



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:08 PM GMT

PDB ID : 1E7F  
Title : HUMAN SERUM ALBUMIN COMPLEXED WITH DODECANOIC ACID  
(LAURIC ACID)  
Authors : Bhattacharya, A.A.; Gruene, T.; Curry, S.  
Deposited on : 2000-08-29  
Resolution : 2.43 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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

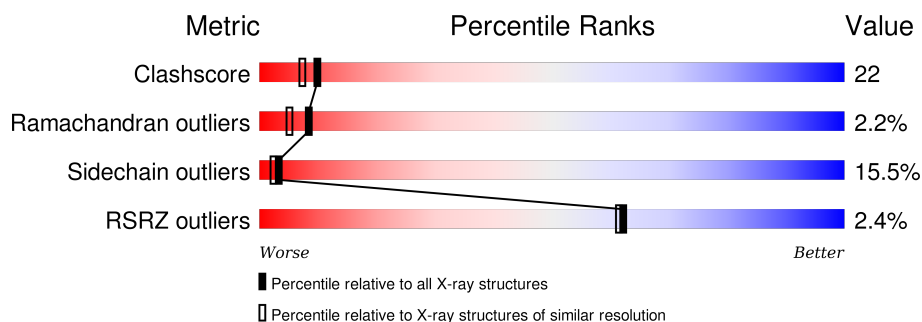
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.43 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	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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.

Mol	Chain	Length	Quality of chain
1	A	585	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DAO	A	1006	-	-	-	X

## 2 Entry composition [i](#)

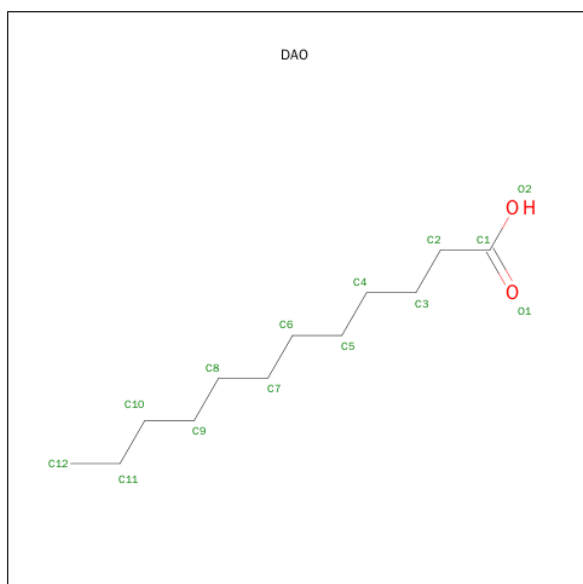
There are 3 unique types of molecules in this entry. The entry contains 4504 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4375	2778	736	820	41			

- Molecule 2 is LAURIC ACID (three-letter code: DAO) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			14	12	2		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			14	12	2		
2	A	1	Total	C	O	0	0
			13	11	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 14 12 2	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 10 10	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	26	Total O 26 26	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	188.50Å 38.90Å 95.77Å 90.00° 104.63° 90.00°	Depositor
Resolution (Å)	12.00 – 2.43 11.98 – 2.44	Depositor EDS
% Data completeness (in resolution range)	92.0 (12.00-2.43) 92.6 (11.98-2.44)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.43Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.225 , 0.276 0.240 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	54.1	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 61.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 23655 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4504	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAO

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	0.38	0/4461	0.58	1/6059 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	563	ASP	N-CA-C	-6.73	92.84	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	4375	0	4096	192	0
2	A	103	0	162	9	0
3	A	26	0	0	3	0
All	All	4504	0	4258	193	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 22.

All (193) 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:301:ASP:O	1:A:303:PRO:HD3	1.70	0.92
1:A:267:ASN:N	1:A:267:ASN:HD22	1.71	0.87
1:A:150:TYR:H	1:A:196:GLN:HE22	1.19	0.87
1:A:225:LYS:HG3	1:A:299:PRO:HD3	1.59	0.84
1:A:440:HIS:H	1:A:440:HIS:CD2	1.95	0.84
1:A:95:GLU:HB3	1:A:96:PRO:HD3	1.59	0.83
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.59	0.83
1:A:69:LEU:HD22	2:A:1008:DAO:H21	1.60	0.82
1:A:138:TYR:O	1:A:142:ILE:HG22	1.82	0.80
1:A:383:GLU:HG3	1:A:384:PRO:HD3	1.64	0.80
1:A:274:LYS:HG3	1:A:296:ASP:HA	1.67	0.77
1:A:383:GLU:HG3	1:A:384:PRO:CD	2.15	0.76
1:A:119:GLU:HB2	1:A:122:VAL:CG2	2.16	0.76
1:A:95:GLU:HB3	1:A:96:PRO:CD	2.17	0.75
1:A:10:ARG:O	1:A:14:LEU:HB2	1.88	0.74
1:A:150:TYR:H	1:A:196:GLN:NE2	1.86	0.73
1:A:142:ILE:HG12	1:A:154:LEU:HD11	1.71	0.73
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.70	0.72
1:A:415:VAL:HB	1:A:418:VAL:HG23	1.72	0.72
1:A:119:GLU:O	1:A:122:VAL:HG23	1.91	0.70
1:A:479:GLU:HG2	1:A:483:ASN:HB2	1.73	0.70
1:A:131:GLU:OE2	1:A:162:LYS:HE3	1.92	0.69
1:A:225:LYS:HG3	1:A:299:PRO:CD	2.22	0.69
1:A:177:CYS:O	1:A:180:PRO:HD2	1.93	0.69
1:A:381:VAL:O	1:A:384:PRO:HD2	1.93	0.68
1:A:480:SER:C	1:A:482:VAL:H	1.97	0.68
1:A:440:HIS:HD2	1:A:440:HIS:H	1.39	0.67
1:A:32:GLN:OE1	1:A:110:PRO:HG3	1.93	0.66
1:A:267:ASN:N	1:A:267:ASN:ND2	2.44	0.66
1:A:409:VAL:O	1:A:413:LYS:HG3	1.95	0.66
1:A:465:GLU:O	1:A:468:PRO:HD3	1.96	0.64
1:A:303:PRO:O	1:A:337:ARG:NH1	2.31	0.64
1:A:224:PRO:HG3	3:A:2013:HOH:O	1.98	0.64
1:A:516:LEU:HD22	1:A:520:GLU:CB	2.28	0.64
2:A:1002:DAO:H121	2:A:1008:DAO:H71	1.81	0.63
1:A:120:VAL:HG13	1:A:178:LEU:HD23	1.81	0.62
1:A:567:CYS:O	1:A:571:GLU:HB2	2.00	0.62
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.29	0.62
1:A:356:THR:HG21	1:A:373:VAL:CG2	2.30	0.62
1:A:315:VAL:HG11	1:A:370:TYR:CZ	2.34	0.61
1:A:142:ILE:HG13	1:A:142:ILE:O	1.99	0.60
1:A:153:GLU:HG3	3:A:2019:HOH:O	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ALA:HA	2:A:1007:DAO:H102	1.84	0.60
1:A:529:LEU:O	1:A:533:VAL:HG23	2.00	0.60
1:A:424:VAL:O	1:A:428:ARG:HG3	2.01	0.60
1:A:156:PHE:CE2	1:A:160:ARG:HD2	2.37	0.60
1:A:173:ASP:HB3	1:A:176:ALA:HB3	1.84	0.59
1:A:383:GLU:HG3	1:A:384:PRO:N	2.17	0.59
1:A:86:GLU:O	1:A:89:ASP:HB2	2.02	0.59
1:A:137:LYS:O	1:A:141:GLU:HG2	2.02	0.59
1:A:356:THR:HG21	1:A:373:VAL:HG21	1.84	0.59
1:A:173:ASP:O	1:A:176:ALA:N	2.36	0.58
1:A:372:LYS:O	1:A:375:ASP:HB2	2.04	0.58
1:A:72:ASP:O	1:A:76:THR:HG23	2.04	0.57
1:A:286:LYS:O	1:A:290:ILE:HG13	2.04	0.57
1:A:523:ILE:N	1:A:523:ILE:HD13	2.18	0.57
1:A:480:SER:O	1:A:482:VAL:N	2.38	0.57
1:A:344:VAL:HG22	1:A:450:GLU:OE2	2.05	0.57
1:A:386:ASN:O	1:A:390:GLN:HG3	2.05	0.56
1:A:119:GLU:HB2	1:A:122:VAL:HG23	1.87	0.56
1:A:217:ALA:HB2	1:A:331:LEU:HD13	1.88	0.55
1:A:8:ALA:O	1:A:12:LYS:HG3	2.06	0.55
1:A:95:GLU:O	1:A:96:PRO:C	2.42	0.55
1:A:440:HIS:N	1:A:440:HIS:CD2	2.69	0.54
1:A:430:LEU:CD1	1:A:456:VAL:HG11	2.36	0.54
1:A:433:VAL:HG22	1:A:452:TYR:HB3	1.89	0.54
1:A:417:GLN:NE2	1:A:494:ASP:OD2	2.37	0.54
1:A:452:TYR:O	1:A:455:VAL:HG23	2.08	0.54
1:A:64:LYS:HB2	1:A:69:LEU:HG	1.89	0.53
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.42	0.53
1:A:417:GLN:O	1:A:469:VAL:HG11	2.08	0.53
1:A:94:GLN:O	1:A:98:ARG:HB2	2.08	0.53
1:A:225:LYS:HG3	1:A:299:PRO:CG	2.39	0.53
1:A:480:SER:C	1:A:482:VAL:N	2.62	0.53
1:A:563:ASP:O	1:A:566:THR:HB	2.09	0.53
1:A:378:LYS:HB3	1:A:379:PRO:CD	2.36	0.52
1:A:562:ASP:C	1:A:564:LYS:N	2.58	0.52
1:A:118:PRO:HG2	1:A:123:MET:HG3	1.92	0.52
1:A:260:LEU:O	1:A:264:ILE:HG13	2.10	0.52
1:A:222:ARG:C	1:A:224:PRO:HD3	2.31	0.51
1:A:36:PHE:CE1	1:A:137:LYS:HA	2.45	0.51
1:A:387:LEU:O	1:A:391:ASN:HB2	2.11	0.51
1:A:220:SER:OG	1:A:335:ALA:HB3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:CYS:O	1:A:93:LYS:HG3	2.12	0.50
1:A:434:GLY:O	1:A:438:CYS:SG	2.69	0.50
1:A:442:GLU:HA	1:A:445:ARG:HD2	1.94	0.50
1:A:46:VAL:O	1:A:49:PHE:HB3	2.12	0.50
1:A:296:ASP:OD1	1:A:297:GLU:N	2.44	0.50
1:A:264:ILE:HG23	1:A:271:ILE:HD13	1.93	0.50
1:A:419:SER:OG	1:A:421:PRO:HD2	2.12	0.50
1:A:369:CYS:C	1:A:371:ALA:H	2.13	0.50
1:A:420:THR:N	1:A:421:PRO:HD2	2.27	0.50
1:A:530:VAL:HG12	1:A:534:LYS:HE3	1.94	0.50
1:A:415:VAL:HG11	1:A:473:VAL:HG23	1.93	0.49
1:A:413:LYS:HE2	1:A:537:PRO:O	2.12	0.49
1:A:141:GLU:O	1:A:145:ARG:HD2	2.12	0.49
1:A:10:ARG:NH2	1:A:255:ASP:OD1	2.45	0.49
1:A:517:SER:O	1:A:520:GLU:N	2.45	0.49
1:A:46:VAL:HG22	2:A:1008:DAO:H31	1.94	0.49
1:A:222:ARG:O	1:A:224:PRO:HD3	2.13	0.49
1:A:175:ALA:O	1:A:179:LEU:HB2	2.13	0.49
1:A:513:ILE:HD11	1:A:555:VAL:HG13	1.95	0.49
1:A:221:GLN:HG2	1:A:339:PRO:HA	1.95	0.48
1:A:430:LEU:HD21	2:A:1004:DAO:H62	1.95	0.48
1:A:311:GLU:O	1:A:312:SER:C	2.51	0.48
1:A:224:PRO:HB3	1:A:336:ARG:HB2	1.96	0.48
1:A:314:ASP:OD1	1:A:314:ASP:N	2.47	0.47
1:A:245:CYS:HA	1:A:253:CYS:HB2	1.97	0.47
1:A:238:LEU:HD21	2:A:1007:DAO:H31	1.96	0.47
1:A:50:ALA:O	1:A:54:VAL:HG23	2.14	0.47
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.97	0.46
1:A:220:SER:O	1:A:336:ARG:HB3	2.15	0.46
1:A:133:THR:O	1:A:137:LYS:HB2	2.15	0.46
1:A:216:VAL:CG2	1:A:235:VAL:HG21	2.46	0.46
1:A:49:PHE:CD2	2:A:1008:DAO:H22	2.51	0.46
1:A:518:GLU:O	1:A:522:GLN:HG3	2.16	0.46
1:A:383:GLU:OE2	1:A:485:ARG:NH2	2.43	0.46
1:A:95:GLU:O	1:A:98:ARG:N	2.44	0.46
1:A:260:LEU:HD12	1:A:260:LEU:O	2.16	0.46
1:A:401:TYR:CE1	1:A:522:GLN:HG2	2.51	0.46
1:A:519:LYS:O	1:A:523:ILE:HG12	2.16	0.45
1:A:364:ALA:O	1:A:366:PRO:HD3	2.15	0.45
1:A:37:GLU:CD	1:A:37:GLU:H	2.19	0.45
1:A:211:PHE:HE2	1:A:239:THR:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:O	1:A:20:LYS:HG3	2.17	0.45
1:A:136:LYS:HA	1:A:136:LYS:HD3	1.56	0.45
1:A:161:TYR:CE1	1:A:185:LEU:HD23	2.52	0.45
1:A:107:ASP:O	1:A:147:PRO:HG3	2.16	0.45
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.99	0.45
1:A:290:ILE:O	1:A:293:VAL:HB	2.16	0.45
1:A:397:GLN:HG3	1:A:397:GLN:H	1.52	0.45
1:A:211:PHE:HZ	1:A:242:HIS:CD2	2.34	0.45
1:A:27:PHE:HE1	1:A:74:LEU:HD12	1.82	0.45
1:A:81:ARG:O	1:A:85:GLY:HA2	2.16	0.45
1:A:238:LEU:HD22	1:A:242:HIS:CD2	2.52	0.44
1:A:530:VAL:CG1	1:A:534:LYS:HE3	2.47	0.44
1:A:458:ASN:O	1:A:462:VAL:HG23	2.17	0.44
1:A:479:GLU:HG2	1:A:483:ASN:CB	2.45	0.44
1:A:120:VAL:HA	1:A:123:MET:HE2	1.99	0.44
1:A:216:VAL:HG22	1:A:235:VAL:HG21	1.99	0.44
1:A:140:TYR:O	1:A:144:ARG:HG2	2.16	0.44
1:A:367:HIS:HA	1:A:370:TYR:CZ	2.53	0.44
1:A:507:PHE:CD1	2:A:1005:DAO:H102	2.53	0.44
1:A:548:MET:HG2	2:A:1005:DAO:H51	1.99	0.43
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.99	0.43
1:A:27:PHE:CE1	1:A:74:LEU:HD12	2.53	0.43
1:A:173:ASP:OD2	1:A:176:ALA:HB2	2.18	0.43
1:A:408:LEU:HD13	1:A:427:SER:HB2	1.99	0.43
1:A:267:ASN:H	1:A:267:ASN:HD22	1.62	0.43
1:A:415:VAL:HB	1:A:418:VAL:CG2	2.46	0.43
1:A:517:SER:O	1:A:518:GLU:C	2.56	0.43
1:A:295:ASN:ND2	1:A:339:PRO:HB3	2.34	0.43
1:A:214:TRP:CH2	1:A:218:ARG:HD3	2.53	0.43
1:A:42:LEU:HD22	1:A:73:LYS:HD2	2.00	0.43
1:A:383:GLU:CG	1:A:384:PRO:HD3	2.43	0.43
1:A:109:ASN:O	1:A:110:PRO:C	2.57	0.43
1:A:383:GLU:OE2	1:A:485:ARG:NH1	2.50	0.42
1:A:10:ARG:HG3	1:A:66:LEU:HD11	2.00	0.42
1:A:151:ALA:CB	1:A:152:PRO:CD	2.95	0.42
1:A:445:ARG:O	1:A:448:CYS:HB3	2.20	0.42
1:A:509:PHE:CE1	1:A:551:PHE:HE2	2.37	0.42
1:A:14:LEU:HD12	1:A:14:LEU:HA	1.90	0.42
1:A:545:LYS:HA	1:A:548:MET:CE	2.50	0.42
1:A:112:LEU:HD22	1:A:144:ARG:NH1	2.35	0.42
1:A:502:PHE:CE2	1:A:503:ASN:O	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:HG22	1:A:256:ASP:HB3	2.00	0.42
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.60	0.42
1:A:305:LEU:O	1:A:307:ALA:N	2.53	0.42
1:A:208:GLU:HG2	1:A:212:LYS:HD2	2.01	0.42
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.89	0.42
1:A:341:TYR:OH	1:A:381:VAL:HG11	2.20	0.41
1:A:21:ALA:O	1:A:25:ILE:HG13	2.19	0.41
1:A:513:ILE:CD1	1:A:555:VAL:HG13	2.50	0.41
1:A:399:GLY:O	1:A:403:PHE:HB2	2.20	0.41
1:A:485:ARG:HB3	1:A:486:PRO:HD3	2.03	0.41
1:A:227:GLU:O	1:A:230:GLU:N	2.50	0.41
1:A:173:ASP:O	1:A:174:LYS:C	2.59	0.41
1:A:513:ILE:HG13	1:A:514:CYS:N	2.34	0.41
1:A:330:PHE:HZ	1:A:377:PHE:CE2	2.38	0.41
1:A:349:LEU:HD23	1:A:380:LEU:HD23	2.03	0.41
1:A:368:GLU:HA	1:A:371:ALA:HB2	2.02	0.41
1:A:357:LEU:HA	1:A:357:LEU:HD23	1.93	0.41
1:A:399:GLY:O	1:A:403:PHE:CB	2.69	0.41
1:A:231:VAL:HG21	1:A:332:TYR:CD1	2.56	0.41
1:A:532:LEU:HD11	1:A:583:LEU:CD1	2.51	0.41
1:A:331:LEU:HA	1:A:331:LEU:HD23	1.92	0.40
1:A:540:THR:HG22	1:A:541:LYS:H	1.86	0.40
1:A:286:LYS:HB2	3:A:2018:HOH:O	2.20	0.40
1:A:222:ARG:HD3	1:A:293:VAL:HG12	2.04	0.40
1:A:30:TYR:O	1:A:32:GLN:HG3	2.22	0.40
1:A:571:GLU:HA	1:A:571:GLU:OE1	2.22	0.40
1:A:430:LEU:HD12	1:A:456:VAL:HG11	2.02	0.40
1:A:544:LEU:HD12	1:A:544:LEU:HA	1.89	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	580/585 (99%)	498 (86%)	69 (12%)	13 (2%)	8 5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	303	PRO
1	A	511	ALA
1	A	95	GLU
1	A	306	ALA
1	A	481	LEU
1	A	174	LYS
1	A	312	SER
1	A	441	PRO
1	A	299	PRO
1	A	205	LYS
1	A	151	ALA
1	A	366	PRO

### 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	439/511 (86%)	371 (84%)	68 (16%)	3 2

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	7	VAL
1	A	32	GLN
1	A	51	LYS
1	A	57	GLU
1	A	73	LYS
1	A	74	LEU
1	A	79	THR

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Mol	Chain	Res	Type
1	A	81	ARG
1	A	93	LYS
1	A	95	GLU
1	A	96	PRO
1	A	103	LEU
1	A	106	LYS
1	A	107	ASP
1	A	114	ARG
1	A	121	ASP
1	A	122	VAL
1	A	123	MET
1	A	132	GLU
1	A	136	LYS
1	A	140	TYR
1	A	142	ILE
1	A	144	ARG
1	A	152	PRO
1	A	166	THR
1	A	185	LEU
1	A	190	LYS
1	A	192	SER
1	A	205	LYS
1	A	222	ARG
1	A	233	LYS
1	A	238	LEU
1	A	267	ASN
1	A	285	GLU
1	A	286	LYS
1	A	287	SER
1	A	293	VAL
1	A	299	PRO
1	A	302	LEU
1	A	312	SER
1	A	314	ASP
1	A	331	LEU
1	A	334	TYR
1	A	337	ARG
1	A	383	GLU
1	A	390	GLN
1	A	397	GLN
1	A	410	ARG
1	A	419	SER

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Mol	Chain	Res	Type
1	A	423	LEU
1	A	427	SER
1	A	440	HIS
1	A	441	PRO
1	A	451	ASP
1	A	453	LEU
1	A	455	VAL
1	A	457	LEU
1	A	467	THR
1	A	472	ARG
1	A	480	SER
1	A	484	ARG
1	A	496	THR
1	A	503	ASN
1	A	512	ASP
1	A	523	ILE
1	A	540	THR
1	A	544	LEU

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	105	HIS
1	A	196	GLN
1	A	242	HIS
1	A	247	HIS
1	A	267	ASN
1	A	440	HIS
1	A	503	ASN
1	A	535	HIS

### 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

8 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$
2	DAO	A	1001	-	9,12,13	0.24	0	9,12,13	0.88	1 (11%)
2	DAO	A	1002	-	10,13,13	0.18	0	10,13,13	0.95	1 (10%)
2	DAO	A	1003	-	9,12,13	0.28	0	9,12,13	0.81	0
2	DAO	A	1004	-	10,13,13	0.17	0	10,13,13	0.88	1 (10%)
2	DAO	A	1005	-	9,12,13	0.23	0	9,12,13	0.89	1 (11%)
2	DAO	A	1006	-	10,13,13	0.27	0	10,13,13	0.82	1 (10%)
2	DAO	A	1007	-	11,11,13	0.35	0	10,10,13	0.55	0
2	DAO	A	1008	-	9,9,13	0.20	0	8,8,13	0.55	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	DAO	A	1001	-	-	0/8/10/11	0/0/0/0
2	DAO	A	1002	-	-	0/9/11/11	0/0/0/0
2	DAO	A	1003	-	-	0/8/10/11	0/0/0/0
2	DAO	A	1004	-	-	0/9/11/11	0/0/0/0
2	DAO	A	1005	-	-	0/8/10/11	0/0/0/0
2	DAO	A	1006	-	-	0/9/11/11	0/0/0/0
2	DAO	A	1007	-	-	0/9/9/11	0/0/0/0
2	DAO	A	1008	-	-	0/7/7/11	0/0/0/0

There are no bond length outliers.



All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	DAO	C4-C3-C2	-2.29	104.24	113.90
2	A	1001	DAO	C4-C3-C2	-2.22	104.51	113.90
2	A	1004	DAO	C4-C3-C2	-2.16	104.77	113.90
2	A	1005	DAO	C4-C3-C2	-2.16	104.77	113.90
2	A	1006	DAO	C4-C3-C2	-2.09	105.08	113.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	DAO	1	0
2	A	1004	DAO	1	0
2	A	1005	DAO	2	0
2	A	1007	DAO	2	0
2	A	1008	DAO	4	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](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	582/585 (99%)	-0.15	14 (2%) 62 61	32, 59, 91, 100	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	HIS	4.6
1	A	301	ASP	3.4
1	A	559	CYS	3.2
1	A	178	LEU	2.9
1	A	80	LEU	2.8
1	A	561	ALA	2.8
1	A	95	GLU	2.7
1	A	128	HIS	2.6
1	A	558	CYS	2.1
1	A	362	ALA	2.1
1	A	566	THR	2.1
1	A	365	ASP	2.0
1	A	370	TYR	2.0
1	A	390	GLN	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DAO	A	1006	14/14	0.85	0.19	3.13	55,68,92,92	0
2	DAO	A	1008	10/14	0.91	0.17	1.58	64,66,75,75	0
2	DAO	A	1003	13/14	0.95	0.16	1.06	55,58,63,64	0
2	DAO	A	1007	12/14	0.87	0.15	0.93	53,60,79,81	0
2	DAO	A	1005	13/14	0.91	0.15	0.74	53,59,68,69	0
2	DAO	A	1002	14/14	0.93	0.14	0.39	53,58,62,64	0
2	DAO	A	1004	14/14	0.94	0.12	0.16	49,54,63,66	0
2	DAO	A	1001	13/14	0.95	0.12	-0.10	77,81,82,83	0

## 6.5 Other polymers

There are no such residues in this entry.