



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:21 PM GMT

PDB ID : 1OLM  
Title : SUPERNATANT PROTEIN FACTOR IN COMPLEX WITH RRR-ALPHA-  
-TOCOPHERYLQUINONE: A LINK BETWEEN OXIDIZED VITAMIN E  
AND CHOLESTEROL BIOSYNTHESIS  
Authors : Stocker, A.; Baumann, U.  
Deposited on : 2003-08-08  
Resolution : 1.95 Å(reported)

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

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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

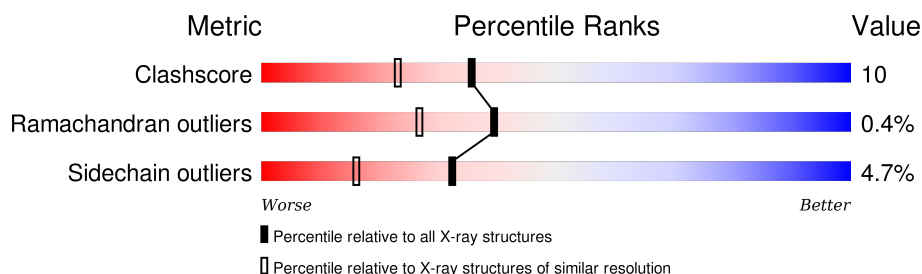
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	403	 79% 15% . .
1	C	403	 81% 13% . .
2	E	403	 78% 17% ..

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10464 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 SEC14-LIKE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	2
			3183	2038	544	582	19			
1	C	385	Total	C	N	O	S	0	0	1
			3106	1993	525	570	18			

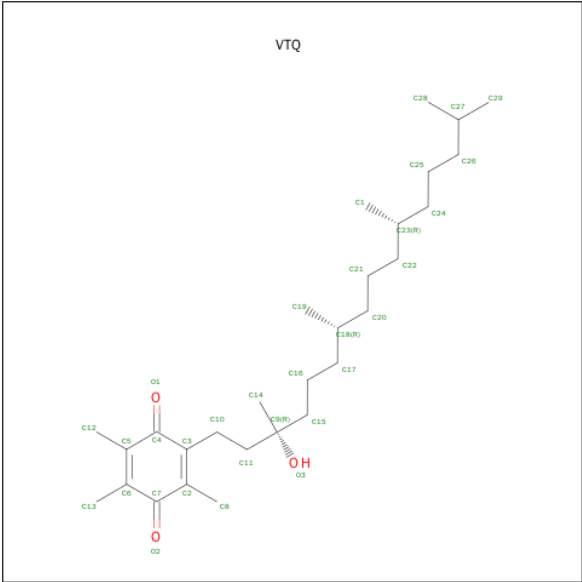
- Molecule 2 is a protein called SEC14-LIKE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	397	Total	C	N	O	S	0	0	0
			3204	2052	547	586	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	322	LYS	THR	CONFLICT	UNP 076054

- Molecule 3 is RRR-ALPHA-TOCOPHERYLQUINONE (three-letter code: VTQ) (formula:  $C_{29}H_{50}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			32	29	3		
3	C	1	Total	C	O	0	0
			32	29	3		
3	E	1	Total	C	O	0	0
			32	29	3		

- Molecule 4 is water.

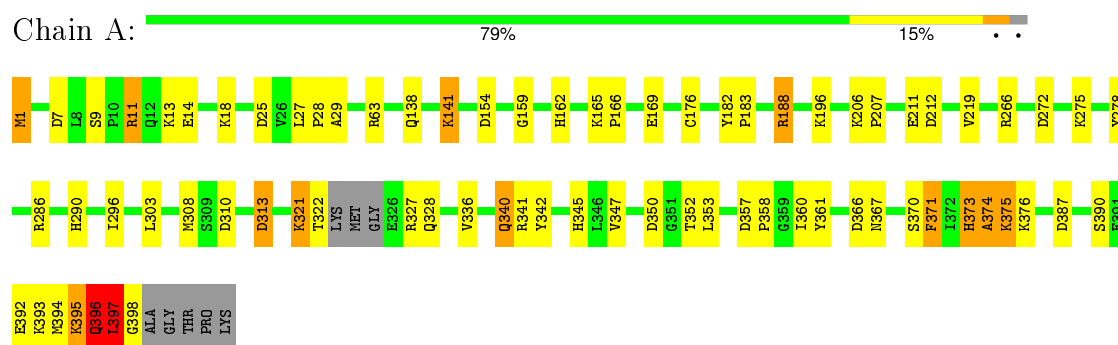
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	299	Total	O	0	0
			299	299		
4	C	295	Total	O	0	0
			295	295		
4	E	281	Total	O	0	0
			281	281		

### 3 Residue-property plots

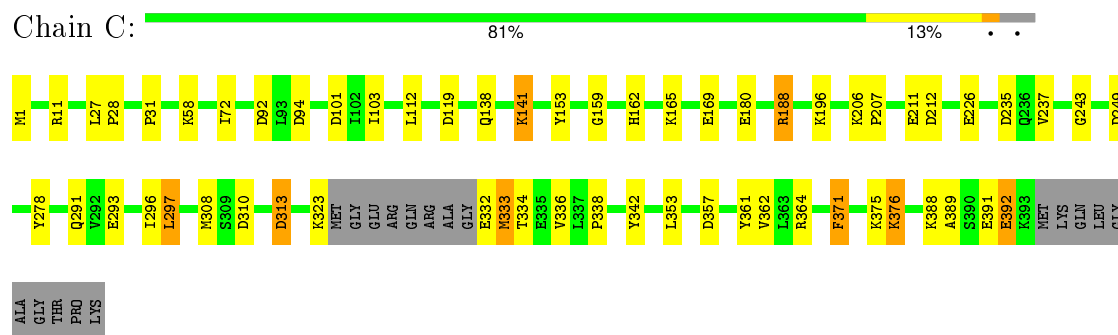
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

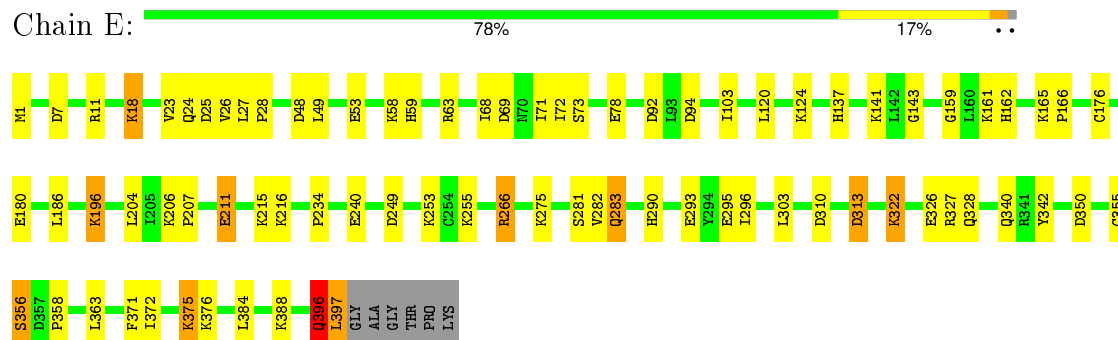
#### • Molecule 1: SEC14-LIKE PROTEIN 2



#### • Molecule 1: SEC14-LIKE PROTEIN 2



#### • Molecule 2: SEC14-LIKE PROTEIN 2



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.86Å 84.62Å 87.45Å 116.20° 102.64° 100.24°	Depositor
Resolution (Å)	19.65 – 1.95	Depositor
% Data completeness (in resolution range)	100.0 (19.65-1.95)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.180 , 0.211	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10464	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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: VTQ

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	0.49	1/3258 (0.0%)	0.68	9/4401 (0.2%)
1	C	0.49	0/3181	0.70	10/4301 (0.2%)
2	E	0.44	0/3280	0.68	9/4430 (0.2%)
All	All	0.47	1/9719 (0.0%)	0.69	28/13132 (0.2%)

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
2	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	397	LEU	C-N	-5.19	1.23	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	313	ASP	CB-CG-OD2	7.73	125.25	118.30
1	C	310	ASP	CB-CG-OD2	6.75	124.37	118.30
2	E	92	ASP	CB-CG-OD2	6.68	124.31	118.30
2	E	313	ASP	CB-CG-OD2	6.48	124.13	118.30
2	E	350	ASP	CB-CG-OD2	6.04	123.74	118.30
1	C	212	ASP	CB-CG-OD2	5.59	123.33	118.30
2	E	48	ASP	CB-CG-OD2	5.54	123.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ASP	CB-CG-OD2	5.51	123.26	118.30
2	E	69	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	92	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	25	ASP	CB-CG-OD2	5.49	123.24	118.30
2	E	7	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	357	ASP	CB-CG-OD2	5.38	123.14	118.30
2	E	25	ASP	CB-CG-OD2	5.31	123.08	118.30
2	E	94	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	272	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	310	ASP	CB-CG-OD2	5.26	123.03	118.30
2	E	249	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	212	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	235	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	119	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	154	ASP	CB-CG-OD2	5.17	122.96	118.30
1	C	94	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	350	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	387	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	249	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	101	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	366	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	373	HIS	Peptide
2	E	396	GLN	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3183	0	3183	72	0
1	C	3106	0	3101	52	0
2	E	3204	0	3204	61	0
3	A	32	0	50	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	32	0	50	3	0
3	E	32	0	50	1	0
4	A	299	0	0	22	1
4	C	295	0	0	13	1
4	E	281	0	0	27	0
All	All	10464	0	9638	186	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 10.

All (186) 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:C:188:ARG:HD3	4:C:2156:HOH:O	1.41	1.19
1:C:364:ARG:HD3	4:C:2274:HOH:O	1.38	1.19
1:A:176:CYS:HB3	4:A:2162:HOH:O	1.44	1.14
1:C:188:ARG:HH11	1:C:188:ARG:HG2	0.99	1.11
1:A:211:GLU:HG3	4:A:2180:HOH:O	1.48	1.09
1:A:371:PHE:O	1:A:371:PHE:HD1	1.32	1.08
2:E:27:LEU:HB3	4:E:2014:HOH:O	0.91	1.07
1:C:188:ARG:HH11	1:C:188:ARG:CG	1.72	1.02
2:E:397:LEU:HD22	4:E:2279:HOH:O	1.63	0.97
1:C:291:GLN:HE21	1:C:364:ARG:HE	0.98	0.96
3:A:1322:VTQ:H8C1	4:A:2298:HOH:O	1.63	0.96
1:A:188:ARG:HH11	1:A:188:ARG:CG	1.80	0.93
2:E:388:LYS:HE3	4:E:2273:HOH:O	1.67	0.93
1:C:188:ARG:HG2	1:C:188:ARG:NH1	1.82	0.92
1:A:188:ARG:NH1	1:A:188:ARG:CB	2.34	0.91
1:A:188:ARG:HH11	1:A:188:ARG:CB	1.84	0.90
1:C:159:GLY:H	1:C:162:HIS:HD2	1.21	0.88
1:A:1:MET:HE3	4:A:2001:HOH:O	1.74	0.87
1:C:138:GLN:HE22	1:C:141:LYS:HE2	1.39	0.86
1:A:371:PHE:CD1	1:A:371:PHE:O	2.25	0.86
2:E:322:LYS:H	2:E:328:GLN:HE22	1.24	0.85
3:E:1398:VTQ:H8C1	4:E:2281:HOH:O	1.77	0.85
1:A:371:PHE:HA	4:A:2283:HOH:O	1.76	0.84
1:A:290:HIS:HD2	4:A:2246:HOH:O	1.61	0.82
1:A:313:ASP:HB2	1:A:342:TYR:O	1.79	0.81
2:E:137:HIS:HD2	4:E:2093:HOH:O	1.63	0.81
2:E:159:GLY:H	2:E:162:HIS:HD2	1.28	0.81
1:A:188:ARG:HB3	1:A:188:ARG:NH1	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ALA:HB3	4:A:2028:HOH:O	1.81	0.80
1:A:188:ARG:HG2	1:A:188:ARG:HH11	1.48	0.78
2:E:137:HIS:HE1	4:E:2095:HOH:O	1.65	0.78
1:C:291:GLN:NE2	1:C:364:ARG:HE	1.81	0.77
1:C:297:LEU:HD12	4:C:2236:HOH:O	1.83	0.77
1:A:371:PHE:C	1:A:371:PHE:HD1	1.88	0.76
1:A:188:ARG:HH11	1:A:188:ARG:HB3	1.51	0.76
1:C:291:GLN:HE21	1:C:364:ARG:NE	1.81	0.75
1:A:159:GLY:H	1:A:162:HIS:HD2	1.35	0.75
2:E:240:GLU:OE1	4:E:2168:HOH:O	2.04	0.75
1:C:159:GLY:H	1:C:162:HIS:CD2	2.06	0.73
2:E:340:GLN:HG3	4:E:2239:HOH:O	1.87	0.73
2:E:397:LEU:CD2	4:E:2279:HOH:O	2.27	0.73
1:A:396:GLN:O	1:A:397:LEU:C	2.29	0.72
1:C:391:GLU:O	1:C:392:GLU:C	2.30	0.71
2:E:49:LEU:HB3	4:E:2034:HOH:O	1.91	0.70
1:C:364:ARG:HD2	4:C:2273:HOH:O	1.90	0.69
1:A:1:MET:HA	4:A:2001:HOH:O	1.94	0.67
2:E:11:ARG:HB2	2:E:11:ARG:NH1	2.10	0.67
1:C:196:LYS:HD2	4:C:2165:HOH:O	1.95	0.67
1:C:58:LYS:HE2	1:C:180:GLU:OE2	1.95	0.67
1:A:373:HIS:O	1:A:375:LYS:N	2.28	0.66
2:E:159:GLY:H	2:E:162:HIS:CD2	2.09	0.66
2:E:397:LEU:HD13	4:E:2156:HOH:O	1.95	0.66
2:E:23:VAL:HG12	2:E:53:GLU:HG3	1.78	0.65
1:A:159:GLY:H	1:A:162:HIS:CD2	2.14	0.65
2:E:28:PRO:HD2	4:E:2013:HOH:O	1.96	0.65
1:A:138:GLN:HE22	1:A:141:LYS:NZ	1.93	0.65
2:E:397:LEU:CD1	4:E:2156:HOH:O	2.44	0.65
1:C:138:GLN:NE2	1:C:141:LYS:HE2	2.09	0.65
2:E:355:CYS:O	4:E:2256:HOH:O	2.14	0.64
1:A:321:LYS:HD3	1:A:328:GLN:NE2	2.14	0.63
1:A:371:PHE:CD1	1:A:371:PHE:C	2.62	0.63
1:A:396:GLN:O	1:A:398:GLY:N	2.32	0.62
2:E:58:LYS:NZ	2:E:180:GLU:OE2	2.33	0.62
1:A:1:MET:CE	1:A:7:ASP:OD1	2.48	0.62
2:E:23:VAL:HG23	2:E:27:LEU:HD21	1.82	0.61
2:E:253:LYS:HD3	2:E:255:LYS:HE2	1.83	0.61
2:E:234:PRO:HD3	4:E:2161:HOH:O	2.00	0.61
1:A:322:THR:N	4:A:2256:HOH:O	2.34	0.61
2:E:211:GLU:HG3	4:E:2150:HOH:O	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HG3	1:A:9:SER:HB3	1.83	0.60
2:E:59:HIS:O	2:E:63:ARG:HG3	2.02	0.59
1:C:103:ILE:HD12	3:C:1323:VTQ:H8C3	1.84	0.59
1:A:1:MET:HE2	1:A:7:ASP:OD1	2.02	0.59
2:E:322:LYS:H	2:E:328:GLN:NE2	1.98	0.57
1:A:278:TYR:CE1	1:A:308:MET:HG2	2.40	0.57
1:C:11:ARG:NH1	1:C:11:ARG:HB2	2.21	0.56
1:A:296:ILE:HG13	1:A:361:TYR:CD1	2.41	0.56
1:C:188:ARG:NH1	1:C:188:ARG:CG	2.43	0.56
2:E:23:VAL:O	2:E:27:LEU:HG	2.07	0.55
2:E:165:LYS:HB3	2:E:166:PRO:HD3	1.89	0.55
2:E:283:GLN:CG	4:E:2215:HOH:O	2.54	0.55
2:E:371:PHE:HB3	4:E:2260:HOH:O	2.07	0.54
1:C:389:ALA:O	1:C:392:GLU:HB2	2.07	0.54
1:C:103:ILE:CD1	3:C:1323:VTQ:H8C3	2.39	0.53
1:A:278:TYR:CZ	1:A:308:MET:HG2	2.44	0.52
1:C:291:GLN:HE22	1:C:364:ARG:HH21	1.57	0.52
1:C:1:MET:CA	4:C:2002:HOH:O	2.56	0.52
1:A:27:LEU:N	1:A:28:PRO:CD	2.72	0.52
1:A:1:MET:HE1	4:A:2007:HOH:O	2.11	0.51
2:E:137:HIS:CD2	4:E:2093:HOH:O	2.49	0.51
1:A:321:LYS:HD3	1:A:328:GLN:HE21	1.74	0.51
1:A:303:LEU:O	1:A:352:THR:HA	2.11	0.51
1:C:1:MET:HA	4:C:2002:HOH:O	2.10	0.51
1:A:345:HIS:CD2	1:A:345:HIS:H	2.29	0.51
3:A:1322:VTQ:H111	3:A:1322:VTQ:O1	2.12	0.50
2:E:282:VAL:HG11	2:E:290:HIS:CE1	2.46	0.50
1:A:286:ARG:CD	4:A:2282:HOH:O	2.60	0.50
2:E:356:SER:O	2:E:358:PRO:HD3	2.11	0.49
1:A:138:GLN:HE22	1:A:141:LYS:HZ2	1.59	0.49
1:C:296:ILE:HD12	1:C:361:TYR:CD1	2.47	0.49
2:E:72:ILE:HG22	4:E:2049:HOH:O	2.12	0.49
1:C:211:GLU:HG2	4:C:2172:HOH:O	2.13	0.49
1:C:278:TYR:CZ	1:C:308:MET:HG2	2.48	0.48
1:C:206:LYS:N	1:C:207:PRO:CD	2.76	0.48
1:C:31:PRO:HD2	4:C:2022:HOH:O	2.13	0.48
1:A:286:ARG:HD2	4:A:2282:HOH:O	2.13	0.48
2:E:206:LYS:N	2:E:207:PRO:CD	2.75	0.48
1:A:138:GLN:HE22	1:A:141:LYS:HZ3	1.62	0.48
1:A:341:ARG:CD	4:A:2260:HOH:O	2.61	0.48
1:C:153:TYR:CZ	3:C:1323:VTQ:H221	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:HIS:O	1:A:374:ALA:C	2.52	0.47
2:E:73:SER:HB3	4:E:2049:HOH:O	2.14	0.47
1:C:291:GLN:NE2	1:C:364:ARG:HH21	2.12	0.47
1:A:211:GLU:CG	4:A:2180:HOH:O	2.28	0.47
1:C:159:GLY:N	1:C:162:HIS:HD2	2.01	0.47
1:C:323:LYS:N	4:C:2249:HOH:O	2.46	0.47
1:C:332:GLU:HB3	4:C:2250:HOH:O	2.13	0.47
1:A:1:MET:HE1	1:A:7:ASP:OD1	2.14	0.47
2:E:283:GLN:HG3	4:E:2215:HOH:O	2.15	0.47
1:A:321:LYS:HB2	1:A:360:ILE:HB	1.97	0.47
1:A:188:ARG:CZ	1:A:188:ARG:CB	2.92	0.47
1:C:27:LEU:N	1:C:28:PRO:CD	2.77	0.47
1:C:58:LYS:CE	1:C:180:GLU:OE2	2.61	0.46
2:E:204:LEU:HD21	2:E:384:LEU:HD22	1.96	0.46
2:E:159:GLY:N	2:E:162:HIS:HD2	2.04	0.46
2:E:275:LYS:HE3	4:E:2203:HOH:O	2.14	0.46
2:E:11:ARG:CZ	2:E:11:ARG:HB2	2.45	0.46
1:A:63:ARG:NH1	4:A:2068:HOH:O	2.49	0.46
1:C:376:LYS:HB3	1:C:376:LYS:HE2	1.62	0.46
1:C:313:ASP:HB2	1:C:342:TYR:O	2.15	0.45
1:A:11:ARG:HB2	1:A:11:ARG:HE	1.50	0.45
1:C:226:GLU:CD	4:C:2189:HOH:O	2.54	0.45
1:C:388:LYS:HE3	1:C:388:LYS:HB3	1.54	0.45
1:C:293:GLU:HG2	1:C:362:VAL:HG22	1.99	0.45
2:E:196:LYS:H	2:E:196:LYS:CE	2.30	0.45
1:C:333:MET:HB3	1:C:333:MET:HE3	1.77	0.45
1:A:340:GLN:HG2	1:A:342:TYR:CZ	2.52	0.45
1:A:206:LYS:N	1:A:207:PRO:CD	2.80	0.45
1:C:11:ARG:HH11	1:C:11:ARG:HB2	1.81	0.44
1:C:278:TYR:CE1	1:C:308:MET:HG2	2.52	0.44
1:A:367:ASN:OD1	1:A:370:SER:HB3	2.17	0.44
1:A:390:SER:O	1:A:394:MET:HG2	2.17	0.44
1:A:1:MET:CA	4:A:2001:HOH:O	2.60	0.44
1:A:340:GLN:HG2	1:A:342:TYR:CE1	2.53	0.44
2:E:281:SER:OG	2:E:376:LYS:HE3	2.18	0.44
1:A:357:ASP:HA	1:A:358:PRO:HD3	1.90	0.44
2:E:313:ASP:HB2	2:E:342:TYR:O	2.16	0.44
2:E:322:LYS:N	2:E:328:GLN:HE22	2.04	0.44
2:E:18:LYS:HG2	2:E:49:LEU:HD13	1.99	0.44
1:A:341:ARG:HD3	4:A:2260:HOH:O	2.17	0.44
2:E:161:LYS:HE3	2:E:162:HIS:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:VAL:CG1	1:A:353:LEU:HD21	2.47	0.44
1:A:188:ARG:HB2	1:A:188:ARG:CZ	2.48	0.44
1:C:165:LYS:O	1:C:169:GLU:HG3	2.18	0.44
1:A:290:HIS:HE1	2:E:143:GLY:O	2.01	0.44
2:E:375:LYS:HE3	2:E:375:LYS:HB2	1.63	0.43
2:E:293:GLU:OE1	4:E:2220:HOH:O	2.21	0.43
2:E:186:LEU:O	2:E:216:LYS:NZ	2.41	0.43
2:E:326:GLU:H	2:E:326:GLU:HG2	1.62	0.43
2:E:266:ARG:HG2	4:E:2065:HOH:O	2.17	0.43
2:E:295:GLU:C	2:E:296:ILE:HD12	2.39	0.43
1:A:396:GLN:HG3	1:A:396:GLN:H	1.48	0.43
1:A:327:ARG:HD2	1:C:338:PRO:HB2	2.00	0.42
1:A:219:VAL:HG11	1:A:394:MET:CE	2.48	0.42
1:A:395:LYS:HD3	4:A:2296:HOH:O	2.19	0.42
2:E:266:ARG:CG	4:E:2065:HOH:O	2.67	0.42
1:A:392:GLU:HG2	4:A:2296:HOH:O	2.19	0.42
2:E:396:GLN:O	2:E:397:LEU:HG	2.19	0.42
2:E:28:PRO:HA	4:E:2015:HOH:O	2.19	0.42
1:C:188:ARG:NH1	1:C:188:ARG:CB	2.83	0.41
1:A:188:ARG:HB2	1:A:188:ARG:NH1	2.29	0.41
2:E:363:LEU:HD12	2:E:363:LEU:N	2.35	0.41
1:A:286:ARG:HD3	4:A:2282:HOH:O	2.20	0.41
1:A:169:GLU:OE1	4:A:2155:HOH:O	2.22	0.41
1:C:237:VAL:HB	1:C:243:GLY:HA3	2.03	0.41
2:E:176:CYS:O	2:E:180:GLU:HG3	2.21	0.41
1:C:332:GLU:CB	4:C:2250:HOH:O	2.69	0.41
1:A:182:TYR:N	1:A:183:PRO:CD	2.83	0.41
2:E:68:ILE:O	2:E:71:ILE:HG22	2.20	0.41
1:C:112:LEU:HD23	1:C:112:LEU:HA	1.89	0.41
2:E:124:LYS:HA	2:E:124:LYS:HD2	1.93	0.40
1:A:165:LYS:HB3	1:A:166:PRO:HD3	2.03	0.40
2:E:27:LEU:N	2:E:28:PRO:CD	2.84	0.40
1:A:14:GLU:HG2	1:A:18:LYS:NZ	2.36	0.40
1:A:176:CYS:CB	4:A:2162:HOH:O	2.30	0.40
1:C:336:VAL:HG11	1:C:353:LEU:HD21	2.04	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)
4:A:2107:HOH:O	4:C:2057:HOH:O[1_554]	2.09	0.11

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	391/403 (97%)	377 (96%)	11 (3%)	3 (1%)	24	11
1	C	381/403 (94%)	372 (98%)	7 (2%)	2 (0%)	34	21
2	E	395/403 (98%)	379 (96%)	16 (4%)	0	100	100
All	All	1167/1209 (96%)	1128 (97%)	34 (3%)	5 (0%)	39	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	GLN
1	C	392	GLU
1	A	397	LEU
1	C	371	PHE
1	A	374	ALA

### 5.3.2 Protein sidechains

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	350/356 (98%)	332 (95%)	18 (5%)	29	13
1	C	343/356 (96%)	334 (97%)	9 (3%)	54	43
2	E	351/356 (99%)	329 (94%)	22 (6%)	22	8
All	All	1044/1068 (98%)	995 (95%)	49 (5%)	32	16

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	ARG
1	A	13	LYS
1	A	141	LYS
1	A	188	ARG
1	A	196	LYS
1	A	266	ARG
1	A	275	LYS
1	A	321	LYS
1	A	340	GLN
1	A	347	VAL
1	A	371	PHE
1	A	375	LYS
1	A	376	LYS
1	A	393	LYS
1	A	395	LYS
1	A	396	GLN
1	A	397	LEU
1	C	72	ILE
1	C	141	LYS
1	C	188	ARG
1	C	297	LEU
1	C	333	MET
1	C	334	THR
1	C	371	PHE
1	C	375	LYS
1	C	376	LYS
2	E	1	MET
2	E	18	LYS
2	E	24	GLN
2	E	26	VAL
2	E	78	GLU
2	E	103	ILE
2	E	120	LEU
2	E	141	LYS
2	E	196	LYS
2	E	211	GLU
2	E	215	LYS
2	E	266	ARG
2	E	283	GLN
2	E	303	LEU
2	E	310	ASP
2	E	322	LYS

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Mol	Chain	Res	Type
2	E	327	ARG
2	E	356	SER
2	E	372	ILE
2	E	375	LYS
2	E	396	GLN
2	E	397	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	162	HIS
1	A	276	GLN
1	A	290	HIS
1	A	328	GLN
1	A	339	ASN
1	A	345	HIS
1	C	32	ASN
1	C	138	GLN
1	C	162	HIS
1	C	231	HIS
1	C	291	GLN
2	E	137	HIS
2	E	138	GLN
2	E	162	HIS
2	E	290	HIS
2	E	328	GLN
2	E	396	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

3 ligands are 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$
3	VTQ	A	1322	-	30,32,32	0.85	2 (6%)	37,44,44	0.92	2 (5%)
3	VTQ	C	1323	-	30,32,32	0.87	2 (6%)	37,44,44	0.80	0
3	VTQ	E	1398	-	30,32,32	0.84	1 (3%)	37,44,44	0.82	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
3	VTQ	A	1322	-	-	0/25/49/49	0/1/1/1
3	VTQ	C	1323	-	-	0/25/49/49	0/1/1/1
3	VTQ	E	1398	-	-	0/25/49/49	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1323	VTQ	C3-C4	-2.63	1.38	1.46
3	A	1322	VTQ	C3-C4	-2.50	1.39	1.46
3	E	1398	VTQ	C3-C4	-2.44	1.39	1.46
3	C	1323	VTQ	C5-C4	-2.11	1.38	1.47
3	A	1322	VTQ	C5-C4	-2.08	1.38	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1322	VTQ	C11-C10-C3	-2.16	104.17	112.20
3	A	1322	VTQ	C10-C11-C9	-2.02	111.20	116.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1322	VTQ	2	0
3	C	1323	VTQ	3	0
3	E	1398	VTQ	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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