Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:15 PM GMT

PDB ID	:	1ESE
Title	:	THE MOLECULAR MECHANISM OF ENANTIORECOGNITION BY ESTERASES
Authors	:	Wei, Y.; Schottel, J.L.; Derewenda, U.; Swenson, L.; Patkar, S.; Derewenda, Z.S.
Deposited on	:	1994-10-07
Resolution	:	2.40 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 ⓘ symbol.

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

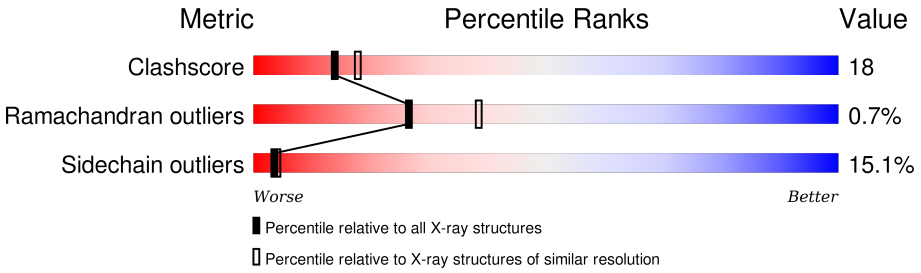
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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	306	42% 39% 14% 5% •

2 Entry composition

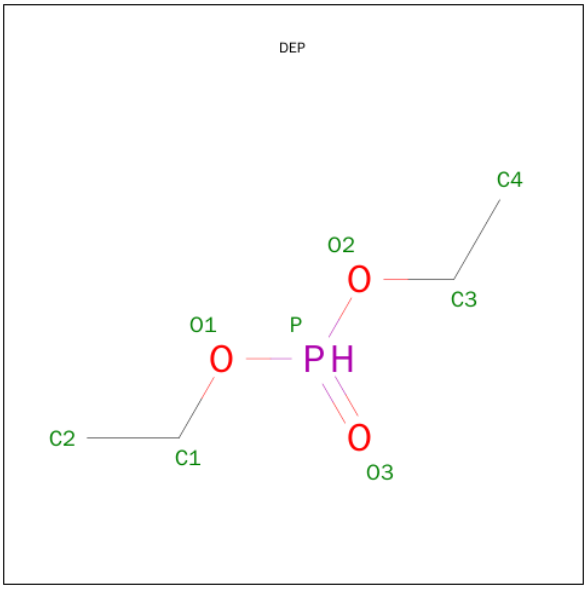
There are 3 unique types of molecules in this entry. The entry contains 2476 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	302	2295	1442	390	456	7	0	0	0

- Molecule 2 is DIETHYL PHOSPHONATE (three-letter code: DEP) (formula: $C_4H_{11}O_3P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	8	4	3	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	173	173	173	0	0

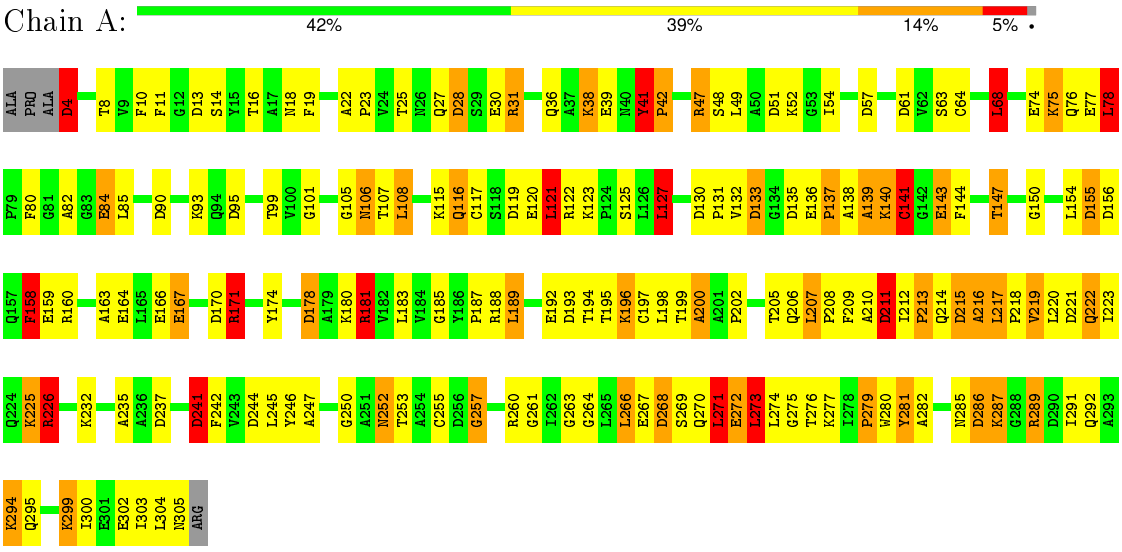
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: ESTERASE

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	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	130.39Å 48.52Å 70.19Å 90.00° 117.74° 90.00°	Depositor
Resolution (Å)	7.50 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (7.50-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2476	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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: DEP

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	2/2344 (0.1%)	2.49	145/3185 (4.6%)

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	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	GLU	CD-OE1	8.42	1.34	1.25
1	A	272	GLU	CD-OE2	6.95	1.33	1.25

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	160	ARG	NE-CZ-NH1	18.87	129.73	120.30
1	A	95	ASP	CB-CG-OD2	-16.88	103.11	118.30
1	A	289	ARG	NE-CZ-NH2	-15.82	112.39	120.30
1	A	156	ASP	CB-CG-OD2	-15.42	104.42	118.30
1	A	135	ASP	CB-CG-OD2	-13.82	105.86	118.30
1	A	192	GLU	CA-CB-CG	12.99	141.97	113.40
1	A	237	ASP	CB-CG-OD2	-12.46	107.08	118.30
1	A	95	ASP	CB-CG-OD1	12.09	129.18	118.30
1	A	237	ASP	CB-CG-OD1	11.84	128.96	118.30
1	A	28	ASP	CB-CG-OD1	11.69	128.82	118.30
1	A	28	ASP	CB-CG-OD2	-11.12	108.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	232	LYS	CA-CB-CG	11.11	137.84	113.40
1	A	160	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	A	51	ASP	CB-CG-OD2	-10.26	109.06	118.30
1	A	221	ASP	CB-CG-OD1	-10.24	109.09	118.30
1	A	160	ARG	CD-NE-CZ	9.94	137.52	123.60
1	A	133	ASP	CB-CG-OD1	9.87	127.18	118.30
1	A	206	GLN	CA-CB-CG	-9.87	91.70	113.40
1	A	222	GLN	CA-CB-CG	9.55	134.41	113.40
1	A	4	ASP	CB-CG-OD2	-9.42	109.82	118.30
1	A	57	ASP	CB-CG-OD1	-9.27	109.96	118.30
1	A	31	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	A	163	ALA	CB-CA-C	9.21	123.92	110.10
1	A	170	ASP	CB-CG-OD1	9.21	126.59	118.30
1	A	156	ASP	CB-CG-OD1	8.84	126.25	118.30
1	A	188	ARG	NE-CZ-NH2	8.55	124.58	120.30
1	A	274	LEU	CB-CA-C	8.25	125.88	110.20
1	A	270	GLN	CG-CD-OE1	8.18	137.96	121.60
1	A	160	ARG	CG-CD-NE	8.16	128.94	111.80
1	A	167	GLU	OE1-CD-OE2	8.15	133.08	123.30
1	A	132	VAL	CB-CA-C	8.02	126.64	111.40
1	A	181	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	192	GLU	CG-CD-OE1	7.80	133.91	118.30
1	A	143	GLU	CA-CB-CG	7.77	130.50	113.40
1	A	130	ASP	CB-CG-OD1	7.53	125.07	118.30
1	A	286	ASP	CB-CG-OD2	7.52	125.07	118.30
1	A	41	TYR	CB-CA-C	7.52	125.43	110.40
1	A	52	LYS	C-N-CA	7.50	138.05	122.30
1	A	27	GLN	CA-CB-CG	7.47	129.82	113.40
1	A	281	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	A	241	ASP	CB-CG-OD2	-7.35	111.69	118.30
1	A	171	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	171	ARG	CD-NE-CZ	-7.33	113.34	123.60
1	A	273	LEU	CB-CA-C	7.15	123.79	110.20
1	A	57	ASP	CB-CG-OD2	7.14	124.73	118.30
1	A	135	ASP	OD1-CG-OD2	7.12	136.82	123.30
1	A	48	SER	CB-CA-C	-7.10	96.61	110.10
1	A	51	ASP	OD1-CG-OD2	7.06	136.71	123.30
1	A	244	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	216	ALA	CB-CA-C	6.94	120.50	110.10
1	A	302	GLU	O-C-N	-6.92	111.63	122.70
1	A	174	TYR	CB-CG-CD1	6.89	125.13	121.00
1	A	78	LEU	CB-CG-CD2	-6.88	99.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	116	GLN	N-CA-CB	6.86	122.95	110.60
1	A	164	GLU	O-C-N	-6.79	111.83	122.70
1	A	19	PHE	O-C-N	6.77	134.71	123.20
1	A	125	SER	N-CA-CB	6.69	120.53	110.50
1	A	292	GLN	O-C-N	6.64	133.32	122.70
1	A	61	ASP	O-C-N	6.63	133.30	122.70
1	A	64	CYS	O-C-N	6.62	134.45	123.20
1	A	275	GLY	N-CA-C	-6.48	96.90	113.10
1	A	121	LEU	O-C-N	6.47	133.05	122.70
1	A	273	LEU	CA-C-N	6.46	131.42	117.20
1	A	130	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	119	ASP	N-CA-CB	6.33	121.99	110.60
1	A	292	GLN	N-CA-CB	6.31	121.96	110.60
1	A	232	LYS	N-CA-CB	6.29	121.93	110.60
1	A	160	ARG	CA-CB-CG	6.18	127.00	113.40
1	A	74	GLU	OE1-CD-OE2	6.16	130.70	123.30
1	A	268	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	28	ASP	N-CA-CB	-6.08	99.65	110.60
1	A	121	LEU	CA-C-O	-6.05	107.39	120.10
1	A	273	LEU	CA-C-O	-6.02	107.47	120.10
1	A	294	LYS	CA-C-O	6.02	132.73	120.10
1	A	302	GLU	C-N-CA	6.00	136.70	121.70
1	A	252	ASN	N-CA-CB	5.97	121.35	110.60
1	A	141	CYS	CA-C-N	5.96	128.11	116.20
1	A	174	TYR	CB-CG-CD2	-5.94	117.43	121.00
1	A	18	ASN	CB-CG-ND2	5.92	130.91	116.70
1	A	213	PRO	C-N-CA	5.92	136.50	121.70
1	A	181	ARG	NH1-CZ-NH2	-5.84	112.97	119.40
1	A	211	ASP	CB-CA-C	-5.81	98.77	110.40
1	A	188	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
1	A	219	VAL	CA-CB-CG1	5.80	119.60	110.90
1	A	38	LYS	CA-CB-CG	5.80	126.15	113.40
1	A	137	PRO	N-CA-CB	-5.79	96.23	102.60
1	A	61	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	68	LEU	CA-CB-CG	5.75	128.54	115.30
1	A	279	PRO	O-C-N	-5.75	113.50	122.70
1	A	133	ASP	N-CA-CB	5.72	120.90	110.60
1	A	122	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	289	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	A	221	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	281	TYR	CA-CB-CG	5.69	124.21	113.40
1	A	242	PHE	CB-CG-CD2	-5.68	116.82	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	GLU	OE1-CD-OE2	5.62	130.05	123.30
1	A	74	GLU	CG-CD-OE2	-5.62	107.06	118.30
1	A	22	ALA	CB-CA-C	5.60	118.50	110.10
1	A	93	LYS	CD-CE-NZ	5.60	124.57	111.70
1	A	270	GLN	CG-CD-NE2	-5.58	103.30	116.70
1	A	164	GLU	N-CA-CB	-5.49	100.71	110.60
1	A	127	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	159	GLU	CB-CG-CD	-5.47	99.42	114.20
1	A	235	ALA	N-CA-CB	-5.47	102.44	110.10
1	A	206	GLN	OE1-CD-NE2	5.44	134.42	121.90
1	A	61	ASP	N-CA-CB	5.44	120.40	110.60
1	A	200	ALA	CB-CA-C	5.44	118.26	110.10
1	A	178	ASP	N-CA-CB	-5.44	100.81	110.60
1	A	192	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	A	155	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	A	246	TYR	CB-CG-CD2	5.41	124.25	121.00
1	A	271	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	158	PHE	CB-CA-C	5.41	121.22	110.40
1	A	139	ALA	CB-CA-C	-5.39	102.01	110.10
1	A	108	LEU	N-CA-CB	5.38	121.16	110.40
1	A	250	GLY	C-N-CA	5.36	135.11	121.70
1	A	99	THR	CA-CB-CG2	5.36	119.91	112.40
1	A	226	ARG	CA-C-O	5.35	131.33	120.10
1	A	302	GLU	OE1-CD-OE2	-5.34	116.90	123.30
1	A	61	ASP	N-CA-C	-5.33	96.61	111.00
1	A	187	PRO	CB-CA-C	5.30	125.25	112.00
1	A	209	PHE	CA-C-O	-5.28	109.02	120.10
1	A	166	GLU	CB-CG-CD	5.25	128.38	114.20
1	A	90	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	A	84	GLU	CA-CB-CG	5.21	124.87	113.40
1	A	247	ALA	N-CA-CB	5.20	117.37	110.10
1	A	8	THR	CA-CB-CG2	5.19	119.67	112.40
1	A	47	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	A	159	GLU	CA-C-O	-5.18	109.21	120.10
1	A	13	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	A	25	THR	CA-CB-OG1	-5.16	98.17	109.00
1	A	164	GLU	CA-C-N	5.10	128.42	117.20
1	A	27	GLN	C-N-CA	5.09	134.42	121.70
1	A	225	LYS	C-N-CA	5.08	134.40	121.70
1	A	31	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	14	SER	N-CA-CB	5.07	118.10	110.50
1	A	49	LEU	CB-CA-C	5.07	119.83	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	143	GLU	CG-CD-OE2	5.06	128.42	118.30
1	A	141	CYS	CA-C-O	-5.05	109.49	120.10
1	A	106	ASN	CB-CG-OD1	-5.04	111.52	121.60
1	A	272	GLU	CB-CG-CD	-5.03	100.62	114.20
1	A	158	PHE	CB-CG-CD2	5.03	124.32	120.80
1	A	10	PHE	N-CA-CB	5.02	119.64	110.60
1	A	36	GLN	O-C-N	5.02	130.74	122.70
1	A	38	LYS	CA-C-O	5.00	130.61	120.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	ARG	Sidechain
1	A	31	ARG	Sidechain

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	2295	0	2210	83	1
2	A	8	0	10	1	0
3	A	173	0	0	12	1
All	All	2476	0	2220	83	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 18.

All (83) 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:120:GLU:HG2	1:A:266:LEU:HD21	1.50	0.93
1:A:193:ASP:OD1	1:A:195:THR:OG1	2.02	0.75
1:A:193:ASP:O	1:A:196:LYS:HG3	1.86	0.75
1:A:213:PRO:O	1:A:216:ALA:HB3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:THR:HG23	1:A:217:LEU:HD12	1.71	0.70
1:A:158:PHE:CZ	1:A:226:ARG:HB3	2.28	0.69
1:A:75:LYS:HG3	1:A:85:LEU:O	1.93	0.68
1:A:138:ALA:O	1:A:141:CYS:HB3	1.95	0.67
1:A:105:GLY:HA3	2:A:400:DEP:H41	1.78	0.65
1:A:120:GLU:HB2	1:A:211:ASP:OD2	1.95	0.65
1:A:139:ALA:HA	1:A:213:PRO:HG3	1.79	0.64
1:A:263:GLY:HA3	1:A:280:TRP:CG	2.33	0.63
1:A:210:ALA:HB2	1:A:266:LEU:HD22	1.80	0.63
1:A:281:TYR:O	1:A:282:ALA:HB3	1.98	0.62
1:A:195:THR:O	1:A:198:LEU:HB2	2.00	0.61
1:A:180:LYS:HE3	3:A:648:HOH:O	1.99	0.61
1:A:255:CYS:HA	3:A:548:HOH:O	2.00	0.60
1:A:141:CYS:SG	1:A:216:ALA:HB1	2.42	0.59
1:A:257:GLY:O	1:A:260:ARG:NH1	2.35	0.59
1:A:54:ILE:HG13	3:A:640:HOH:O	2.03	0.59
1:A:269:SER:OG	1:A:271:LEU:HB2	2.01	0.58
1:A:193:ASP:HB3	1:A:196:LYS:HD2	1.85	0.58
1:A:291:ILE:O	1:A:295:GLN:HG2	2.03	0.58
1:A:143:GLU:O	1:A:147:THR:N	2.37	0.57
1:A:272:GLU:HA	1:A:276:THR:O	2.04	0.57
1:A:39:GLU:OE1	1:A:47:ARG:NH2	2.37	0.57
1:A:300:ILE:O	1:A:304:LEU:HG	2.05	0.56
1:A:195:THR:HA	1:A:198:LEU:HD12	1.87	0.55
1:A:16:THR:HA	1:A:41:TYR:CE2	2.43	0.54
1:A:219:VAL:O	1:A:223:ILE:HG13	2.08	0.53
1:A:263:GLY:HA3	1:A:280:TRP:CD1	2.45	0.52
1:A:41:TYR:CG	1:A:42:PRO:HD3	2.45	0.52
1:A:140:LYS:HA	1:A:143:GLU:OE2	2.09	0.52
1:A:214:GLN:HA	1:A:217:LEU:HG	1.91	0.51
1:A:47:ARG:NH2	3:A:532:HOH:O	2.32	0.51
1:A:4:ASP:N	3:A:642:HOH:O	2.44	0.51
1:A:117:CYS:HB3	1:A:212:ILE:HG23	1.94	0.50
1:A:200:ALA:HB2	1:A:207:LEU:HD23	1.94	0.49
1:A:185:GLY:O	1:A:245:LEU:HD12	2.12	0.48
1:A:68:LEU:HB3	1:A:107:THR:OG1	2.14	0.48
1:A:75:LYS:HG2	1:A:84:GLU:HB3	1.96	0.48
1:A:76:GLN:O	1:A:84:GLU:HA	2.14	0.48
1:A:273:LEU:HA	1:A:273:LEU:HD12	1.72	0.48
1:A:305:ASN:ND2	3:A:650:HOH:O	2.46	0.47
1:A:68:LEU:HD22	1:A:106:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:O	1:A:277:LYS:HA	2.14	0.47
1:A:268:ASP:HB3	1:A:277:LYS:CB	2.44	0.47
1:A:267:GLU:O	1:A:279:PRO:HA	2.14	0.47
1:A:116:GLN:O	1:A:138:ALA:HA	2.15	0.47
1:A:120:GLU:O	1:A:123:LYS:HD2	2.16	0.46
1:A:78:LEU:HB3	1:A:82:ALA:HB3	1.98	0.46
1:A:133:ASP:HB3	1:A:136:GLU:HB2	1.97	0.45
1:A:178:ASP:HB2	3:A:622:HOH:O	2.16	0.45
1:A:215:ASP:O	1:A:218:PRO:HD2	2.17	0.45
1:A:268:ASP:HB3	1:A:277:LYS:HB3	1.98	0.45
1:A:196:LYS:NZ	1:A:196:LYS:HB3	2.32	0.45
1:A:181:ARG:HD3	3:A:658:HOH:O	2.17	0.45
1:A:141:CYS:SG	1:A:216:ALA:CB	3.06	0.44
1:A:295:GLN:HG3	3:A:600:HOH:O	2.17	0.44
1:A:199:THR:HG22	1:A:200:ALA:O	2.18	0.44
1:A:11:PHE:O	1:A:101:GLY:HA3	2.18	0.44
1:A:115:LYS:HG2	1:A:121:LEU:HB3	1.99	0.44
1:A:131:PRO:HD2	3:A:591:HOH:O	2.17	0.44
1:A:23:PRO:HB2	3:A:671:HOH:O	2.18	0.43
1:A:194:THR:O	1:A:194:THR:HG22	2.18	0.43
1:A:210:ALA:CB	1:A:266:LEU:HD22	2.46	0.43
1:A:167:GLU:OE2	1:A:171:ARG:NE	2.46	0.43
1:A:299:LYS:HA	1:A:299:LYS:HD3	1.92	0.43
1:A:241:ASP:CG	1:A:303:ILE:HD11	2.38	0.43
1:A:76:GLN:O	1:A:85:LEU:N	2.41	0.42
1:A:220:LEU:HA	1:A:220:LEU:HD23	1.68	0.42
1:A:267:GLU:HB2	3:A:546:HOH:O	2.20	0.42
1:A:189:LEU:O	1:A:253:THR:HB	2.19	0.42
1:A:294:LYS:HD2	1:A:295:GLN:NE2	2.35	0.42
1:A:287:LYS:HD2	1:A:291:ILE:HD11	2.02	0.41
1:A:264:GLY:O	1:A:280:TRP:HB2	2.21	0.41
1:A:144:PHE:CE1	1:A:150:GLY:HA3	2.56	0.41
1:A:183:LEU:HA	1:A:183:LEU:HD12	1.88	0.41
1:A:127:LEU:HG	1:A:281:TYR:CG	2.56	0.41
1:A:252:ASN:O	1:A:261:GLY:N	2.52	0.41
1:A:197:CYS:O	1:A:208:PRO:HD2	2.21	0.41
1:A:285:ASN:O	1:A:289:ARG:N	2.41	0.40
1:A:154:LEU:O	1:A:158:PHE:HB2	2.21	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:80:PHE:N	3:A:664:HOH:O[2_654]	2.07	0.13

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	300/306 (98%)	271 (90%)	27 (9%)	2 (1%)	26 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	GLY
1	A	202	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	239/241 (99%)	203 (85%)	36 (15%)	3 4

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

Mol	Chain	Res	Type
1	A	4	ASP
1	A	28	ASP
1	A	38	LYS
1	A	41	TYR

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Mol	Chain	Res	Type
1	A	42	PRO
1	A	63	SER
1	A	68	LEU
1	A	75	LYS
1	A	78	LEU
1	A	108	LEU
1	A	121	LEU
1	A	127	LEU
1	A	137	PRO
1	A	140	LYS
1	A	141	CYS
1	A	147	THR
1	A	155	ASP
1	A	158	PHE
1	A	171	ARG
1	A	189	LEU
1	A	196	LYS
1	A	205	THR
1	A	207	LEU
1	A	211	ASP
1	A	215	ASP
1	A	217	LEU
1	A	222	GLN
1	A	225	LYS
1	A	226	ARG
1	A	241	ASP
1	A	266	LEU
1	A	271	LEU
1	A	273	LEU
1	A	286	ASP
1	A	287	LYS
1	A	299	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	94	GLN
1	A	228	ASN
1	A	295	GLN

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

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
2	DEP	A	400	1	2,7,7	1.76	0	2,7,7	1.53	0

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
2	DEP	A	400	1	-	0/2/6/6	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	DEP	1	0

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

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.