



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:40 PM UTC

PDB ID : 4E99 / pdb_00004e99
Title : Human Serum Albumin Complex with Perfluorooctane Sulfonate Potassium
Authors : Luo, Z.P.; Shi, X.L.; Huang, M.D.
Deposited on : 2012-03-20
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

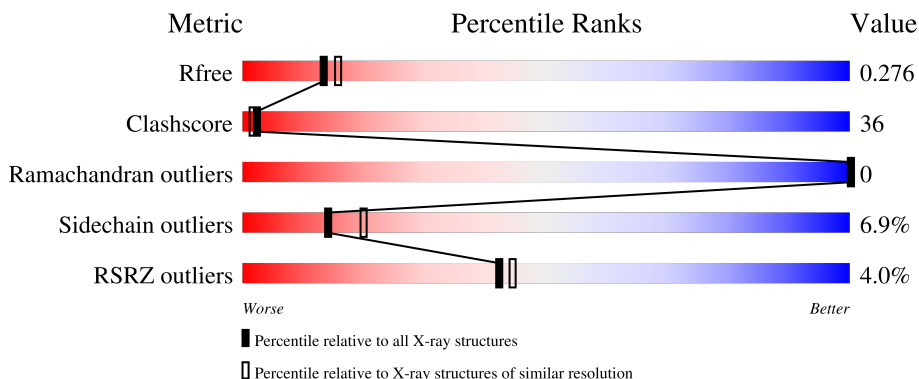
1 Overall quality at a glance i

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))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of 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 $\leq 5\%$. 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	P8S	A	601	-	-	X	-

2 Entry composition [i](#)

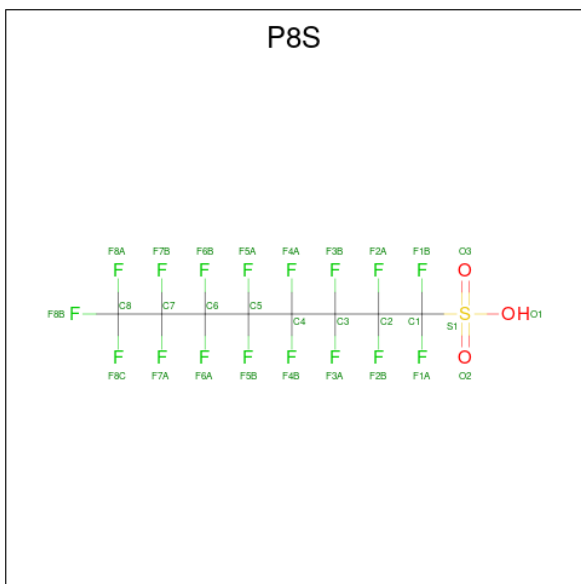
There are 3 unique types of molecules in this entry. The entry contains 4436 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	554	4326	2728	730	828	40	0	1	0

- Molecule 2 is heptadecafluoro-1-octanesulfonic acid (CCD ID: P8S) (formula: $C_8HF_{17}O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	O	S		
2	A	1	29	8	17	3	1	0	0
2	A	1	29	8	17	3	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total	O	0	0
			52	52		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.47Å 83.76Å 56.00Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	54.46 – 2.30 54.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (54.46-2.30) 99.0 (54.46-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.238 , 0.278 0.237 , 0.276	Depositor DCC
R_{free} test set	1102 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtrriage
Anisotropy	0.596	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.027 for l,-k,h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4436	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P8S

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	1.20	2/4411 (0.0%)	1.25	30/5973 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	HIS	CG-ND1	-5.47	1.32	1.38
1	A	146	HIS	CG-ND1	-5.14	1.32	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	LEU	N-CA-C	-8.53	101.98	111.28
1	A	15	GLY	N-CA-C	-7.55	103.17	112.68
1	A	280	GLU	N-CA-C	-6.43	105.47	113.38
1	A	351	LYS	N-CA-C	-6.19	104.45	111.14
1	A	196	GLN	N-CA-C	-6.14	104.49	112.23
1	A	213	ALA	N-CA-C	-6.08	104.57	111.07
1	A	544	LEU	N-CA-C	-6.03	104.63	111.14
1	A	117	ARG	CA-C-N	-6.00	114.58	120.52
1	A	117	ARG	C-N-CA	-6.00	114.58	120.52
1	A	477	CYS	N-CA-C	5.96	120.28	112.89
1	A	495	GLU	N-CA-C	-5.93	106.04	113.28
1	A	393	GLU	N-CA-C	-5.88	104.78	111.14
1	A	66	LEU	N-CA-C	-5.88	104.87	111.28
1	A	302	LEU	CA-C-N	-5.86	114.72	120.52
1	A	302	LEU	C-N-CA	-5.86	114.72	120.52
1	A	536	LYS	CA-C-N	-5.82	114.76	120.52
1	A	536	LYS	C-N-CA	-5.82	114.76	120.52
1	A	298	MET	N-CA-C	-5.63	102.03	110.24
1	A	114	ARG	N-CA-C	-5.46	102.31	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	LYS	N-CA-C	-5.43	105.36	111.28
1	A	434	GLY	N-CA-C	-5.40	106.23	112.50
1	A	314	ASP	N-CA-C	-5.34	106.63	112.72
1	A	223	PHE	CA-C-N	-5.30	114.20	119.56
1	A	223	PHE	C-N-CA	-5.30	114.20	119.56
1	A	467	THR	CA-C-N	-5.26	114.37	119.90
1	A	467	THR	C-N-CA	-5.26	114.37	119.90
1	A	308	ASP	N-CA-C	5.26	118.86	112.23
1	A	498	VAL	CA-C-N	-5.24	114.31	119.92
1	A	498	VAL	C-N-CA	-5.24	114.31	119.92
1	A	91	CYS	CA-CB-SG	-5.02	102.85	114.40

There are no chirality outliers.

There are no planarity outliers.

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	4326	0	4133	297	0
2	A	58	0	2	13	0
3	A	52	0	0	1	0
All	All	4436	0	4135	303	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 36.

All (303) 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:233:LYS:HE3	1:A:237:ASP:OD2	1.40	1.19
1:A:513:ILE:HD12	1:A:516:LEU:HD12	1.41	0.98
1:A:305:LEU:HD11	1:A:333:GLU:HB3	1.45	0.97
1:A:310:VAL:HG13	1:A:371:ALA:HA	1.49	0.93
1:A:310:VAL:CG1	1:A:371:ALA:HA	2.04	0.86
1:A:347:LEU:HB3	1:A:482:VAL:HG21	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214[A]:TRP:CD1	1:A:343:VAL:HG11	2.12	0.84
1:A:392:CYS:CB	1:A:445:ARG:HH21	1.88	0.84
1:A:31:LEU:HB2	1:A:39:HIS:HE1	1.43	0.82
1:A:165:PHE:O	1:A:169:CYS:HB2	1.82	0.80
1:A:392:CYS:HB3	1:A:445:ARG:NH2	1.95	0.80
1:A:233:LYS:CE	1:A:237:ASP:OD2	2.27	0.80
1:A:392:CYS:HB3	1:A:445:ARG:HH21	1.47	0.79
1:A:420:THR:HG21	1:A:531:GLU:OE2	1.83	0.78
1:A:503:ASN:ND2	1:A:505:GLU:HG2	1.99	0.77
1:A:475:LYS:HE3	1:A:479:GLU:OE1	1.85	0.76
1:A:348:ARG:HG3	1:A:482:VAL:CG1	2.15	0.76
1:A:168:CYS:HB2	1:A:178:LEU:HD13	1.68	0.75
1:A:104:GLN:HG3	1:A:105:HIS:CD2	2.22	0.74
1:A:12:LYS:HE2	1:A:54:VAL:HG13	1.70	0.73
1:A:310:VAL:HG22	1:A:373:VAL:CG1	2.18	0.73
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.72	0.72
1:A:67:HIS:CE1	1:A:249:ASP:OD1	2.42	0.72
1:A:249:ASP:HB3	1:A:252:GLU:CG	2.20	0.72
1:A:383:GLU:OE1	1:A:485:ARG:NH2	2.22	0.72
1:A:30:TYR:HE1	1:A:103:LEU:HD12	1.56	0.71
1:A:31:LEU:HB2	1:A:39:HIS:CE1	2.25	0.71
1:A:348:ARG:HG3	1:A:482:VAL:HG13	1.72	0.71
1:A:232:SER:O	1:A:236:THR:HG23	1.92	0.70
1:A:342:SER:HA	1:A:447:PRO:HA	1.72	0.70
1:A:305:LEU:HD22	1:A:334:TYR:HD1	1.55	0.69
1:A:141:GLU:OE1	1:A:145:ARG:NH1	2.21	0.69
1:A:414:LYS:NZ	2:A:601:P8S:O3	2.24	0.69
1:A:385:GLN:HG3	1:A:446:MET:HE2	1.75	0.69
1:A:452:TYR:O	1:A:456:VAL:HG23	1.93	0.68
1:A:334:TYR:HE2	1:A:349:LEU:HD13	1.58	0.68
2:A:601:P8S:F4B	2:A:601:P8S:F6A	1.84	0.68
1:A:66:LEU:O	1:A:70:PHE:HD1	1.77	0.67
1:A:30:TYR:CD1	1:A:102:PHE:HB3	2.30	0.67
1:A:416:PRO:O	1:A:534:LYS:HE2	1.95	0.67
1:A:139:LEU:HD21	1:A:158:ALA:HB2	1.77	0.66
1:A:90:CYS:O	1:A:91:CYS:HB2	1.96	0.66
1:A:152:PRO:HB2	1:A:257:ARG:HH11	1.61	0.66
1:A:11:PHE:HE2	1:A:47:THR:HG23	1.59	0.66
1:A:292:GLU:HG2	1:A:292:GLU:O	1.96	0.66
1:A:310:VAL:HG13	1:A:371:ALA:CA	2.26	0.65
1:A:306:ALA:HB1	1:A:311:GLU:OE2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:HG2	1:A:252:GLU:HG3	1.76	0.65
1:A:290:ILE:O	1:A:293:VAL:HG22	1.97	0.65
1:A:424:VAL:O	1:A:428:ARG:HG3	1.97	0.65
1:A:413:LYS:HB3	1:A:493:VAL:HG22	1.79	0.64
1:A:513:ILE:HD13	1:A:524:LYS:HG2	1.80	0.64
1:A:222:ARG:NH2	1:A:222:ARG:HG3	2.12	0.63
1:A:214[A]:TRP:HD1	1:A:343:VAL:HG11	1.61	0.63
1:A:310:VAL:HG22	1:A:373:VAL:HG12	1.81	0.63
1:A:418:VAL:O	1:A:534:LYS:NZ	2.31	0.63
1:A:39:HIS:O	1:A:43:VAL:HG23	1.97	0.63
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.81	0.62
1:A:23:VAL:HG13	1:A:70:PHE:HE2	1.65	0.62
1:A:333:GLU:O	1:A:337:ARG:NH1	2.33	0.62
1:A:23:VAL:HG13	1:A:70:PHE:CE2	2.35	0.62
1:A:32:GLN:OE1	1:A:107:ASP:N	2.29	0.61
1:A:153:GLU:O	1:A:157:PHE:HD1	1.82	0.61
1:A:214[B]:TRP:CD1	1:A:343:VAL:HG11	2.35	0.61
1:A:347:LEU:HB3	1:A:482:VAL:CG2	2.30	0.61
1:A:529:LEU:HD13	1:A:548:MET:HG3	1.81	0.61
1:A:5:SER:HB3	1:A:57:GLU:HG2	1.81	0.61
1:A:305:LEU:HD11	1:A:333:GLU:CB	2.27	0.61
1:A:305:LEU:HD22	1:A:334:TYR:CD1	2.35	0.60
1:A:222:ARG:CG	1:A:222:ARG:HH21	2.15	0.60
1:A:152:PRO:HG3	1:A:254:ALA:HA	1.81	0.60
1:A:453:LEU:HD23	1:A:485:ARG:HD3	1.82	0.60
1:A:37:GLU:HA	1:A:40:VAL:CG2	2.32	0.60
1:A:69:LEU:O	1:A:73:LYS:HG2	2.02	0.59
1:A:472:ARG:NH1	1:A:492:GLU:O	2.26	0.59
1:A:222:ARG:HG3	1:A:222:ARG:HH21	1.68	0.59
1:A:387:LEU:HG	1:A:391:ASN:HD22	1.67	0.59
1:A:484:ARG:HD2	3:A:725:HOH:O	2.01	0.59
1:A:278:CYS:O	1:A:281:LYS:HB2	2.03	0.58
1:A:31:LEU:HD13	1:A:34:CYS:SG	2.43	0.58
1:A:513:ILE:HA	1:A:516:LEU:HD12	1.85	0.58
1:A:104:GLN:HG3	1:A:105:HIS:HD2	1.65	0.58
1:A:31:LEU:HG	1:A:74:LEU:HD22	1.86	0.58
1:A:430:LEU:O	1:A:433:VAL:HG22	2.03	0.58
1:A:101:CYS:O	1:A:105:HIS:HD2	1.86	0.58
1:A:127:PHE:CE1	1:A:131:GLU:HG2	2.39	0.58
1:A:408:LEU:HD12	1:A:427:SER:HB2	1.84	0.58
1:A:453:LEU:HG	1:A:485:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:TYR:HE1	1:A:103:LEU:CD1	2.18	0.57
1:A:156:PHE:CZ	1:A:160:ARG:HD2	2.39	0.57
1:A:278:CYS:O	1:A:286:LYS:HG3	2.04	0.57
1:A:160:ARG:NH2	1:A:188:GLU:OE2	2.36	0.57
1:A:433:VAL:HG12	1:A:452:TYR:CD2	2.39	0.57
1:A:408:LEU:HD21	1:A:526:GLN:O	2.05	0.56
1:A:198:LEU:HD13	1:A:458:ASN:HB2	1.87	0.56
1:A:12:LYS:NZ	1:A:57:GLU:OE2	2.29	0.56
1:A:19:PHE:O	1:A:23:VAL:HG23	2.04	0.56
1:A:462:VAL:O	1:A:465:GLU:HG2	2.05	0.56
1:A:408:LEU:CD1	1:A:424:VAL:HA	2.36	0.56
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.87	0.56
1:A:414:LYS:HE2	1:A:491:LEU:O	2.06	0.56
1:A:312:SER:O	1:A:370:TYR:OH	2.22	0.55
1:A:347:LEU:CB	1:A:482:VAL:HG21	2.34	0.55
1:A:50:ALA:O	1:A:54:VAL:HG23	2.06	0.55
1:A:408:LEU:HD11	1:A:424:VAL:HA	1.88	0.55
1:A:323:LYS:HE2	1:A:354:GLU:OE2	2.07	0.55
1:A:398:LEU:HB3	1:A:402:LYS:HB2	1.90	0.54
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.90	0.54
1:A:127:PHE:CD2	1:A:165:PHE:HB3	2.41	0.54
1:A:345:LEU:O	1:A:349:LEU:HG	2.08	0.54
1:A:442:GLU:HA	1:A:445:ARG:HD3	1.88	0.54
2:A:601:P8S:F6B	2:A:601:P8S:F8A	2.04	0.54
1:A:218:ARG:HH12	1:A:295:ASN:HD21	1.55	0.54
1:A:400:GLU:OE1	1:A:435:SER:HB3	2.08	0.54
1:A:383:GLU:CD	1:A:485:ARG:HH22	2.15	0.54
1:A:499:PRO:HG3	1:A:537:PRO:HD2	1.89	0.54
1:A:123:MET:HB3	1:A:165:PHE:HE2	1.73	0.53
1:A:221:GLN:NE2	1:A:341:TYR:O	2.40	0.53
1:A:244:GLU:HG2	1:A:252:GLU:CG	2.39	0.53
1:A:347:LEU:CB	1:A:482:VAL:CG2	2.85	0.53
1:A:233:LYS:HE3	1:A:237:ASP:CG	2.26	0.53
1:A:257:ARG:NE	1:A:287:SER:HB3	2.24	0.53
1:A:315:VAL:HB	1:A:370:TYR:CZ	2.44	0.53
1:A:384:PRO:O	1:A:388:ILE:HG12	2.09	0.53
1:A:67:HIS:HE1	1:A:249:ASP:OD1	1.90	0.53
1:A:205:LYS:NZ	1:A:465:GLU:OE1	2.25	0.53
1:A:407:LEU:HD13	1:A:430:LEU:HB3	1.90	0.53
1:A:31:LEU:HB3	1:A:34:CYS:HB2	1.91	0.52
1:A:11:PHE:HZ	1:A:51:LYS:HE3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ASP:HB3	1:A:252:GLU:HG2	1.90	0.52
1:A:392:CYS:SG	1:A:445:ARG:NH2	2.82	0.52
1:A:101:CYS:O	1:A:105:HIS:CD2	2.62	0.52
1:A:388:ILE:O	1:A:392:CYS:HB2	2.10	0.52
1:A:153:GLU:OE2	1:A:288:HIS:ND1	2.31	0.52
1:A:404:GLN:HG2	1:A:428:ARG:HA	1.93	0.51
1:A:222:ARG:NH2	1:A:222:ARG:CG	2.73	0.51
1:A:38:ASP:N	1:A:38:ASP:OD1	2.42	0.51
1:A:387:LEU:HD22	1:A:485:ARG:NH1	2.25	0.51
1:A:220:SER:HB2	1:A:335:ALA:HB3	1.92	0.51
1:A:25:ILE:O	1:A:29:GLN:HG3	2.11	0.51
1:A:46:VAL:CG2	1:A:73:LYS:HG3	2.41	0.51
1:A:479:GLU:O	1:A:480:SER:C	2.54	0.50
1:A:24:LEU:HA	1:A:43:VAL:HG21	1.93	0.50
1:A:433:VAL:HG12	1:A:452:TYR:CG	2.47	0.50
1:A:28:ALA:HB3	1:A:143:ALA:HB3	1.93	0.50
1:A:225:LYS:HA	1:A:299:PRO:HG3	1.94	0.50
1:A:312:SER:HB3	1:A:315:VAL:HG23	1.93	0.50
1:A:424:VAL:HG11	1:A:523:ILE:HG23	1.94	0.50
1:A:108:ASP:OD1	1:A:197:ARG:NE	2.30	0.50
1:A:428:ARG:NH1	1:A:526:GLN:OE1	2.35	0.50
1:A:209:ARG:NH2	1:A:354:GLU:OE2	2.45	0.50
1:A:30:TYR:CD2	1:A:74:LEU:HD11	2.47	0.49
1:A:225:LYS:NZ	1:A:297:GLU:HB2	2.27	0.49
1:A:319:TYR:O	1:A:323:LYS:HA	2.12	0.49
1:A:387:LEU:HG	1:A:391:ASN:ND2	2.26	0.49
1:A:10:ARG:NH1	1:A:255:ASP:OD2	2.43	0.49
1:A:71:GLY:O	1:A:75:CYS:SG	2.70	0.49
1:A:352:THR:OG1	1:A:380:LEU:HD11	2.12	0.49
1:A:449:ALA:O	1:A:453:LEU:HB2	2.12	0.49
1:A:540:THR:H	1:A:543:GLN:NE2	2.11	0.49
1:A:278:CYS:HA	1:A:281:LYS:HD2	1.94	0.49
1:A:211:PHE:O	1:A:214[A]:TRP:HB3	2.13	0.49
1:A:222:ARG:HA	1:A:295:ASN:HD22	1.78	0.49
1:A:504:ALA:O	1:A:508:THR:OG1	2.28	0.49
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.13	0.49
1:A:306:ALA:O	1:A:311:GLU:HB2	2.13	0.49
1:A:99:ASN:O	1:A:103:LEU:HD13	2.13	0.48
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.94	0.48
1:A:391:ASN:OD1	1:A:410:ARG:NH1	2.39	0.48
1:A:475:LYS:HG2	1:A:479:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:THR:HB	1:A:530:VAL:CG1	2.43	0.48
1:A:540:THR:OG1	1:A:543:GLN:HG3	2.13	0.48
1:A:108:ASP:CG	1:A:197:ARG:HE	2.17	0.48
1:A:224:PRO:HG2	1:A:297:GLU:O	2.12	0.48
1:A:310:VAL:HG21	1:A:374:PHE:CD1	2.48	0.48
1:A:426:VAL:HG13	1:A:456:VAL:HG12	1.96	0.48
1:A:417:GLN:NE2	1:A:494:ASP:OD2	2.37	0.48
2:A:601:P8S:F3B	2:A:601:P8S:F1B	2.11	0.48
1:A:160:ARG:NH1	1:A:188:GLU:OE1	2.45	0.48
1:A:408:LEU:HD21	1:A:530:VAL:HG23	1.94	0.48
1:A:554:PHE:CZ	1:A:568:PHE:HD1	2.31	0.48
1:A:334:TYR:CE2	1:A:349:LEU:HD13	2.44	0.48
1:A:398:LEU:HB3	1:A:402:LYS:CB	2.44	0.48
1:A:36:PHE:O	1:A:40:VAL:HG22	2.14	0.47
1:A:39:HIS:HD2	1:A:140:TYR:CE1	2.31	0.47
1:A:282:PRO:HG2	1:A:285:GLU:HB2	1.96	0.47
2:A:601:P8S:F7A	2:A:601:P8S:F5A	2.08	0.47
1:A:275:LEU:O	1:A:276:LYS:C	2.57	0.47
1:A:453:LEU:HD23	1:A:485:ARG:CD	2.45	0.47
2:A:601:P8S:F3B	2:A:601:P8S:F5B	2.01	0.47
1:A:298:MET:HE2	1:A:339:PRO:HD3	1.97	0.47
1:A:257:ARG:CZ	1:A:287:SER:HB3	2.45	0.47
1:A:284:LEU:HD12	1:A:284:LEU:H	1.79	0.47
1:A:7:VAL:HA	1:A:66:LEU:HD21	1.96	0.47
1:A:474:THR:O	1:A:478:THR:HG23	2.15	0.47
1:A:495:GLU:OE1	1:A:495:GLU:N	2.48	0.47
2:A:602:P8S:F2B	2:A:602:P8S:F4A	2.13	0.47
1:A:133:THR:O	1:A:137:LYS:HG3	2.14	0.47
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.39	0.47
1:A:107:ASP:O	1:A:110:PRO:HD3	2.16	0.46
1:A:219:LEU:HD12	1:A:235:VAL:HG23	1.96	0.46
1:A:213:ALA:HA	2:A:602:P8S:F4A	2.05	0.46
1:A:264:ILE:HD13	1:A:290:ILE:HG21	1.97	0.46
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.77	0.46
1:A:249:ASP:O	1:A:252:GLU:HG2	2.15	0.46
1:A:339:PRO:O	1:A:447:PRO:HG3	2.16	0.46
1:A:389:LYS:NZ	1:A:389:LYS:HB3	2.30	0.46
1:A:420:THR:HG22	1:A:534:LYS:NZ	2.31	0.46
1:A:212:LYS:HZ1	1:A:236:THR:HG22	1.81	0.46
1:A:512:ASP:O	1:A:516:LEU:HG	2.16	0.46
1:A:278:CYS:HB3	1:A:289:CYS:HB3	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASP:O	1:A:42:LEU:HG	2.17	0.45
1:A:503:ASN:CG	1:A:505:GLU:HG2	2.42	0.45
1:A:453:LEU:CD1	2:A:601:P8S:F5B	2.55	0.45
1:A:457:LEU:HD23	1:A:457:LEU:HA	1.74	0.45
1:A:394:LEU:O	1:A:398:LEU:HG	2.17	0.45
1:A:543:GLN:O	1:A:547:VAL:HG22	2.17	0.45
1:A:128:HIS:NE2	1:A:169:CYS:HB3	2.31	0.45
1:A:217:ALA:HB3	1:A:343:VAL:HG13	1.98	0.45
1:A:348:ARG:CG	1:A:482:VAL:CG1	2.91	0.45
1:A:353:TYR:HD1	1:A:373:VAL:HG21	1.82	0.44
1:A:150:TYR:CZ	1:A:242:HIS:CE1	3.05	0.44
1:A:281:LYS:HB3	1:A:285:GLU:HB3	1.98	0.44
1:A:426:VAL:HG21	1:A:460:LEU:HB2	2.00	0.44
1:A:310:VAL:HG12	1:A:371:ALA:HA	1.92	0.44
1:A:349:LEU:HD22	1:A:377:PHE:CG	2.53	0.44
1:A:495:GLU:C	1:A:497:TYR:H	2.24	0.44
1:A:165:PHE:CE2	1:A:178:LEU:HD21	2.52	0.44
1:A:395:PHE:CZ	1:A:435:SER:HA	2.53	0.44
1:A:521:ARG:HG3	1:A:522:GLN:N	2.32	0.44
1:A:127:PHE:CG	1:A:165:PHE:HB3	2.53	0.43
1:A:212:LYS:HB3	2:A:602:P8S:F5A	2.07	0.43
1:A:418:VAL:HG21	1:A:473:VAL:HG21	1.99	0.43
1:A:485:ARG:NH1	1:A:489:SER:OG	2.51	0.43
1:A:30:TYR:CE1	1:A:103:LEU:HD12	2.45	0.43
1:A:264:ILE:HA	1:A:271:ILE:CD1	2.49	0.43
1:A:420:THR:HA	1:A:423:LEU:HB2	2.00	0.43
1:A:554:PHE:CZ	1:A:568:PHE:HA	2.53	0.43
1:A:22:LEU:HG	1:A:155:LEU:HD11	2.01	0.43
1:A:347:LEU:HB2	1:A:482:VAL:HG22	2.00	0.43
1:A:354:GLU:O	1:A:358:GLU:HG2	2.17	0.43
1:A:357:LEU:O	1:A:361:CYS:HB2	2.18	0.43
1:A:198:LEU:HG	1:A:214[A]:TRP:CH2	2.54	0.43
1:A:420:THR:O	1:A:421:PRO:C	2.61	0.43
1:A:513:ILE:HA	1:A:516:LEU:CD1	2.48	0.43
1:A:310:VAL:HG11	1:A:371:ALA:O	2.18	0.43
1:A:408:LEU:HG	1:A:530:VAL:HG22	2.01	0.42
1:A:334:TYR:HE2	1:A:349:LEU:CD1	2.30	0.42
1:A:370:TYR:O	1:A:373:VAL:HG12	2.19	0.42
1:A:98:ARG:O	1:A:101:CYS:HB3	2.20	0.42
1:A:19:PHE:CE2	1:A:23:VAL:HG21	2.54	0.42
1:A:46:VAL:HG22	1:A:73:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PHE:CE1	1:A:285:GLU:HG3	2.55	0.42
1:A:414:LYS:NZ	2:A:601:P8S:S1	2.93	0.42
1:A:414:LYS:O	1:A:472:ARG:NH1	2.47	0.42
1:A:565:GLU:H	1:A:565:GLU:HG2	1.50	0.42
1:A:222:ARG:HA	1:A:295:ASN:HA	2.02	0.42
1:A:327:LEU:HD23	1:A:327:LEU:HA	1.87	0.42
1:A:487:CYS:O	1:A:491:LEU:HG	2.20	0.42
1:A:261:ALA:HB2	1:A:287:SER:OG	2.20	0.42
1:A:502:PHE:CB	1:A:535:HIS:NE2	2.83	0.42
1:A:11:PHE:CZ	1:A:51:LYS:HE3	2.55	0.42
1:A:438:CYS:O	1:A:445:ARG:NH1	2.53	0.42
1:A:24:LEU:HA	1:A:43:VAL:CG2	2.49	0.42
1:A:135:LEU:HD11	1:A:158:ALA:O	2.19	0.42
1:A:420:THR:HG22	1:A:534:LYS:HZ2	1.83	0.42
1:A:244:GLU:OE1	1:A:256:ASP:OD2	2.38	0.42
1:A:343:VAL:O	1:A:347:LEU:HG	2.19	0.41
1:A:345:LEU:HD21	1:A:381:VAL:HG22	2.02	0.41
1:A:420:THR:HB	1:A:530:VAL:HG11	2.01	0.41
1:A:513:ILE:HG21	1:A:568:PHE:CZ	2.55	0.41
1:A:8:ALA:HB2	1:A:53:CYS:HB3	2.02	0.41
1:A:12:LYS:HE2	1:A:54:VAL:CG1	2.44	0.41
1:A:437:CYS:SG	1:A:449:ALA:HA	2.60	0.41
1:A:456:VAL:O	1:A:459:GLN:HB2	2.20	0.41
1:A:96:PRO:O	1:A:100:GLU:HG2	2.20	0.41
1:A:120:VAL:O	1:A:124:CYS:HB2	2.20	0.41
1:A:127:PHE:CE2	1:A:165:PHE:HB3	2.56	0.41
1:A:298:MET:HB2	1:A:298:MET:HE3	1.68	0.41
1:A:446:MET:N	1:A:447:PRO:HD2	2.36	0.41
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.50	0.41
1:A:215:ALA:HB1	1:A:235:VAL:HG22	2.03	0.41
1:A:453:LEU:HD11	2:A:601:P8S:F5B	2.10	0.41
1:A:212:LYS:NZ	1:A:236:THR:HG22	2.35	0.41
1:A:427:SER:O	1:A:430:LEU:HB2	2.20	0.41
1:A:540:THR:OG1	1:A:543:GLN:CG	2.69	0.41
1:A:6:GLU:OE2	1:A:10:ARG:NE	2.54	0.41
1:A:173:ASP:HB3	1:A:176:ALA:HB3	2.01	0.41
1:A:222:ARG:HA	1:A:295:ASN:ND2	2.35	0.41
1:A:529:LEU:HD13	1:A:548:MET:CG	2.48	0.41
1:A:554:PHE:CZ	1:A:568:PHE:CD1	3.09	0.41
1:A:513:ILE:CD1	1:A:516:LEU:HD12	2.29	0.41
1:A:380:LEU:O	1:A:384:PRO:CD	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ASN:ND2	1:A:505:GLU:OE2	2.48	0.40
1:A:101:CYS:HA	1:A:104:GLN:HG2	2.03	0.40
1:A:211:PHE:CE2	1:A:239:THR:HA	2.56	0.40
1:A:420:THR:N	1:A:421:PRO:CD	2.84	0.40
1:A:453:LEU:CD2	1:A:485:ARG:CD	2.99	0.40
1:A:139:LEU:CD2	1:A:158:ALA:HB2	2.49	0.40
1:A:219:LEU:O	1:A:223:PHE:N	2.47	0.40
1:A:392:CYS:SG	2:A:601:P8S:F8B	2.69	0.40
1:A:252:GLU:CD	1:A:252:GLU:H	2.28	0.40
1:A:529:LEU:O	1:A:533:VAL:HG23	2.21	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	551/585 (94%)	534 (97%)	17 (3%)	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	464/511 (91%)	432 (93%)	32 (7%)	14 20

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	100	GLU
1	A	103	LEU
1	A	116	VAL
1	A	117	ARG
1	A	124	CYS
1	A	169	CYS
1	A	212	LYS
1	A	222	ARG
1	A	233	LYS
1	A	245	CYS
1	A	252	GLU
1	A	270	SER
1	A	277	GLU
1	A	292	GLU
1	A	293	VAL
1	A	305	LEU
1	A	317	LYS
1	A	365	ASP
1	A	389	LYS
1	A	419	SER
1	A	420	THR
1	A	435	SER
1	A	450	GLU
1	A	472	ARG
1	A	479	GLU
1	A	496	THR
1	A	506	THR
1	A	543	GLN
1	A	547	VAL
1	A	563	ASP
1	A	565	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	61	ASN
1	A	67	HIS
1	A	104	GLN
1	A	105	HIS

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Mol	Chain	Res	Type
1	A	295	ASN
1	A	318	ASN
1	A	397	GLN
1	A	483	ASN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	P8S	A	601	-	28,28,28	1.57	2 (7%)	50,54,54	1.32	8 (16%)
2	P8S	A	602	-	28,28,28	1.59	3 (10%)	50,54,54	0.95	2 (4%)

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	P8S	A	601	-	-	36/72/72/72	-
2	P8S	A	602	-	-	19/72/72/72	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	P8S	C1-S1	-6.81	1.65	1.83
2	A	601	P8S	C1-S1	-6.58	1.66	1.83
2	A	601	P8S	O3-S1	2.53	1.49	1.42
2	A	602	P8S	O3-S1	2.41	1.49	1.42
2	A	602	P8S	O2-S1	2.35	1.49	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	P8S	C1-C2-C3	-3.45	105.53	116.11
2	A	601	P8S	C2-C1-S1	-3.01	105.52	116.18
2	A	601	P8S	C4-C5-C6	-2.91	104.27	116.45
2	A	602	P8S	O1-S1-C1	2.85	112.13	101.77
2	A	601	P8S	C3-C4-C5	-2.27	106.92	116.45
2	A	601	P8S	O2-S1-O3	-2.20	109.34	117.52
2	A	601	P8S	C8-C7-C6	-2.18	107.15	117.11
2	A	602	P8S	C8-C7-C6	-2.16	107.25	117.11
2	A	601	P8S	O1-S1-C1	2.10	109.40	101.77
2	A	601	P8S	F3A-C3-F3B	2.01	115.70	107.33

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	P8S	F1B-C1-C2-C3
2	A	601	P8S	F1A-C1-C2-C3
2	A	601	P8S	S1-C1-C2-C3
2	A	601	P8S	F1A-C1-C2-F2B
2	A	601	P8S	S1-C1-C2-F2B
2	A	602	P8S	C1-C2-C3-C4
2	A	602	P8S	C1-C2-C3-F3A
2	A	601	P8S	C4-C5-C6-C7
2	A	601	P8S	C2-C3-C4-C5
2	A	601	P8S	F7B-C7-C8-F8B
2	A	601	P8S	F7A-C7-C8-F8C
2	A	601	P8S	F3A-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	A	601	P8S	C2-C3-C4-F4A
2	A	601	P8S	F5B-C5-C6-C7
2	A	601	P8S	C4-C5-C6-F6B
2	A	602	P8S	C3-C4-C5-C6
2	A	602	P8S	C3-C4-C5-F5A
2	A	601	P8S	F1B-C1-C2-F2A
2	A	601	P8S	C6-C7-C8-F8A
2	A	602	P8S	F4A-C4-C5-C6
2	A	601	P8S	F7B-C7-C8-F8C
2	A	601	P8S	F7A-C7-C8-F8A
2	A	601	P8S	F7B-C7-C8-F8A
2	A	601	P8S	C6-C7-C8-F8B
2	A	601	P8S	C6-C7-C8-F8C
2	A	601	P8S	F7A-C7-C8-F8B
2	A	602	P8S	F2A-C2-C3-F3A
2	A	601	P8S	F1A-C1-C2-F2A
2	A	601	P8S	F5B-C5-C6-F6B
2	A	601	P8S	F3A-C3-C4-F4A
2	A	602	P8S	F2B-C2-C3-F3A
2	A	602	P8S	F2B-C2-C3-F3B
2	A	602	P8S	F2A-C2-C3-F3B
2	A	602	P8S	F2A-C2-C3-C4
2	A	601	P8S	F3B-C3-C4-F4B
2	A	602	P8S	F7B-C7-C8-F8C
2	A	602	P8S	C6-C7-C8-F8C
2	A	602	P8S	F2B-C2-C3-C4
2	A	601	P8S	F3B-C3-C4-F4A
2	A	601	P8S	F5A-C5-C6-F6A
2	A	601	P8S	C2-C3-C4-F4B
2	A	601	P8S	F1B-C1-C2-F2B
2	A	602	P8S	F7B-C7-C8-F8B
2	A	602	P8S	F7A-C7-C8-F8C
2	A	601	P8S	F3B-C3-C4-C5
2	A	601	P8S	F5B-C5-C6-F6A
2	A	602	P8S	C1-C2-C3-F3B
2	A	601	P8S	S1-C1-C2-F2A
2	A	601	P8S	F3A-C3-C4-F4B
2	A	601	P8S	F5A-C5-C6-F6B
2	A	602	P8S	F7A-C7-C8-F8B
2	A	601	P8S	C4-C5-C6-F6A
2	A	602	P8S	F7B-C7-C8-F8A
2	A	601	P8S	F5A-C5-C6-C7

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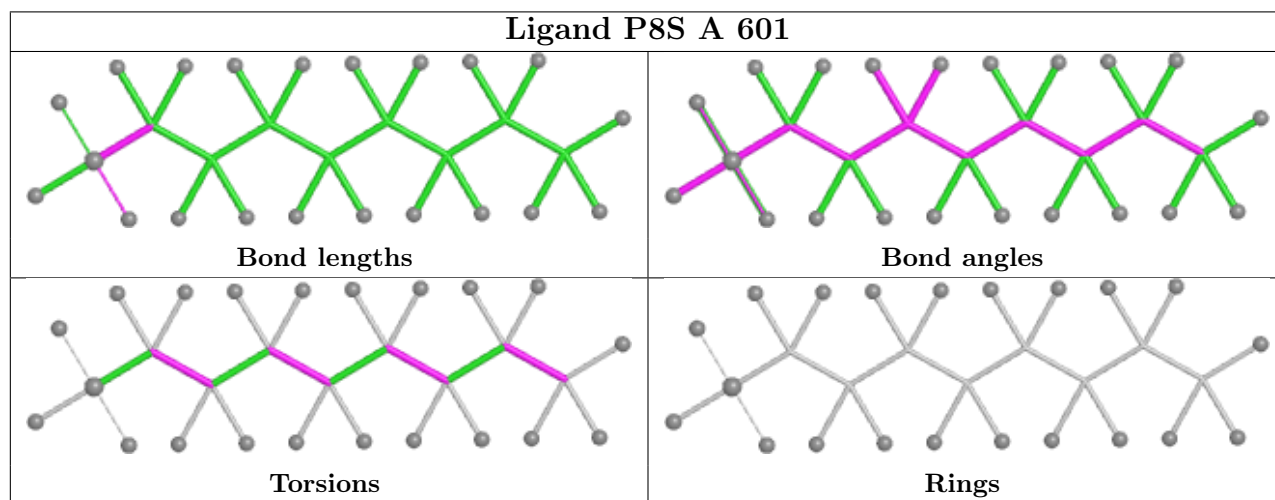
Mol	Chain	Res	Type	Atoms
2	A	602	P8S	C6-C7-C8-F8B

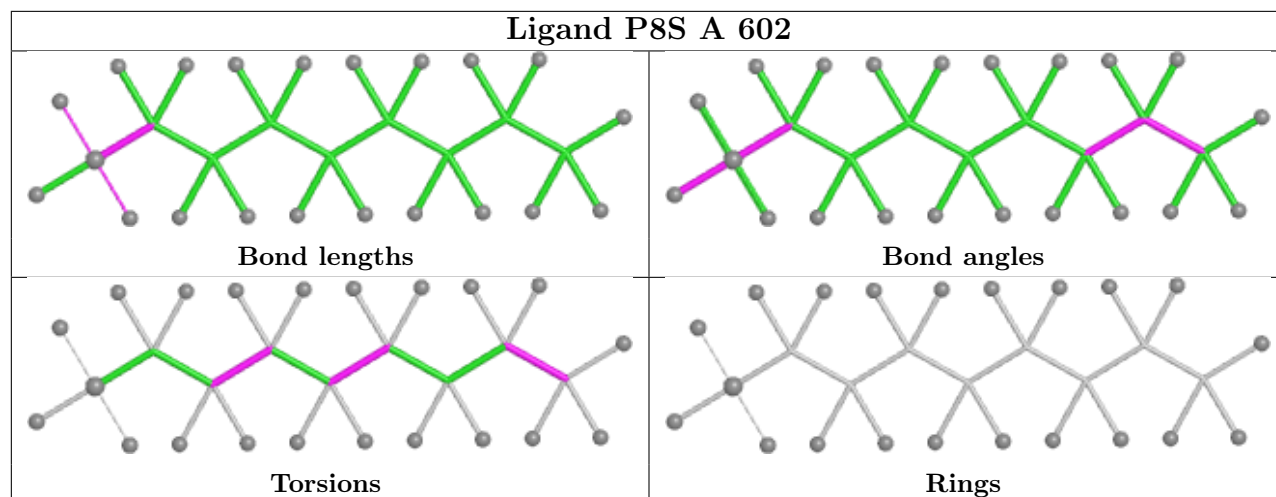
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	P8S	10	0
2	A	602	P8S	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 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	554/585 (94%)	0.55	22 (3%) 42 44	21, 58, 85, 97	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214[A]	TRP	4.1
1	A	493	VAL	3.5
1	A	443	ALA	3.3
1	A	441	PRO	3.1
1	A	452	TYR	3.0
1	A	511	ALA	3.0
1	A	509	PHE	2.8
1	A	5	SER	2.7
1	A	176	ALA	2.6
1	A	92	ALA	2.5
1	A	347	LEU	2.5
1	A	518	GLU	2.5
1	A	217	ALA	2.4
1	A	122	VAL	2.4
1	A	370	TYR	2.3
1	A	463	LEU	2.2
1	A	433	VAL	2.2
1	A	548	MET	2.2
1	A	300	ALA	2.2
1	A	371	ALA	2.1
1	A	449	ALA	2.0
1	A	356	THR	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](#)

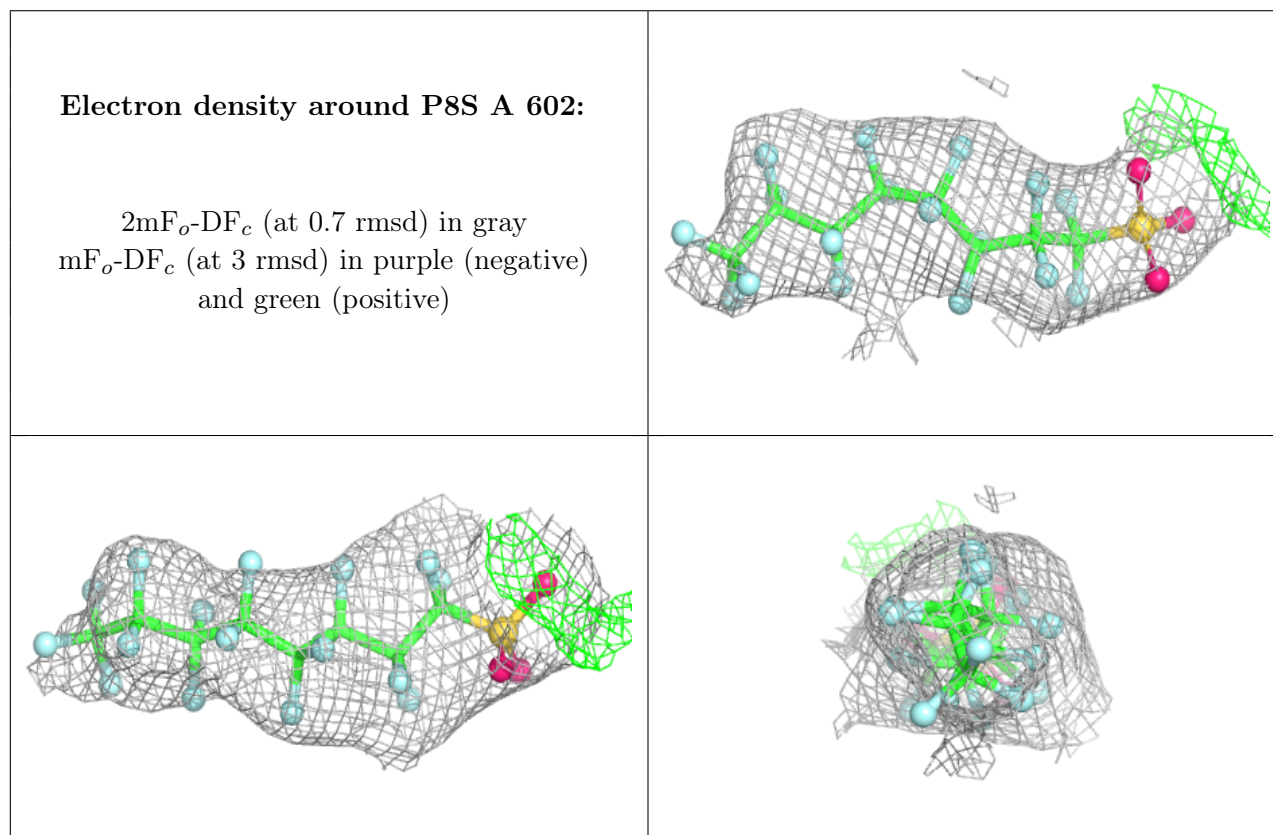
There are no oligosaccharides in this entry.

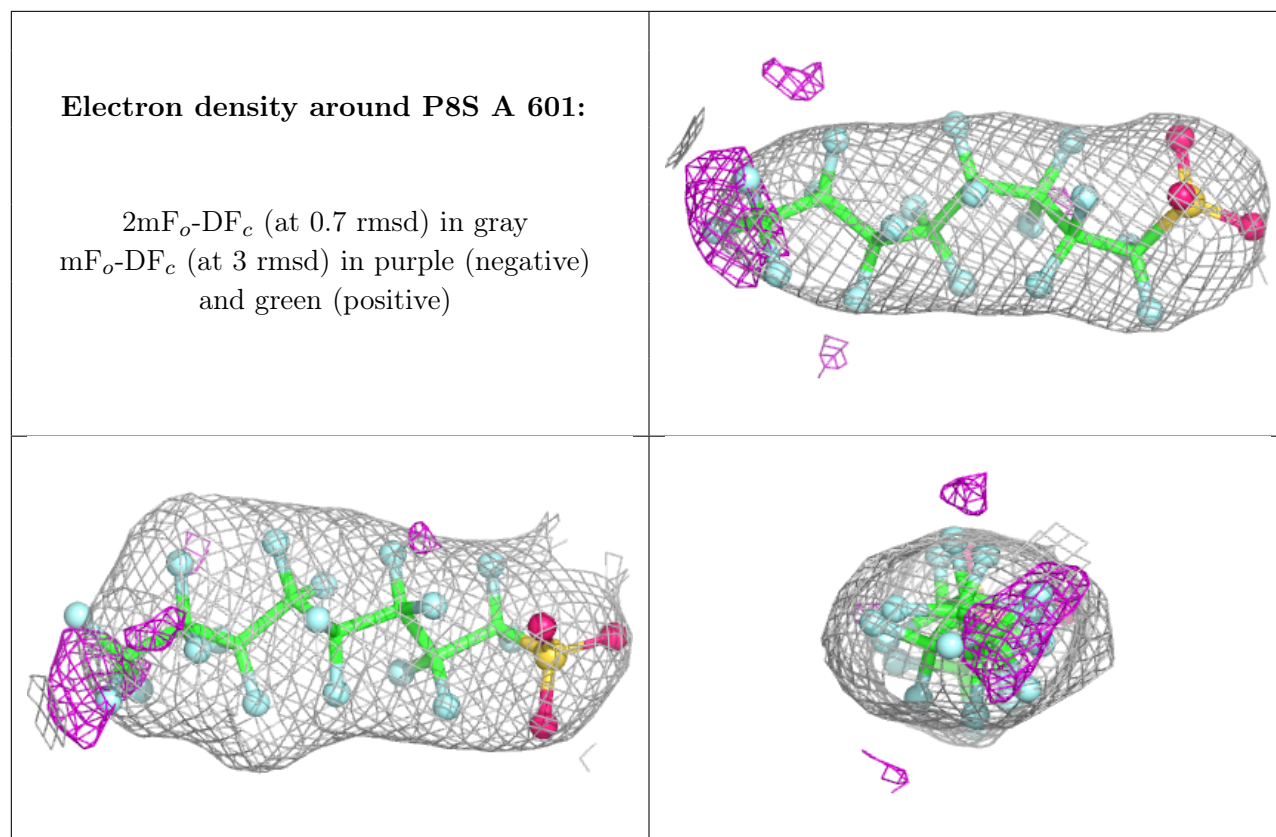
6.4 Ligands [i](#)

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. 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	B-factors(Å ²)	Q<0.9
2	P8S	A	602	29/29	0.84	0.11	53,63,72,75	29
2	P8S	A	601	29/29	0.91	0.08	55,65,73,75	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.