Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:42 am BST

PDB ID	:	1ESD
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	:	2.30 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
https://www.wwpdb.org/validation/2017/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:

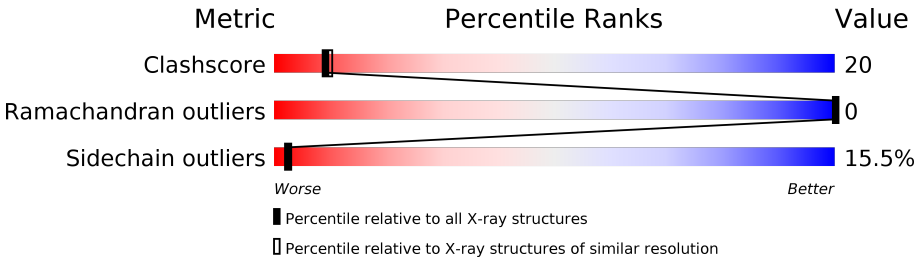
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	42% 39% 14%

2 Entry composition

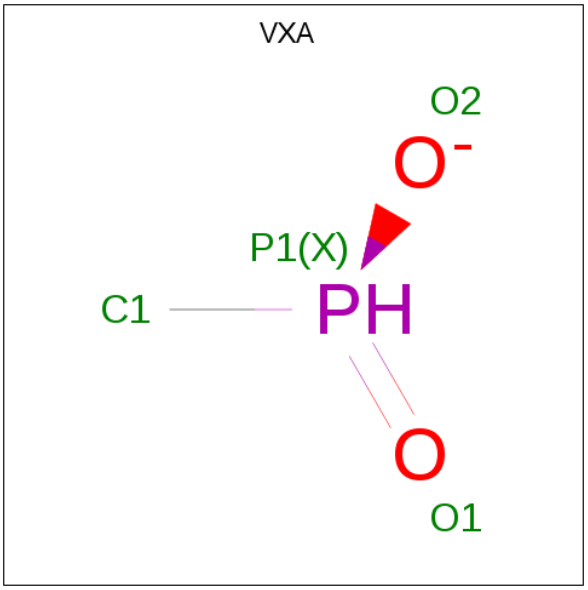
There are 3 unique types of molecules in this entry. The entry contains 2484 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 METHYLPHOSPHONIC ACID ESTER GROUP (three-letter code: VXA) (formula: CH_4O_2P).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	185	185	185	0	0

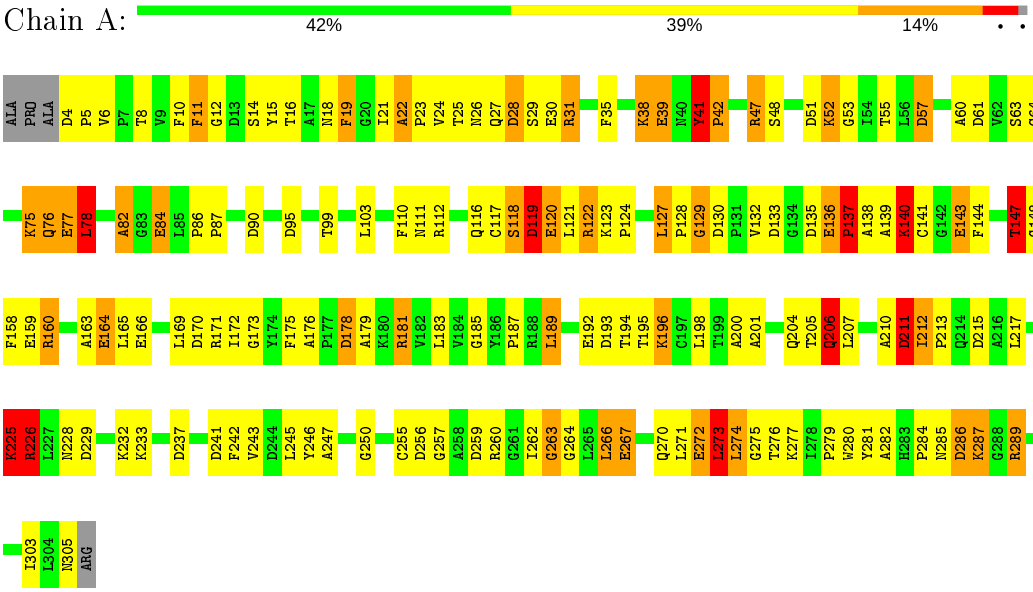
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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 is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	131.13Å 48.60Å 70.35Å 90.00° 118.03° 90.00°	Depositor
Resolution (Å)	7.50 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (7.50-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2484	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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: VXA

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	1.10	3/2344 (0.1%)	2.50	141/3185 (4.4%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	GLU	CD-OE1	9.41	1.35	1.25
1	A	272	GLU	CD-OE2	8.35	1.34	1.25
1	A	117	CYS	CB-SG	-5.94	1.72	1.81

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289	ARG	NE-CZ-NH1	16.91	128.75	120.30
1	A	237	ASP	CB-CG-OD1	16.15	132.83	118.30
1	A	192	GLU	CA-CB-CG	16.06	148.72	113.40
1	A	112	ARG	NE-CZ-NH2	-14.67	112.96	120.30
1	A	237	ASP	CB-CG-OD2	-14.30	105.43	118.30
1	A	232	LYS	CA-CB-CG	14.18	144.60	113.40
1	A	181	ARG	NE-CZ-NH1	13.71	127.16	120.30
1	A	156	ASP	CB-CG-OD2	-12.72	106.85	118.30
1	A	28	ASP	CB-CG-OD2	-11.98	107.52	118.30
1	A	31	ARG	NE-CZ-NH2	-11.86	114.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	206	GLN	CA-CB-CG	-10.93	89.37	113.40
1	A	221	ASP	CB-CG-OD1	-10.35	108.98	118.30
1	A	95	ASP	CB-CG-OD1	10.21	127.49	118.30
1	A	226	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	A	192	GLU	CG-CD-OE1	10.00	138.29	118.30
1	A	222	GLN	CA-CB-CG	9.79	134.93	113.40
1	A	286	ASP	CB-CG-OD2	9.68	127.01	118.30
1	A	119	ASP	CB-CG-OD2	-9.66	109.60	118.30
1	A	38	LYS	CA-CB-CG	9.56	134.44	113.40
1	A	140	LYS	CD-CE-NZ	9.35	133.21	111.70
1	A	164	GLU	OE1-CD-OE2	-9.19	112.28	123.30
1	A	28	ASP	CB-CG-OD1	9.15	126.54	118.30
1	A	221	ASP	CB-CG-OD2	9.13	126.51	118.30
1	A	259	ASP	CB-CG-OD1	9.11	126.50	118.30
1	A	274	LEU	CB-CA-C	9.09	127.47	110.20
1	A	206	GLN	O-C-N	8.85	136.86	122.70
1	A	289	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	A	156	ASP	CB-CG-OD1	8.61	126.05	118.30
1	A	242	PHE	CB-CG-CD1	8.58	126.81	120.80
1	A	242	PHE	CB-CG-CD2	-8.56	114.81	120.80
1	A	120	GLU	CA-CB-CG	8.39	131.86	113.40
1	A	47	ARG	NE-CZ-NH1	-8.35	116.13	120.30
1	A	286	ASP	CB-CG-OD1	-8.33	110.80	118.30
1	A	82	ALA	CB-CA-C	8.27	122.51	110.10
1	A	170	ASP	CB-CG-OD1	8.18	125.66	118.30
1	A	122	ARG	NE-CZ-NH2	8.17	124.38	120.30
1	A	132	VAL	CB-CA-C	8.10	126.79	111.40
1	A	259	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	A	51	ASP	CB-CG-OD1	-7.79	111.29	118.30
1	A	143	GLU	CG-CD-OE2	7.66	133.62	118.30
1	A	77	GLU	CA-CB-CG	7.57	130.04	113.40
1	A	60	ALA	O-C-N	7.47	134.65	122.70
1	A	119	ASP	N-CA-CB	7.38	123.88	110.60
1	A	78	LEU	CB-CG-CD2	-7.34	98.53	111.00
1	A	159	GLU	O-C-N	7.16	134.16	122.70
1	A	143	GLU	OE1-CD-OE2	-7.11	114.77	123.30
1	A	11	PHE	CB-CG-CD2	7.09	125.77	120.80
1	A	206	GLN	N-CA-CB	7.01	123.22	110.60
1	A	68	LEU	CA-CB-CG	7.00	131.41	115.30
1	A	275	GLY	N-CA-C	-7.00	95.61	113.10
1	A	136	GLU	CG-CD-OE2	-6.99	104.32	118.30
1	A	41	TYR	CB-CG-CD2	-6.99	116.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	170	ASP	CA-C-O	-6.87	105.67	120.10
1	A	211	ASP	CB-CA-C	-6.85	96.71	110.40
1	A	135	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	A	112	ARG	CD-NE-CZ	6.83	133.16	123.60
1	A	95	ASP	CB-CG-OD2	-6.82	112.17	118.30
1	A	26	ASN	C-N-CA	6.58	138.16	121.70
1	A	42	PRO	O-C-N	-6.56	112.20	122.70
1	A	18	ASN	CB-CG-OD1	-6.52	108.56	121.60
1	A	163	ALA	CB-CA-C	6.42	119.73	110.10
1	A	6	VAL	CA-C-O	-6.39	106.67	120.10
1	A	181	ARG	NH1-CZ-NH2	-6.39	112.37	119.40
1	A	192	GLU	CG-CD-OE2	-6.37	105.57	118.30
1	A	225	LYS	C-N-CA	6.36	137.60	121.70
1	A	61	ASP	N-CA-C	-6.35	93.86	111.00
1	A	130	ASP	CB-CG-OD2	-6.32	112.62	118.30
1	A	39	GLU	CG-CD-OE2	6.25	130.80	118.30
1	A	170	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	A	305	ASN	CA-C-O	-6.24	107.00	120.10
1	A	192	GLU	OE1-CD-OE2	-6.21	115.85	123.30
1	A	99	THR	N-CA-CB	6.20	122.07	110.30
1	A	61	ASP	N-CA-CB	6.19	121.74	110.60
1	A	147	THR	OG1-CB-CG2	6.16	124.16	110.00
1	A	28	ASP	N-CA-CB	-6.09	99.63	110.60
1	A	57	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	206	GLN	CB-CA-C	-6.08	98.23	110.40
1	A	183	LEU	CB-CA-C	6.06	121.71	110.20
1	A	76	GLN	N-CA-CB	6.02	121.44	110.60
1	A	256	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	53	GLY	CA-C-O	-6.02	109.77	120.60
1	A	232	LYS	CG-CD-CE	5.98	129.83	111.90
1	A	112	ARG	NH1-CZ-NH2	5.98	125.97	119.40
1	A	18	ASN	CB-CG-ND2	5.95	130.99	116.70
1	A	270	GLN	CG-CD-OE1	5.95	133.50	121.60
1	A	273	LEU	CA-C-O	-5.94	107.63	120.10
1	A	117	CYS	CA-CB-SG	-5.94	103.31	114.00
1	A	173	GLY	C-N-CA	5.88	136.41	121.70
1	A	143	GLU	CB-CG-CD	5.85	129.99	114.20
1	A	19	PHE	CB-CG-CD1	-5.84	116.71	120.80
1	A	75	LYS	CB-CA-C	-5.83	98.73	110.40
1	A	41	TYR	CB-CA-C	5.81	122.01	110.40
1	A	229	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	31	ARG	NE-CZ-NH1	5.71	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	ASP	OD1-CG-OD2	5.68	134.09	123.30
1	A	194	THR	CA-CB-OG1	-5.68	97.08	109.00
1	A	271	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	60	ALA	CA-C-O	-5.62	108.31	120.10
1	A	178	ASP	N-CA-CB	-5.59	100.54	110.60
1	A	147	THR	N-CA-CB	-5.59	99.68	110.30
1	A	129	GLY	C-N-CA	5.59	135.67	121.70
1	A	273	LEU	CA-C-N	5.58	129.47	117.20
1	A	27	GLN	CA-CB-CG	5.57	125.64	113.40
1	A	147	THR	CA-CB-OG1	-5.55	97.34	109.00
1	A	133	ASP	N-CA-CB	5.54	120.58	110.60
1	A	212	ILE	CB-CA-C	5.53	122.66	111.60
1	A	225	LYS	O-C-N	-5.52	113.87	122.70
1	A	287	LYS	CA-CB-CG	5.50	125.49	113.40
1	A	48	SER	N-CA-CB	5.45	118.67	110.50
1	A	137	PRO	N-CA-CB	-5.41	96.65	102.60
1	A	47	ARG	CD-NE-CZ	-5.40	116.04	123.60
1	A	166	GLU	CG-CD-OE2	-5.40	107.50	118.30
1	A	14	SER	O-C-N	-5.38	114.10	122.70
1	A	22	ALA	N-CA-CB	5.38	117.63	110.10
1	A	110	PHE	CB-CA-C	5.38	121.16	110.40
1	A	192	GLU	N-CA-CB	5.38	120.28	110.60
1	A	121	LEU	CB-CA-C	5.30	120.27	110.20
1	A	285	ASN	CB-CA-C	5.29	120.98	110.40
1	A	64	CYS	O-C-N	5.25	132.12	123.20
1	A	35	PHE	CB-CG-CD2	-5.24	117.13	120.80
1	A	8	THR	CA-CB-CG2	5.23	119.72	112.40
1	A	86	PRO	N-CA-CB	-5.23	96.85	102.60
1	A	52	LYS	CB-CG-CD	-5.20	98.07	111.60
1	A	267	GLU	OE1-CD-OE2	5.20	129.54	123.30
1	A	21	ILE	CB-CA-C	5.20	121.99	111.60
1	A	159	GLU	CA-C-O	-5.19	109.20	120.10
1	A	263	GLY	O-C-N	-5.18	114.39	123.20
1	A	250	GLY	C-N-CA	5.14	134.56	121.70
1	A	181	ARG	CD-NE-CZ	-5.13	116.41	123.60
1	A	247	ALA	CA-C-N	5.13	126.46	116.20
1	A	140	LYS	CA-CB-CG	5.13	124.68	113.40
1	A	11	PHE	CB-CG-CD1	-5.13	117.21	120.80
1	A	246	TYR	O-C-N	-5.13	114.50	122.70
1	A	25	THR	CA-CB-CG2	5.12	119.58	112.40
1	A	217	LEU	CB-CA-C	5.10	119.89	110.20
1	A	24	VAL	N-CA-CB	-5.09	100.29	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	57	ASP	CB-CA-C	5.09	120.58	110.40
1	A	255	CYS	N-CA-CB	-5.08	101.46	110.60
1	A	256	ASP	CA-CB-CG	-5.06	102.27	113.40
1	A	120	GLU	N-CA-CB	-5.05	101.51	110.60
1	A	155	ASP	O-C-N	5.01	130.72	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	90	0
2	A	4	0	3	0	0
3	A	185	0	0	22	0
All	All	2484	0	2213	90	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 20.

All (90) 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:206:GLN:HB2	3:A:643:HOH:O	1.63	0.97
1:A:195:THR:HA	1:A:198:LEU:HD12	1.57	0.86
1:A:206:GLN:NE2	3:A:642:HOH:O	2.15	0.80
1:A:281:TYR:O	1:A:282:ALA:HB3	1.86	0.76
1:A:272:GLU:HA	1:A:276:THR:O	1.87	0.75
1:A:193:ASP:O	1:A:196:LYS:HG3	1.89	0.72
1:A:119:ASP:HA	1:A:122:ARG:HG3	1.72	0.71
1:A:52:LYS:HD2	3:A:580:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:THR:O	1:A:198:LEU:HB2	1.92	0.68
1:A:224:GLN:HG2	3:A:670:HOH:O	1.94	0.67
1:A:169:LEU:O	1:A:181:ARG:NH1	2.29	0.66
1:A:178:ASP:HB2	3:A:570:HOH:O	1.97	0.65
1:A:206:GLN:O	3:A:676:HOH:O	2.14	0.65
1:A:206:GLN:HG2	3:A:649:HOH:O	1.98	0.63
1:A:243:VAL:HG22	1:A:299:LYS:HG2	1.82	0.61
1:A:120:GLU:HB2	1:A:211:ASP:OD2	2.01	0.60
1:A:224:GLN:NE2	3:A:670:HOH:O	2.34	0.60
1:A:185:GLY:O	1:A:245:LEU:HD12	2.03	0.59
1:A:78:LEU:HB3	1:A:82:ALA:HB3	1.83	0.59
1:A:147:THR:HG22	3:A:632:HOH:O	2.02	0.59
1:A:263:GLY:HA3	1:A:280:TRP:CG	2.38	0.59
1:A:158:PHE:CZ	1:A:226:ARG:HB3	2.40	0.57
1:A:136:GLU:HG2	3:A:630:HOH:O	2.05	0.57
1:A:228:ASN:HA	3:A:505:HOH:O	2.05	0.55
1:A:4:ASP:N	3:A:578:HOH:O	2.38	0.55
1:A:200:ALA:HA	3:A:676:HOH:O	2.06	0.55
1:A:294:LYS:HD2	1:A:295:GLN:HE21	1.71	0.55
1:A:128:PRO:HB3	3:A:658:HOH:O	2.07	0.55
1:A:264:GLY:O	1:A:280:TRP:HB2	2.07	0.55
1:A:19:PHE:HB2	3:A:501:HOH:O	2.08	0.54
1:A:187:PRO:HG2	1:A:262:ILE:HD11	1.90	0.53
1:A:172:ILE:HG21	1:A:181:ARG:HG2	1.91	0.53
1:A:111:ASN:ND2	1:A:128:PRO:O	2.38	0.52
1:A:136:GLU:HG3	1:A:144:PHE:CD1	2.44	0.52
1:A:120:GLU:HG2	1:A:266:LEU:HD21	1.92	0.52
1:A:294:LYS:HD2	1:A:295:GLN:NE2	2.25	0.52
1:A:263:GLY:HA3	1:A:280:TRP:CD1	2.45	0.52
1:A:111:ASN:HD22	1:A:129:GLY:HA3	1.75	0.52
1:A:171:ARG:O	1:A:175:PHE:HD2	1.94	0.51
1:A:137:PRO:O	1:A:138:ALA:C	2.49	0.50
1:A:111:ASN:ND2	1:A:129:GLY:HA3	2.27	0.50
1:A:189:LEU:HD12	1:A:262:ILE:HG13	1.94	0.50
1:A:140:LYS:HE3	1:A:143:GLU:CD	2.32	0.50
1:A:267:GLU:O	1:A:279:PRO:HA	2.12	0.50
1:A:172:ILE:CG2	1:A:181:ARG:HD3	2.43	0.49
1:A:241:ASP:CB	1:A:303:ILE:HD11	2.43	0.49
1:A:245:LEU:N	3:A:520:HOH:O	2.45	0.49
1:A:69:ILE:CD1	1:A:165:LEU:HG	2.43	0.49
1:A:210:ALA:HB2	1:A:266:LEU:CD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ARG:NH1	3:A:637:HOH:O	2.35	0.48
1:A:5:PRO:HA	1:A:55:THR:HG22	1.93	0.48
1:A:69:ILE:HD13	1:A:165:LEU:CD2	2.43	0.48
1:A:76:GLN:O	1:A:84:GLU:HA	2.14	0.48
1:A:210:ALA:HB2	1:A:266:LEU:HD22	1.95	0.48
1:A:69:ILE:HD13	1:A:165:LEU:HG	1.96	0.47
1:A:257:GLY:O	1:A:260:ARG:NH1	2.47	0.47
1:A:241:ASP:CG	1:A:303:ILE:HD11	2.34	0.47
1:A:200:ALA:HB2	1:A:207:LEU:HD23	1.95	0.47
1:A:136:GLU:HA	1:A:136:GLU:OE2	2.14	0.47
1:A:128:PRO:HG2	3:A:672:HOH:O	2.15	0.47
1:A:158:PHE:CZ	1:A:226:ARG:HD2	2.50	0.47
1:A:22:ALA:HB1	1:A:23:PRO:HA	1.97	0.47
1:A:87:PRO:O	1:A:90:ASP:HB2	2.14	0.47
1:A:127:LEU:HD22	1:A:128:PRO:HD2	1.97	0.46
1:A:143:GLU:O	1:A:147:THR:N	2.40	0.46
1:A:12:GLY:HA2	1:A:103:LEU:HG	1.96	0.46
1:A:201:ALA:O	1:A:204:GLN:HB2	2.16	0.45
1:A:176:ALA:O	1:A:179:ALA:HB3	2.15	0.45
1:A:281:TYR:O	1:A:282:ALA:CB	2.55	0.45
1:A:15:TYR:CE2	1:A:284:PRO:HD3	2.51	0.45
1:A:128:PRO:CB	3:A:658:HOH:O	2.65	0.44
1:A:41:TYR:CG	1:A:42:PRO:HD3	2.53	0.44
1:A:123:LYS:HB3	1:A:124:PRO:HD2	1.99	0.44
1:A:10:PHE:CG	1:A:42:PRO:HB3	2.52	0.44
1:A:137:PRO:HD2	1:A:140:LYS:HB2	2.01	0.43
1:A:78:LEU:HD12	1:A:78:LEU:HA	1.84	0.43
1:A:148:GLY:N	3:A:632:HOH:O	2.50	0.43
1:A:172:ILE:HG22	1:A:181:ARG:HD3	2.01	0.42
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.89	0.41
1:A:273:LEU:HD13	1:A:273:LEU:HA	1.66	0.41
1:A:164:GLU:OE1	3:A:623:HOH:O	2.22	0.41
1:A:11:PHE:O	1:A:16:THR:HG21	2.20	0.41
1:A:116:GLN:O	1:A:138:ALA:HA	2.21	0.41
1:A:225:LYS:HD3	3:A:528:HOH:O	2.21	0.41
1:A:289:ARG:HD2	1:A:289:ARG:O	2.21	0.40
1:A:139:ALA:HA	1:A:213:PRO:HG3	2.03	0.40
1:A:277:LYS:HA	1:A:277:LYS:HD2	1.81	0.40
1:A:299:LYS:HA	1:A:299:LYS:HD3	1.92	0.40
1:A:39:GLU:OE1	1:A:47:ARG:NH2	2.53	0.40
1:A:118:SER:HB2	1:A:212:ILE:CG1	2.51	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	300/306 (98%)	276 (92%)	24 (8%)	0	100 100

There are no Ramachandran outliers to report.

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%)	202 (84%)	37 (16%)	2 2

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	29	SER
1	A	38	LYS
1	A	41	TYR
1	A	57	ASP
1	A	63	SER
1	A	68	LEU
1	A	70	HIS
1	A	75	LYS
1	A	77	GLU

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Mol	Chain	Res	Type
1	A	78	LEU
1	A	84	GLU
1	A	118	SER
1	A	119	ASP
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	160	ARG
1	A	189	LEU
1	A	196	LYS
1	A	205	THR
1	A	206	GLN
1	A	211	ASP
1	A	215	ASP
1	A	222	GLN
1	A	225	LYS
1	A	226	ARG
1	A	233	LYS
1	A	266	LEU
1	A	273	LEU
1	A	274	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	97	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 (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)

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	VXA	A	400	-	0,3,3	0.00	-	0,3,3	0.00	-

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.

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 (i)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.