	110.10
1	A	20	SER	N-CA-CB	10.25	125.87	110.50
1	A	559	ARG	NE-CZ-NH1	10.21	125.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	ASP	CB-CG-OD1	9.98	127.29	118.30
1	A	548	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	A	185	MET	CG-SD-CE	9.58	115.53	100.20
1	A	84	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	A	406	GLN	O-C-N	9.41	137.75	122.70
1	A	506	ARG	NH1-CZ-NH2	-9.39	109.07	119.40
1	A	543	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	A	246	ASP	CB-CG-OD2	9.16	126.54	118.30
1	A	380	ASP	CB-CG-OD1	9.06	126.46	118.30
1	A	280	ASP	CB-CG-OD2	9.01	126.41	118.30
1	A	104	SER	O-C-N	8.92	136.97	122.70
1	A	493	ARG	NH1-CZ-NH2	8.91	129.20	119.40
1	A	465	GLU	OE1-CD-OE2	8.90	133.98	123.30
1	A	318	ASN	CB-CA-C	8.81	128.02	110.40
1	A	114	SER	N-CA-CB	8.80	123.70	110.50
1	A	586	ASP	CB-CG-OD2	8.73	126.16	118.30
1	A	460	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	234	ASP	CB-CG-OD1	8.61	126.05	118.30
1	A	48	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	A	119	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	A	282	ARG	CD-NE-CZ	8.31	135.23	123.60
1	A	589	ARG	CD-NE-CZ	-8.22	112.09	123.60
1	A	190	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	225	ASP	CB-CG-OD1	8.04	125.54	118.30
1	A	466	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	A	532	TYR	CB-CG-CD1	7.97	125.78	121.00
1	A	534	TYR	CB-CG-CD1	-7.88	116.27	121.00
1	A	227	PHE	CB-CG-CD1	-7.88	115.28	120.80
1	A	389	TYR	CB-CG-CD1	-7.73	116.36	121.00
1	A	86	GLU	OE1-CD-OE2	7.69	132.53	123.30
1	A	499	SER	N-CA-CB	7.68	122.02	110.50
1	A	234	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	A	300	GLU	OE1-CD-OE2	7.65	132.48	123.30
1	A	246	ASP	CB-CG-OD1	-7.64	111.42	118.30
1	A	218	THR	O-C-N	7.60	134.86	122.70
1	A	55	TYR	CB-CG-CD1	-7.57	116.46	121.00
1	A	609	ASP	CB-CG-OD1	-7.45	111.59	118.30
1	A	439	ARG	CA-CB-CG	7.32	129.51	113.40
1	A	217	ARG	CG-CD-NE	7.21	126.94	111.80
1	A	338	PHE	CB-CG-CD2	-7.15	115.80	120.80
1	A	92	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	A	375	ARG	NE-CZ-NH1	7.10	123.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	439	ARG	NH1-CZ-NH2	-7.09	111.59	119.40
1	A	55	TYR	CB-CG-CD2	7.08	125.25	121.00
1	A	576	TYR	CB-CG-CD2	7.02	125.22	121.00
1	A	524	ASP	CB-CG-OD2	7.00	124.61	118.30
1	A	254	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	466	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	170	VAL	CA-CB-CG1	6.88	121.22	110.90
1	A	464	PHE	CB-CG-CD1	-6.87	115.99	120.80
1	A	41	THR	CA-CB-CG2	-6.86	102.80	112.40
1	A	588	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	A	19	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	342	LYS	N-CA-CB	-6.71	98.52	110.60
1	A	633	SER	N-CA-CB	6.71	120.56	110.50
1	A	119	ARG	CD-NE-CZ	6.69	132.97	123.60
1	A	517	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	573	LEU	CA-CB-CG	6.57	130.41	115.30
1	A	485	LYS	CB-CG-CD	6.55	128.62	111.60
1	A	20	SER	CB-CA-C	-6.53	97.69	110.10
1	A	543	ARG	NH1-CZ-NH2	6.50	126.56	119.40
1	A	578	THR	OG1-CB-CG2	6.43	124.79	110.00
1	A	406	GLN	CA-C-O	-6.42	106.62	120.10
1	A	586	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	A	318	ASN	N-CA-CB	-6.37	99.13	110.60
1	A	173	ALA	N-CA-CB	6.36	119.01	110.10
1	A	125	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	507	VAL	CA-CB-CG1	6.34	120.41	110.90
1	A	282	ARG	NH1-CZ-NH2	-6.30	112.47	119.40
1	A	26	GLU	CG-CD-OE2	6.29	130.88	118.30
1	A	161	TRP	CB-CG-CD1	6.23	135.10	127.00
1	A	190	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	182	ARG	CA-CB-CG	-6.20	99.75	113.40
1	A	369	GLY	C-N-CA	6.20	137.19	121.70
1	A	208	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	467	SER	C-N-CA	6.18	137.15	121.70
1	A	217	ARG	CD-NE-CZ	6.15	132.21	123.60
1	A	371	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	224	HIS	CA-CB-CG	6.11	123.99	113.60
1	A	217	ARG	CB-CG-CD	6.08	127.41	111.60
1	A	623	MET	CG-SD-CE	-6.02	90.56	100.20
1	A	286	ILE	O-C-N	6.02	133.44	123.20
1	A	297	LYS	CD-CE-NZ	-6.02	97.86	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	460	ARG	NH1-CZ-NH2	6.02	126.02	119.40
1	A	439	ARG	CG-CD-NE	6.01	124.43	111.80
1	A	160	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	532	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	182	ARG	CD-NE-CZ	-5.98	115.22	123.60
1	A	575	ARG	N-CA-CB	-5.98	99.83	110.60
1	A	268	VAL	CA-CB-CG1	5.98	119.87	110.90
1	A	299	GLY	O-C-N	5.96	132.23	122.70
1	A	380	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	108	ASP	CB-CA-C	5.95	122.29	110.40
1	A	160	ARG	CB-CA-C	-5.95	98.51	110.40
1	A	508	PHE	CB-CG-CD1	-5.94	116.64	120.80
1	A	333	ASN	O-C-N	5.93	132.19	122.70
1	A	161	TRP	CB-CG-CD2	-5.89	118.94	126.60
1	A	310	THR	N-CA-CB	5.88	121.47	110.30
1	A	589	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	58	ASP	N-CA-CB	5.88	121.18	110.60
1	A	70	MET	CG-SD-CE	5.87	109.59	100.20
1	A	532	TYR	CB-CA-C	5.82	122.04	110.40
1	A	20	SER	O-C-N	5.81	132.00	122.70
1	A	70	MET	O-C-N	5.81	131.99	122.70
1	A	258	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	578	THR	CA-CB-OG1	-5.80	96.83	109.00
1	A	52	PRO	O-C-N	5.79	131.97	122.70
1	A	639	GLN	N-CA-CB	5.77	120.98	110.60
1	A	338	PHE	CD1-CE1-CZ	-5.75	113.19	120.10
1	A	637	VAL	CA-CB-CG1	5.75	119.52	110.90
1	A	370	LYS	CB-CA-C	-5.74	98.92	110.40
1	A	324	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	453	PHE	CB-CG-CD2	-5.71	116.80	120.80
1	A	99	PRO	O-C-N	5.71	131.83	122.70
1	A	575	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	A	253	TYR	O-C-N	5.64	131.73	122.70
1	A	283	VAL	O-C-N	-5.64	113.68	122.70
1	A	405	TYR	CB-CG-CD1	5.63	124.38	121.00
1	A	609	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	421	GLU	CG-CD-OE1	5.57	129.43	118.30
1	A	216	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	566	SER	O-C-N	5.55	131.58	122.70
1	A	495	TYR	CB-CA-C	5.54	121.48	110.40
1	A	430	PHE	CB-CG-CD1	-5.51	116.94	120.80
1	A	169	ILE	O-C-N	5.51	131.51	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	364	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	459	ARG	CB-CA-C	5.49	121.37	110.40
1	A	278	MET	N-CA-CB	-5.46	100.77	110.60
1	A	274	SER	O-C-N	5.46	131.44	122.70
1	A	200	GLY	N-CA-C	5.46	126.75	113.10
1	A	189	TYR	CB-CG-CD1	5.46	124.27	121.00
1	A	440	THR	CA-CB-OG1	-5.44	97.57	109.00
1	A	30	ALA	CA-C-O	-5.43	108.69	120.10
1	A	385	ASN	CB-CG-OD1	-5.42	110.76	121.60
1	A	243	GLY	C-N-CA	-5.42	110.93	122.30
1	A	522	HIS	O-C-N	5.41	131.36	122.70
1	A	217	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	270	ARG	N-CA-CB	-5.39	100.89	110.60
1	A	10	SER	N-CA-CB	5.39	118.58	110.50
1	A	84	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
1	A	459	ARG	CD-NE-CZ	5.37	131.11	123.60
1	A	20	SER	CA-CB-OG	5.36	125.67	111.20
1	A	614	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	603	SER	O-C-N	5.34	131.24	122.70
1	A	214	VAL	CG1-CB-CG2	-5.31	102.40	110.90
1	A	389	TYR	CB-CG-CD2	5.29	124.18	121.00
1	A	606	VAL	CG1-CB-CG2	5.29	119.36	110.90
1	A	595	THR	CA-CB-OG1	-5.28	97.91	109.00
1	A	449	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	54	THR	N-CA-CB	-5.26	100.31	110.30
1	A	337	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	500	LEU	CB-CG-CD1	-5.25	102.07	111.00
1	A	131	GLU	N-CA-C	-5.25	96.82	111.00
1	A	122	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	543	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	A	635	ILE	CB-CG1-CD1	5.22	128.52	113.90
1	A	296	GLU	CA-CB-CG	5.20	124.83	113.40
1	A	167	LEU	N-CA-CB	-5.20	100.01	110.40
1	A	405	TYR	CG-CD2-CE2	5.19	125.45	121.30
1	A	639	GLN	N-CA-C	-5.17	97.05	111.00
1	A	468	THR	CA-CB-CG2	5.15	119.61	112.40
1	A	300	GLU	CA-CB-CG	5.15	124.74	113.40
1	A	2	SER	CB-CA-C	5.14	119.87	110.10
1	A	588	ARG	CD-NE-CZ	5.14	130.80	123.60
1	A	41	THR	O-C-N	5.13	130.91	122.70
1	A	68	LEU	CB-CA-C	5.13	119.96	110.20
1	A	266	MET	O-C-N	5.13	130.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	386	ALA	CB-CA-C	5.13	117.80	110.10
1	A	416	ILE	N-CA-CB	5.12	122.58	110.80
1	A	489	ASN	OD1-CG-ND2	5.12	133.66	121.90
1	A	71	LEU	N-CA-C	-5.11	97.19	111.00
1	A	249	LYS	C-N-CA	5.11	134.48	121.70
1	A	53	HIS	N-CA-C	-5.11	97.21	111.00
1	A	15	ALA	N-CA-CB	5.11	117.25	110.10
1	A	201	ILE	O-C-N	5.11	130.87	122.70
1	A	137	TRP	CB-CA-C	-5.10	100.19	110.40
1	A	137	TRP	O-C-N	5.09	130.85	122.70
1	A	190	ARG	CD-NE-CZ	5.08	130.71	123.60
1	A	283	VAL	CA-C-O	5.06	130.72	120.10
1	A	338	PHE	CE1-CZ-CE2	5.05	129.10	120.00
1	A	625	SER	O-C-N	5.05	130.78	122.70
1	A	77	ASN	C-N-CA	5.03	134.28	121.70
1	A	282	ARG	CG-CD-NE	5.03	122.36	111.80
1	A	227	PHE	CB-CG-CD2	5.02	124.32	120.80

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	4826	0	4599	105	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	12	0	9	0	0
6	A	326	0	0	11	0
All	All	5171	0	4608	105	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 11.

All (105) 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:22:GLN:NE2	1:A:46:ASN:HB2	1.81	0.96
1:A:506:ARG:HD3	6:A:819:HOH:O	1.68	0.92
1:A:22:GLN:HE21	1:A:46:ASN:HB2	1.33	0.91
1:A:22:GLN:NE2	1:A:43:TYR:H	1.70	0.90
1:A:13:ASN:HB2	6:A:931:HOH:O	1.87	0.72
1:A:35:LYS:HE2	1:A:71:LEU:HD21	1.73	0.70
1:A:298:ASN:HD22	1:A:317:VAL:H	1.39	0.69
1:A:529:THR:HG23	1:A:533:LEU:HD12	1.73	0.69
1:A:326:GLN:HB3	6:A:840:HOH:O	1.93	0.67
1:A:21:ALA:HA	1:A:40:HIS:O	1.95	0.67
1:A:171:PRO:HD2	1:A:511:GLY:HA2	1.78	0.66
1:A:29:LYS:HD2	1:A:37:THR:HB	1.78	0.65
1:A:300:GLU:HG3	1:A:309:TRP:CE3	2.31	0.65
1:A:290:HIS:HD2	6:A:741:HOH:O	1.79	0.65
1:A:174:ALA:HB3	1:A:498:ILE:HD13	1.80	0.62
1:A:9:ILE:HD12	1:A:145:VAL:HG12	1.83	0.61
1:A:84:ARG:NH1	6:A:978:HOH:O	2.34	0.61
1:A:504:ASP:OD1	1:A:506:ARG:HB2	2.01	0.60
1:A:103:GLY:HA3	1:A:166:ASP:O	2.02	0.59
1:A:469:PRO:HB3	1:A:492:VAL:HG13	1.84	0.59
1:A:51:PRO:HD3	1:A:136:PRO:HA	1.86	0.58
1:A:298:ASN:ND2	1:A:317:VAL:H	2.01	0.57
1:A:90:SER:HB2	1:A:96:TRP:CE3	2.40	0.57
1:A:72:PRO:HG2	1:A:109:SER:HA	1.88	0.56
1:A:17:THR:HG22	6:A:944:HOH:O	2.05	0.56
1:A:22:GLN:NE2	1:A:43:TYR:O	2.36	0.55
1:A:290:HIS:CD2	6:A:741:HOH:O	2.56	0.55
1:A:35:LYS:HE2	1:A:71:LEU:CD2	2.36	0.55
1:A:167:LEU:CD1	1:A:171:PRO:HG3	2.37	0.54
1:A:356:TRP:O	1:A:365:VAL:HA	2.06	0.54
1:A:459:ARG:HB2	6:A:849:HOH:O	2.06	0.54
1:A:174:ALA:CB	1:A:498:ILE:HD13	2.38	0.53
1:A:334:HIS:CE1	1:A:581:HIS:HB3	2.42	0.53
1:A:63:GLN:O	1:A:120:PRO:HA	2.08	0.53
1:A:22:GLN:HG3	1:A:42:PHE:HA	1.91	0.52
1:A:402:SER:HB2	1:A:408:SER:HB3	1.91	0.52
1:A:398:THR:O	1:A:414:ALA:HA	2.09	0.52
1:A:174:ALA:HA	1:A:184:LEU:O	2.09	0.52
1:A:227:PHE:O	1:A:244:GLY:HA3	2.10	0.51
1:A:576:TYR:HE2	1:A:634:THR:HG23	1.76	0.51
1:A:260:TRP:C	1:A:261:ILE:HG13	2.31	0.50
1:A:169:ILE:HG22	1:A:191:ASN:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:SER:O	1:A:39:TRP:NE1	2.43	0.50
1:A:52:PRO:HA	1:A:128:ALA:O	2.11	0.49
1:A:39:TRP:O	1:A:139:SER:HA	2.13	0.49
1:A:458:GLN:HA	1:A:468:THR:O	2.13	0.49
1:A:282:ARG:HG2	1:A:303:SER:HA	1.95	0.49
1:A:261:ILE:HA	1:A:262:PRO:HD3	1.70	0.48
1:A:58:ASP:OD1	1:A:60:LYS:N	2.39	0.48
1:A:575:ARG:HD2	1:A:618:TRP:CZ2	2.49	0.48
1:A:448:PRO:HA	1:A:574:ILE:CD1	2.44	0.48
1:A:88:TYR:CE2	1:A:99:PRO:HD3	2.49	0.47
1:A:14:TRP:CD1	1:A:59:MET:HA	2.50	0.47
1:A:402:SER:HB2	1:A:403:PRO:HD2	1.96	0.47
1:A:317:VAL:O	1:A:320:MET:HG2	2.15	0.47
1:A:564:THR:HG21	1:A:568:ILE:HD13	1.97	0.46
1:A:35:LYS:O	6:A:926:HOH:O	2.21	0.46
1:A:59:MET:HB2	1:A:122:ARG:O	2.16	0.46
1:A:20:SER:HB2	1:A:41:THR:HA	1.98	0.46
1:A:89:LEU:CD2	1:A:124:VAL:HG22	2.45	0.46
1:A:448:PRO:HA	1:A:574:ILE:HD11	1.97	0.45
1:A:225:ASP:N	1:A:246:ASP:OD2	2.41	0.45
1:A:68:LEU:HA	1:A:144:ASN:O	2.16	0.45
1:A:5:ILE:HD12	1:A:490:SER:HB3	1.99	0.45
1:A:340:TRP:CG	1:A:341:LYS:N	2.85	0.45
1:A:78:GLN:HG2	1:A:81:TRP:CH2	2.51	0.45
1:A:495:TYR:O	1:A:496:HIS:HB2	2.17	0.45
1:A:182:ARG:HH11	1:A:182:ARG:HD3	1.54	0.45
1:A:56:THR:HG21	1:A:125:ARG:HH21	1.82	0.45
1:A:32:ASP:OD2	1:A:37:THR:OG1	2.35	0.44
1:A:228:CYS:N	1:A:229:PRO:HD3	2.32	0.44
1:A:192:ASP:HA	1:A:514:LEU:HD12	2.00	0.44
1:A:469:PRO:HB3	1:A:492:VAL:CG1	2.47	0.44
1:A:161:TRP:CE2	1:A:489:ASN:HB3	2.53	0.44
1:A:351:SER:O	1:A:371:ARG:NH1	2.45	0.44
1:A:576:TYR:CZ	1:A:619:MET:HG3	2.53	0.44
1:A:253:TYR:CE2	1:A:255:SER:HA	2.53	0.44
1:A:300:GLU:HG3	1:A:309:TRP:CZ3	2.54	0.43
1:A:135:GLN:HB3	1:A:136:PRO:CD	2.48	0.43
1:A:16:VAL:HG12	1:A:57:ILE:HG12	2.00	0.43
1:A:29:LYS:HB3	1:A:37:THR:HB	2.01	0.43
1:A:290:HIS:HE1	6:A:1031:HOH:O	2.02	0.43
1:A:529:THR:HA	1:A:530:PRO:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLY:O	1:A:272:TYR:HB2	2.19	0.43
1:A:67:GLY:HA2	1:A:114:SER:O	2.19	0.43
1:A:11:ARG:O	1:A:12:ASN:C	2.57	0.42
1:A:554:VAL:HG11	1:A:606:VAL:HG21	2.01	0.42
1:A:95:ASN:N	1:A:95:ASN:ND2	2.67	0.42
1:A:560:ILE:HD13	1:A:560:ILE:HG21	1.79	0.42
1:A:208:ASP:OD1	1:A:208:ASP:C	2.56	0.42
1:A:72:PRO:HG2	1:A:109:SER:CA	2.50	0.42
1:A:296:GLU:OE2	1:A:318:ASN:HB2	2.20	0.42
1:A:49:PRO:HB2	6:A:1022:HOH:O	2.18	0.42
1:A:595:THR:O	1:A:602:TYR:HA	2.20	0.42
1:A:95:ASN:N	1:A:95:ASN:HD22	2.17	0.42
1:A:146:PHE:CD1	1:A:146:PHE:N	2.87	0.41
1:A:464:PHE:CD1	1:A:515:CYS:HB3	2.55	0.41
1:A:402:SER:HB2	1:A:403:PRO:CD	2.50	0.41
1:A:69:SER:HB3	1:A:146:PHE:CE1	2.56	0.41
1:A:35:LYS:HG3	1:A:74:GLN:HG3	2.04	0.40
1:A:477:VAL:HA	1:A:478:PRO:HD2	1.98	0.40
1:A:541:ALA:HB1	1:A:628:VAL:HG21	2.04	0.40
1:A:283:VAL:O	1:A:301:VAL:HA	2.22	0.40
1:A:298:ASN:ND2	1:A:316:LYS:HA	2.37	0.40
1:A:183:VAL:O	1:A:206:SER:HA	2.22	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	637/639 (100%)	603 (95%)	31 (5%)	3 (0%)	34 30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	494	VAL
1	A	229	PRO

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	526/526 (100%)	499 (95%)	27 (5%)	29 26

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	17	THR
1	A	20	SER
1	A	61	THR
1	A	62	THR
1	A	68	LEU
1	A	84	ARG
1	A	94	THR
1	A	95	ASN
1	A	98	SER
1	A	108	ASP
1	A	152	THR
1	A	203	LEU
1	A	218	THR
1	A	229	PRO
1	A	256	SER
1	A	305	SER
1	A	350	PRO
1	A	385	ASN
1	A	408	SER
1	A	532	TYR
1	A	536	SER
1	A	545	LYS
1	A	556	VAL

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Mol	Chain	Res	Type
1	A	563	SER
1	A	570	LYS
1	A	639	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	22	GLN
1	A	78	GLN
1	A	95	ASN
1	A	290	HIS
1	A	298	ASN
1	A	597	ASN
1	A	600	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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	ACT	A	701	-	1,3,3	3.96	1 (100%)	0,3,3	0.00	-
5	ACT	A	703	2	1,3,3	3.64	1 (100%)	0,3,3	0.00	-
4	SO4	A	704	-	4,4,4	1.15	0	6,6,6	1.18	1 (16%)
5	ACT	A	705	-	1,3,3	3.53	1 (100%)	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ACT	A	701	-	-	0/0/0/0	0/0/0/0
5	ACT	A	703	2	-	0/0/0/0	0/0/0/0
4	SO4	A	704	-	-	0/0/0/0	0/0/0/0
5	ACT	A	705	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	705	ACT	CH3-C	3.53	1.53	1.48
5	A	703	ACT	CH3-C	3.64	1.53	1.48
5	A	701	ACT	CH3-C	3.96	1.54	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	704	SO4	O2-S-O1	2.64	117.85	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.