Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2017 – 04:45 pm GMT

PDB ID : 1E7I

Title : HUMAN SERUM ALBUMIN COMPLEXED WITH OCTADECANOIC ACID (STEARIC ACID)

Authors : Bhattacharya, A.A.; Gruene, T.; Curry, S.

Deposited on : 2000-08-29

Resolution : 2.70 Å(reported)

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

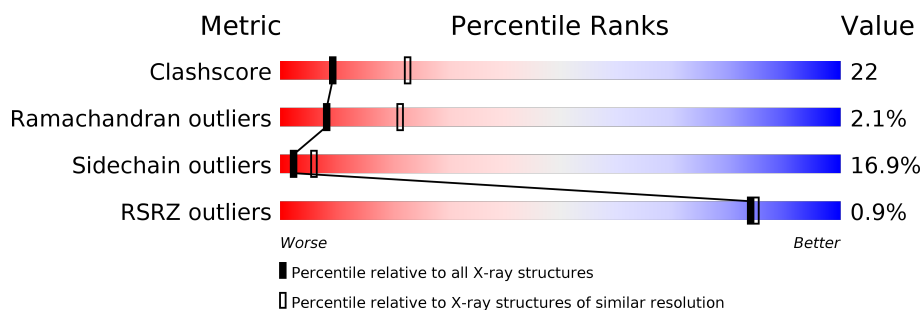|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.70 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	Percentile Ranks	Value
Clashscore		22
Ramachandran outliers		2.1%
Sidechain outliers		16.9%
RSRZ outliers		0.9%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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.

Mol	Chain	Length	Quality of chain
1	A	585	56% 34% 9% •

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	STE	A	1001	-	-	-	X
2	STE	A	1002	-	-	-	X
2	STE	A	1003	-	-	-	X
2	STE	A	1004[A]	-	-	-	X

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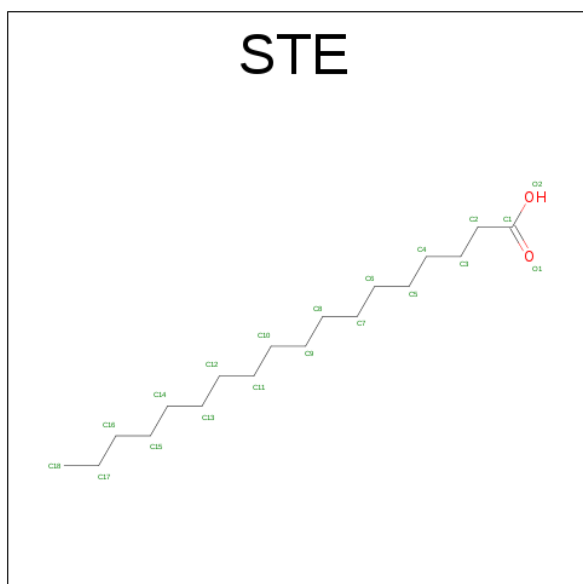| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	STE	A	1004[B]	-	-	-	X
2	STE	A	1006	-	-	-	X
2	STE	A	1007	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4665 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 4496	C 2857	N 752	O 846	S 41	0	0	0

- Molecule 2 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 15	C 13	O 2	0	0
2	A	1	Total 19	C 17	O 2	0	0
2	A	1	Total 19	C 17	O 2	0	0
2	A	1	Total 40	C 36	O 4	0	1
2	A	1	Total 20	C 18	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 19 17 2	0	0
2	A	1	Total C 11 11	0	0

- Molecule 3 is water.

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

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 the various outlier classes 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.

• Molecule 1: SERUM ALBUMIN
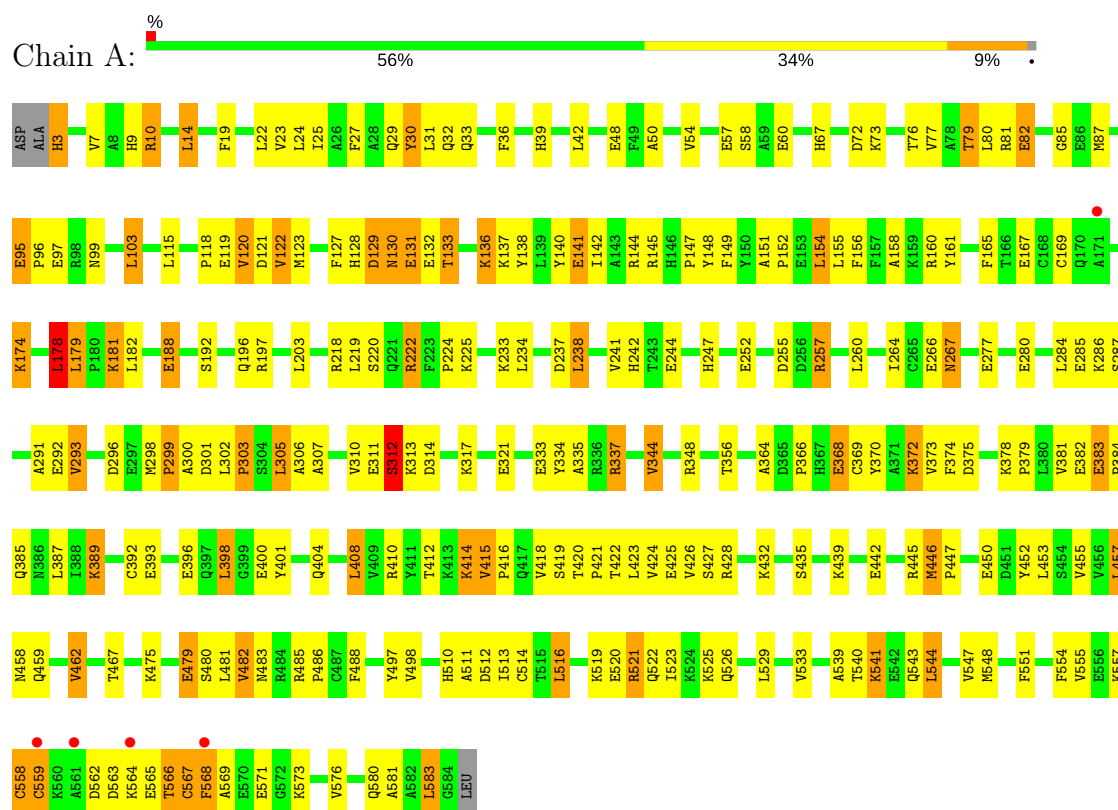
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	189.60Å 38.84Å 95.98Å 90.00° 105.49° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 35.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.8 (40.00-2.70) 92.8 (35.85-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.68Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.258 0.202 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	54.6	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 60.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4665	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: STE

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	0.36	0/4585	0.57	1/6205 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	30	TYR	N-CA-C	-6.31	93.95	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	4496	0	4310	201	0
2	A	143	0	235	15	0
3	A	26	0	0	0	0
All	All	4665	0	4545	201	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 (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:HG3	1:A:10:ARG:HH11	1.04	1.14
1:A:576:VAL:HG12	1:A:580:GLN:HE21	1.23	1.03
1:A:138:TYR:HB3	2:A:1001:STE:H102	1.50	0.94
1:A:372:LYS:C	1:A:372:LYS:HD2	1.93	0.89
1:A:138:TYR:O	1:A:142:ILE:HD12	1.76	0.85
1:A:422:THR:O	1:A:426:VAL:HG23	1.77	0.85
1:A:422:THR:HG21	2:A:1004[B]:STE:O1	1.77	0.85
1:A:10:ARG:HG3	1:A:10:ARG:NH1	1.84	0.84
1:A:95:GLU:CB	1:A:96:PRO:HD3	2.10	0.82
1:A:10:ARG:CG	1:A:10:ARG:HH11	1.91	0.81
1:A:317:LYS:O	1:A:321:GLU:HG3	1.79	0.81
1:A:412:THR:HG22	1:A:423:LEU:HD13	1.65	0.77
1:A:305:LEU:HD21	1:A:337:ARG:CD	2.17	0.75
1:A:521:ARG:O	1:A:525:LYS:HG3	1.89	0.72
1:A:10:ARG:NH2	1:A:255:ASP:OD1	2.23	0.72
1:A:555:VAL:O	1:A:559:CYS:HB2	1.90	0.72
1:A:408:LEU:CD2	1:A:526:GLN:HG2	2.20	0.71
1:A:79:THR:O	1:A:81:ARG:N	2.22	0.71
1:A:383:GLU:HG3	1:A:384:PRO:HD3	1.71	0.71
1:A:576:VAL:HG12	1:A:580:GLN:NE2	2.03	0.70
1:A:424:VAL:O	1:A:428:ARG:HG3	1.92	0.69
1:A:564:LYS:O	1:A:566:THR:N	2.26	0.69
1:A:244:GLU:OE2	1:A:252:GLU:HG3	1.93	0.69
1:A:305:LEU:HD21	1:A:337:ARG:HD2	1.75	0.69
1:A:267:ASN:N	1:A:267:ASN:HD22	1.90	0.67
1:A:218:ARG:HH21	1:A:222:ARG:HH12	1.42	0.67
1:A:372:LYS:O	1:A:375:ASP:HB2	1.95	0.66
1:A:127:PHE:CD2	1:A:165:PHE:HB3	2.31	0.66
1:A:408:LEU:HD13	1:A:427:SER:OG	1.95	0.66
1:A:383:GLU:HG3	1:A:384:PRO:CD	2.26	0.66
1:A:576:VAL:O	1:A:580:GLN:HG3	1.95	0.66
1:A:155:LEU:HD23	1:A:155:LEU:O	1.96	0.66
1:A:160:ARG:NH2	1:A:188:GLU:OE2	2.25	0.66
1:A:119:GLU:O	1:A:122:VAL:HG23	1.95	0.65
1:A:567:CYS:O	1:A:571:GLU:HB2	1.95	0.65
1:A:479:GLU:HG3	1:A:480:SER:H	1.61	0.65
1:A:422:THR:CG2	2:A:1004[B]:STE:O1	2.45	0.65
1:A:392:CYS:O	1:A:396:GLU:HG2	1.96	0.65
1:A:418:VAL:HG21	2:A:1004[B]:STE:H81	1.78	0.65
1:A:167:GLU:HG2	1:A:167:GLU:O	1.95	0.65
1:A:562:ASP:O	1:A:563:ASP:HB3	1.98	0.64
1:A:566:THR:HG22	1:A:567:CYS:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:SER:HB3	1:A:483:ASN:OD1	1.98	0.63
1:A:458:ASN:O	1:A:462:VAL:HG13	2.00	0.62
1:A:127:PHE:O	1:A:127:PHE:CD1	2.53	0.62
1:A:158:ALA:HA	2:A:1001:STE:H122	1.82	0.62
1:A:178:LEU:O	1:A:181:LYS:HG3	2.01	0.61
1:A:267:ASN:N	1:A:267:ASN:ND2	2.45	0.61
1:A:551:PHE:O	1:A:554:PHE:HB3	1.99	0.61
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.83	0.60
1:A:130:ASN:OD1	1:A:133:THR:HG23	2.01	0.60
1:A:10:ARG:CG	1:A:10:ARG:NH1	2.58	0.60
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.84	0.60
1:A:513:ILE:O	1:A:521:ARG:HD2	2.01	0.60
1:A:149:PHE:CD1	1:A:154:LEU:HD12	2.37	0.59
1:A:383:GLU:HG3	1:A:384:PRO:N	2.18	0.59
1:A:401:TYR:CE1	1:A:522:GLN:HG2	2.38	0.59
1:A:511:ALA:O	1:A:514:CYS:HB2	2.03	0.59
1:A:306:ALA:HA	1:A:310:VAL:HG23	1.84	0.58
1:A:378:LYS:O	1:A:382:GLU:HG3	2.03	0.58
1:A:381:VAL:O	1:A:384:PRO:HD2	2.03	0.58
1:A:419:SER:HB3	2:A:1004[B]:STE:O1	2.04	0.58
1:A:149:PHE:CG	1:A:154:LEU:HD12	2.39	0.58
1:A:516:LEU:O	1:A:521:ARG:HD3	2.04	0.57
1:A:516:LEU:HD13	1:A:520:GLU:OE1	2.04	0.57
1:A:566:THR:CG2	1:A:567:CYS:N	2.67	0.57
1:A:237:ASP:O	1:A:241:VAL:HG23	2.05	0.56
1:A:36:PHE:CE1	1:A:137:LYS:HA	2.40	0.56
1:A:529:LEU:O	1:A:533:VAL:HG23	2.06	0.56
1:A:369:CYS:O	1:A:372:LYS:HE2	2.06	0.56
1:A:408:LEU:O	1:A:412:THR:HG23	2.05	0.55
1:A:488:PHE:HB3	2:A:1004[B]:STE:H151	1.88	0.55
1:A:408:LEU:HD23	1:A:526:GLN:HG2	1.88	0.55
1:A:548:MET:HG2	2:A:1005:STE:H61	1.89	0.55
1:A:400:GLU:O	1:A:404:GLN:HG3	2.06	0.55
1:A:475:LYS:O	1:A:479:GLU:HB2	2.07	0.55
1:A:540:THR:HG22	1:A:541:LYS:N	2.23	0.54
1:A:418:VAL:HG21	2:A:1004[B]:STE:C8	2.38	0.54
1:A:95:GLU:CB	1:A:96:PRO:CD	2.82	0.54
1:A:457:LEU:HD11	2:A:1004[B]:STE:H152	1.91	0.53
1:A:127:PHE:CE2	1:A:165:PHE:HB3	2.43	0.53
1:A:127:PHE:CG	1:A:127:PHE:O	2.61	0.53
1:A:510:HIS:HB2	1:A:512:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LYS:C	1:A:566:THR:H	2.12	0.53
1:A:569:ALA:O	1:A:573:LYS:HG3	2.09	0.52
1:A:372:LYS:CD	1:A:372:LYS:C	2.75	0.52
1:A:381:VAL:O	1:A:385:GLN:HG3	2.10	0.52
1:A:563:ASP:C	1:A:563:ASP:OD1	2.48	0.52
1:A:115:LEU:HD11	1:A:141:GLU:CG	2.40	0.51
1:A:483:ASN:C	1:A:486:PRO:HD2	2.30	0.51
1:A:169:CYS:HA	1:A:174:LYS:HD2	1.93	0.51
1:A:299:PRO:O	1:A:300:ALA:HB3	2.11	0.51
1:A:22:LEU:HG	1:A:155:LEU:HD12	1.92	0.51
1:A:539:ALA:HB1	1:A:544:LEU:HD13	1.92	0.51
1:A:81:ARG:O	1:A:85:GLY:N	2.42	0.50
1:A:138:TYR:CB	2:A:1001:STE:H102	2.32	0.50
1:A:25:ILE:O	1:A:29:GLN:HG3	2.11	0.50
1:A:141:GLU:HG3	1:A:145:ARG:NH1	2.26	0.50
1:A:147:PRO:HG2	1:A:148:TYR:HD1	1.77	0.50
1:A:373:VAL:HG12	1:A:374:PHE:N	2.27	0.50
1:A:372:LYS:HD2	1:A:372:LYS:O	2.09	0.50
1:A:348:ARG:HG3	1:A:482:VAL:CG2	2.42	0.49
1:A:115:LEU:HD11	1:A:141:GLU:HG2	1.93	0.49
1:A:291:ALA:HA	2:A:1007:STE:H72	1.93	0.49
1:A:446:MET:N	1:A:447:PRO:CD	2.76	0.49
1:A:558:CYS:SG	1:A:567:CYS:C	2.91	0.49
1:A:511:ALA:HA	1:A:568:PHE:CE2	2.48	0.48
1:A:161:TYR:O	1:A:165:PHE:HD1	1.96	0.48
1:A:557:LYS:CG	1:A:557:LYS:O	2.61	0.48
1:A:291:ALA:HB2	2:A:1007:STE:H52	1.95	0.48
1:A:383:GLU:O	1:A:387:LEU:HG	2.14	0.48
1:A:161:TYR:HE1	1:A:182:LEU:HD22	1.78	0.48
1:A:39:HIS:HD2	1:A:140:TYR:CE1	2.32	0.48
1:A:419:SER:OG	1:A:421:PRO:HD2	2.14	0.48
1:A:540:THR:HB	1:A:543:GLN:HG3	1.95	0.48
1:A:428:ARG:O	1:A:432:LYS:HG3	2.14	0.47
1:A:31:LEU:HB3	1:A:39:HIS:HE1	1.80	0.47
1:A:519:LYS:O	1:A:523:ILE:HG12	2.14	0.47
1:A:120:VAL:HG13	1:A:178:LEU:HD13	1.96	0.47
1:A:129:ASP:O	1:A:130:ASN:HB2	2.15	0.47
1:A:544:LEU:O	1:A:548:MET:HE2	2.15	0.47
1:A:266:GLU:HB3	1:A:267:ASN:ND2	2.29	0.47
1:A:516:LEU:CD1	1:A:520:GLU:HB3	2.45	0.47
1:A:67:HIS:HD2	1:A:99:ASN:ND2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:VAL:HG21	2:A:1004[B]:STE:H102	1.96	0.47
1:A:305:LEU:CD2	1:A:305:LEU:N	2.78	0.46
1:A:133:THR:O	1:A:137:LYS:HB2	2.16	0.46
1:A:442:GLU:HA	1:A:445:ARG:HD2	1.96	0.46
1:A:356:THR:HG21	1:A:373:VAL:CG2	2.45	0.46
1:A:313:LYS:O	1:A:314:ASP:CB	2.64	0.46
1:A:389:LYS:HE2	1:A:393:GLU:OE1	2.16	0.46
1:A:420:THR:HB	1:A:421:PRO:HD3	1.98	0.46
1:A:554:PHE:O	1:A:558:CYS:HB2	2.16	0.46
1:A:234:LEU:O	1:A:238:LEU:HB2	2.15	0.46
1:A:401:TYR:OH	1:A:525:LYS:HE3	2.15	0.46
1:A:512:ASP:O	1:A:516:LEU:HD23	2.16	0.45
1:A:516:LEU:HD12	1:A:520:GLU:HB3	1.98	0.45
1:A:260:LEU:O	1:A:264:ILE:HG13	2.17	0.45
1:A:305:LEU:HD21	1:A:337:ARG:HD3	1.94	0.45
1:A:368:GLU:HA	1:A:368:GLU:OE1	2.16	0.45
1:A:540:THR:HG22	1:A:541:LYS:H	1.80	0.45
1:A:257:ARG:NH1	1:A:287:SER:OG	2.50	0.45
1:A:82:GLU:HG3	1:A:82:GLU:H	1.44	0.45
1:A:50:ALA:O	1:A:54:VAL:HG23	2.17	0.44
1:A:39:HIS:HD2	1:A:140:TYR:HE1	1.65	0.44
1:A:333:GLU:HA	1:A:333:GLU:OE1	2.17	0.44
1:A:555:VAL:O	1:A:559:CYS:N	2.50	0.44
1:A:416:PRO:HB2	1:A:497:TYR:CD1	2.53	0.44
1:A:72:ASP:O	1:A:76:THR:HG23	2.17	0.44
1:A:302:LEU:HA	1:A:303:PRO:HD3	1.86	0.43
1:A:581:ALA:C	1:A:583:LEU:H	2.21	0.43
1:A:401:TYR:OH	2:A:1005:STE:H32	2.19	0.43
1:A:521:ARG:O	1:A:525:LYS:CG	2.63	0.43
1:A:179:LEU:HD13	1:A:179:LEU:N	2.33	0.43
1:A:410:ARG:O	1:A:414:LYS:HG2	2.19	0.43
1:A:566:THR:HG22	1:A:567:CYS:H	1.81	0.43
1:A:19:PHE:O	1:A:23:VAL:HG23	2.18	0.43
1:A:483:ASN:N	1:A:483:ASN:OD1	2.51	0.43
1:A:123:MET:HE1	1:A:182:LEU:HD11	2.01	0.43
1:A:439:LYS:HD3	1:A:439:LYS:HA	1.71	0.43
1:A:480:SER:OG	1:A:482:VAL:CG1	2.67	0.43
1:A:564:LYS:C	1:A:566:THR:N	2.71	0.43
1:A:127:PHE:CD1	1:A:131:GLU:HB2	2.54	0.43
1:A:156:PHE:HZ	1:A:284:LEU:O	2.02	0.42
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD22	1:A:242:HIS:CD2	2.54	0.42
1:A:415:VAL:HB	1:A:418:VAL:HG23	2.01	0.42
1:A:344:VAL:HG22	1:A:450:GLU:OE2	2.18	0.42
1:A:516:LEU:HB3	1:A:520:GLU:HB3	2.02	0.42
1:A:238:LEU:HD22	1:A:242:HIS:HD2	1.85	0.42
1:A:364:ALA:O	1:A:366:PRO:HD3	2.20	0.42
1:A:10:ARG:O	1:A:14:LEU:HB2	2.19	0.42
1:A:220:SER:HB2	1:A:335:ALA:HB3	2.02	0.42
1:A:27:PHE:O	1:A:30:TYR:O	2.37	0.42
1:A:452:TYR:O	1:A:455:VAL:HG22	2.20	0.42
1:A:298:MET:O	1:A:300:ALA:N	2.52	0.42
1:A:310:VAL:O	1:A:370:TYR:HE1	2.03	0.42
1:A:31:LEU:HD21	1:A:77:VAL:HG21	2.02	0.42
1:A:299:PRO:C	1:A:301:ASP:H	2.23	0.42
1:A:378:LYS:CB	1:A:379:PRO:HD3	2.50	0.42
1:A:307:ALA:O	1:A:312:SER:HB3	2.20	0.41
1:A:24:LEU:HD22	1:A:136:LYS:HG3	2.02	0.41
1:A:313:LYS:O	1:A:314:ASP:HB2	2.20	0.41
1:A:218:ARG:NH2	1:A:222:ARG:HH12	2.14	0.41
1:A:511:ALA:HB1	1:A:564:LYS:HD2	2.02	0.41
1:A:103:LEU:HD22	1:A:247:HIS:O	2.21	0.41
1:A:398:LEU:HG	1:A:398:LEU:H	1.60	0.41
1:A:10:ARG:HA	1:A:10:ARG:HD3	1.95	0.41
1:A:543:GLN:O	1:A:547:VAL:HG23	2.19	0.41
1:A:161:TYR:CE1	1:A:182:LEU:HD22	2.55	0.41
1:A:277:GLU:O	1:A:280:GLU:CG	2.69	0.41
1:A:81:ARG:O	1:A:85:GLY:HA2	2.21	0.41
1:A:485:ARG:HB3	1:A:486:PRO:HD3	2.03	0.41
1:A:149:PHE:HB3	1:A:154:LEU:CD1	2.51	0.40
1:A:311:GLU:O	1:A:312:SER:O	2.39	0.40
1:A:3:HIS:NE2	1:A:9:HIS:CE1	2.89	0.40
1:A:192:SER:O	1:A:196:GLN:HG3	2.22	0.40
1:A:480:SER:OG	1:A:482:VAL:HG12	2.22	0.40
1:A:485:ARG:N	1:A:486:PRO:CD	2.85	0.40
1:A:408:LEU:HD21	1:A:526:GLN:HG2	1.99	0.40
1:A:311:GLU:O	1:A:312:SER:C	2.59	0.40

There are no symmetry-related clashes.

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	580/585 (99%)	519 (90%)	49 (8%)	12 (2%)	8	21

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	95	GLU
1	A	130	ASN
1	A	312	SER
1	A	565	GLU
1	A	118	PRO
1	A	178	LEU
1	A	303	PRO
1	A	293	VAL
1	A	299	PRO
1	A	60	GLU
1	A	120	VAL

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	467/511 (91%)	388 (83%)	79 (17%)	2	6

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	7	VAL
1	A	10	ARG
1	A	14	LEU
1	A	32	GLN
1	A	33	GLN
1	A	42	LEU
1	A	48	GLU
1	A	57	GLU
1	A	58	SER
1	A	73	LYS
1	A	79	THR
1	A	82	GLU
1	A	87	MET
1	A	97	GLU
1	A	103	LEU
1	A	121	ASP
1	A	122	VAL
1	A	128	HIS
1	A	129	ASP
1	A	131	GLU
1	A	132	GLU
1	A	133	THR
1	A	136	LYS
1	A	141	GLU
1	A	144	ARG
1	A	154	LEU
1	A	174	LYS
1	A	178	LEU
1	A	179	LEU
1	A	181	LYS
1	A	188	GLU
1	A	197	ARG
1	A	203	LEU
1	A	222	ARG
1	A	225	LYS
1	A	233	LYS
1	A	238	LEU
1	A	257	ARG
1	A	267	ASN
1	A	285	GLU
1	A	286	LYS
1	A	292	GLU

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Mol	Chain	Res	Type
1	A	293	VAL
1	A	305	LEU
1	A	312	SER
1	A	334	TYR
1	A	337	ARG
1	A	344	VAL
1	A	368	GLU
1	A	372	LYS
1	A	383	GLU
1	A	389	LYS
1	A	398	LEU
1	A	408	LEU
1	A	414	LYS
1	A	415	VAL
1	A	425	GLU
1	A	435	SER
1	A	446	MET
1	A	453	LEU
1	A	457	LEU
1	A	459	GLN
1	A	462	VAL
1	A	467	THR
1	A	479	GLU
1	A	481	LEU
1	A	482	VAL
1	A	498	VAL
1	A	516	LEU
1	A	521	ARG
1	A	541	LYS
1	A	544	LEU
1	A	558	CYS
1	A	559	CYS
1	A	566	THR
1	A	567	CYS
1	A	568	PHE
1	A	583	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	39	HIS

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Mol	Chain	Res	Type
1	A	67	HIS
1	A	99	ASN
1	A	105	HIS
1	A	128	HIS
1	A	242	HIS
1	A	267	ASN
1	A	510	HIS
1	A	580	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 ⓘ

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	STE	A	1001	-	11,14,19	0.30	0	10,14,19	0.85	1 (10%)
2	STE	A	1002	-	15,18,19	0.18	0	14,18,19	0.87	1 (7%)
2	STE	A	1003	-	15,18,19	0.33	0	14,18,19	0.71	1 (7%)
2	STE	A	1004[A]	-	16,19,19	0.27	0	15,19,19	0.82	1 (6%)
2	STE	A	1004[B]	-	16,19,19	0.26	0	15,19,19	0.78	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|$ > 2	Counts	RMSZ	#$|Z|$ > 2
2	STE	A	1005	-	16,19,19	0.20	0	15,19,19	0.87	1 (6%)
2	STE	A	1006	-	15,18,19	0.18	0	14,18,19	0.86	1 (7%)
2	STE	A	1007	-	10,10,19	0.24	0	9,9,19	0.60	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	STE	A	1001	-	-	0/10/12/17	0/0/0/0
2	STE	A	1002	-	-	0/14/16/17	0/0/0/0
2	STE	A	1003	-	-	0/14/16/17	0/0/0/0
2	STE	A	1004[A]	-	-	0/15/17/17	0/0/0/0
2	STE	A	1004[B]	-	-	0/15/17/17	0/0/0/0
2	STE	A	1005	-	-	0/15/17/17	0/0/0/0
2	STE	A	1006	-	-	0/14/16/17	0/0/0/0
2	STE	A	1007	-	-	0/8/8/17	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1004[A]	STE	C4-C3-C2	-2.42	104.09	113.70
2	A	1002	STE	C4-C3-C2	-2.36	104.30	113.70
2	A	1004[B]	STE	C4-C3-C2	-2.36	104.33	113.70
2	A	1005	STE	C4-C3-C2	-2.32	104.49	113.70
2	A	1006	STE	C4-C3-C2	-2.27	104.66	113.70
2	A	1001	STE	C4-C3-C2	-2.14	105.20	113.70
2	A	1003	STE	C4-C3-C2	-2.09	105.41	113.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	STE	3	0
2	A	1004[B]	STE	8	0
2	A	1005	STE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1007	STE	2	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 ⓘ

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, 95th 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^2)	Q<0.9
1	A	582/585 (99%)	-0.23	5 (0%)	84	85	24, 54, 85, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	564	LYS	3.7
1	A	568	PHE	2.5
1	A	561	ALA	2.5
1	A	171	ALA	2.3
1	A	559	CYS	2.0

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

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

6.3 Carbohydrates ⓘ

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, 95th 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^2)	Q<0.9
2	STE	A	1001	15/20	0.74	0.57	13.22	74,90,99,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	STE	A	1004[A]	20/20	0.82	0.35	8.47	53,56,57,59	20
2	STE	A	1004[B]	20/20	0.82	0.35	8.34	50,53,56,56	20
2	STE	A	1007	11/20	0.82	0.39	7.25	54,59,59,59	0
2	STE	A	1006	19/20	0.90	0.28	5.96	61,66,80,80	0
2	STE	A	1002	19/20	0.91	0.28	3.60	48,50,62,63	0
2	STE	A	1003	19/20	0.95	0.22	2.10	42,44,46,46	0
2	STE	A	1005	20/20	0.91	0.21	0.96	45,51,61,64	0

6.5 Other polymers ⓘ

There are no such residues in this entry.