



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:31 pm GMT

PDB ID : 4E99
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (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

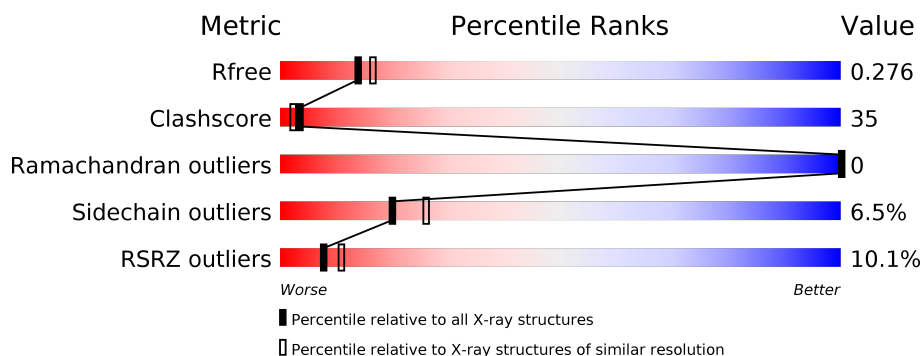
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>10%</div> <div>47%</div> <div>43%</div> <div>5%</div> </div>

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](#)

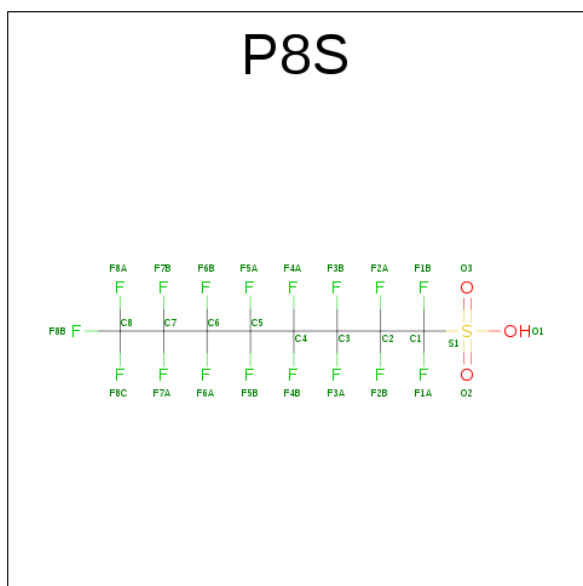
There are 3 unique types of molecules in this entry. The entry contains 4436 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is HEPTADEC AFLUORO-1-OCTANESULFONIC ACID (three-letter code: P8S) (formula: $C_8HF_{17}O_3S$).



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

- 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 34.19 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (54.46-2.30) 99.0 (34.19-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.238 , 0.278 0.237 , 0.276	Depositor DCC
R_{free} test set	1101 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
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

Xtriage'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	0.83	0/4411	0.89	6/5973 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	91	CYS	CA-CB-SG	-6.19	102.85	114.00
1	A	219	LEU	CB-CG-CD1	-5.99	100.81	111.00
1	A	491	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	A	198	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	A	245	CYS	CA-CB-SG	-5.25	104.56	114.00
1	A	246	CYS	CA-CB-SG	-5.08	104.85	114.00

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	291	0
2	A	58	0	2	14	0
3	A	52	0	0	1	0
All	All	4436	0	4135	298	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 35.

All (298) 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
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:348:ARG:HG3	1:A:482:VAL:HG13	1.72	0.71
1:A:31:LEU:HB2	1:A:39:HIS:CE1	2.25	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:420:THR:HG22	1:A:534:LYS:HZ2	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:152:PRO:HB2	1:A:257:ARG:HH11	1.61	0.66
1:A:90:CYS:O	1:A:91:CYS:HB2	1.96	0.66
1:A:11:PHE:HE2	1:A:47:THR:HG23	1.59	0.66
1:A:292:GLU:O	1:A:292:GLU:HG2	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
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:HG3	1:A:222:ARG:NH2	2.12	0.63
1:A:310:VAL:HG22	1:A:373:VAL:HG12	1.81	0.63
1:A:214[A]:TRP:HD1	1:A:343:VAL:HG11	1.61	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:205:LYS:NZ	1:A:465:GLU:OE1	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:418:VAL:O	1:A:534:LYS:NZ	2.31	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
1:A:156:PHE:CZ	1:A:160:ARG:HD2	2.39	0.57
1:A:30:TYR:HE1	1:A:103:LEU:CD1	2.18	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: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: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:127:PHE:CD2	1:A:165:PHE:HB3	2.41	0.54
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.90	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:F8A	2:A:601:P8S:F6B	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: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:257:ARG:NE	1:A:287:SER:HB3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:38:ASP:OD1	1:A:38:ASP:N	2.42	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:CG	1:A:222:ARG:NH2	2.73	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: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: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:30:TYR:CD2	1:A:74:LEU:HD11	2.47	0.49
1:A:10:ARG:NH1	1:A:255:ASP:OD2	2.43	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:71:GLY:O	1:A:75:CYS:SG	2.70	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:ASN:O	1:A:103:LEU:HD13	2.13	0.48
1:A:475:LYS:HG2	1:A:479:GLU:OE1	2.13	0.48
1:A:233:LYS:HE3	1:A:237:ASP:CG	2.26	0.48
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: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
1:A:383:GLU:CD	1:A:485:ARG:HH22	2.15	0.47
2:A:601:P8S:F7A	2:A:601:P8S:F5A	2.08	0.47
1:A:453:LEU:HD23	1:A:485:ARG:CD	2.45	0.47
1:A:12:LYS:NZ	1:A:57:GLU:OE2	2.29	0.47
2:A:601:P8S:F5B	2:A:601:P8S:F3B	2.01	0.47
1:A:284:LEU:H	1:A:284:LEU:HD12	1.79	0.47
1:A:257:ARG:CZ	1:A:287:SER:HB3	2.45	0.47
1:A:495:GLU:N	1:A:495:GLU:OE1	2.48	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
2:A:602:P8S:F4A	2:A:602:P8S:F2B	2.13	0.47
1:A:133:THR:O	1:A:137:LYS:HG3	2.14	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:HA	1:A:430:LEU:HD23	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:HB3	1:A:389:LYS:NZ	2.30	0.46
1:A:479:GLU:O	1:A:480:SER:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:504:ALA:O	1:A:508:THR:OG1	2.28	0.45
2:A:601:P8S:O1	2:A:601:P8S:F2A	2.07	0.45
1:A:38:ASP:O	1:A:42:LEU:HG	2.17	0.45
1:A:453:LEU:CD1	2:A:601:P8S:F5B	2.55	0.45
1:A:457:LEU:HA	1:A:457:LEU:HD23	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:312:SER:O	1:A:370:TYR:OH	2.22	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: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:108:ASP:CG	1:A:197:ARG:HE	2.17	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:513:ILE:HA	1:A:516:LEU:CD1	2.48	0.43
1:A:212:LYS:HZ1	1:A:236:THR:HG22	1.83	0.43
1:A:310:VAL:HG11	1:A:371:ALA:O	2.18	0.43
1:A:275:LEU:O	1:A:276:LYS:C	2.57	0.42
1:A:408:LEU:HG	1:A:530:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:156:PHE:CE1	1:A:285:GLU:HG3	2.55	0.42
1:A:46:VAL:HG22	1:A:73:LYS:HG3	2.01	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:HA	1:A:327:LEU:HD23	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:438:CYS:O	1:A:445:ARG:NH1	2.53	0.42
1:A:11:PHE:CZ	1:A:51:LYS:HE3	2.55	0.42
1:A:135:LEU:HD11	1:A:158:ALA:O	2.19	0.42
1:A:24:LEU:HA	1:A:43:VAL:CG2	2.49	0.42
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.39	0.42
1:A:244:GLU:OE1	1:A:256:ASP:OD2	2.38	0.42
1:A:345:LEU:HD21	1:A:381:VAL:HG22	2.02	0.41
1:A:343:VAL:O	1:A:347:LEU:HG	2.19	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: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:8:ALA:HB2	1:A:53:CYS:HB3	2.02	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:446:MET:N	1:A:447:PRO:HD2	2.36	0.41
1:A:96:PRO:O	1:A:100:GLU:HG2	2.20	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:222:ARG:HA	1:A:295:ASN:ND2	2.35	0.41
1:A:173:ASP:HB3	1:A:176:ALA:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:503:ASN:CG	1:A:505:GLU:HG2	2.42	0.40
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:HG22	1:A:534:LYS:NZ	2.31	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: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%)	434 (94%)	30 (6%)	20	26

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
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	270	SER
1	A	277	GLU
1	A	284	LEU
1	A	292	GLU
1	A	293	VAL
1	A	305	LEU
1	A	365	ASP
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	543	GLN
1	A	547	VAL
1	A	563	ASP
1	A	565	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS

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Mol	Chain	Res	Type
1	A	104	GLN
1	A	105	HIS
1	A	295	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 carbohydrates 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%)	54,54,54	1.32	8 (14%)
2	P8S	A	602	-	28,28,28	1.60	3 (10%)	54,54,54	0.95	3 (5%)

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	-	-	0/72/72/72	0/0/0/0
2	P8S	A	602	-	-	0/72/72/72	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	P8S	C1-S1	-7.12	1.65	1.84
2	A	601	P8S	C1-S1	-6.88	1.66	1.84
2	A	602	P8S	O2-S1	2.08	1.49	1.42
2	A	602	P8S	O3-S1	2.14	1.49	1.42
2	A	601	P8S	O3-S1	2.24	1.49	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	P8S	C1-C2-C3	-3.62	105.53	116.28
2	A	601	P8S	C4-C5-C6	-2.76	104.27	116.68
2	A	601	P8S	C2-C1-S1	-2.70	105.52	115.89
2	A	601	P8S	C3-C4-C5	-2.17	106.92	116.68
2	A	602	P8S	C1-C2-C3	-2.09	110.07	116.28
2	A	601	P8S	C8-C7-C6	-2.04	107.15	117.21
2	A	601	P8S	O2-S1-O3	-2.03	109.34	117.38
2	A	602	P8S	C8-C7-C6	-2.02	107.25	117.21
2	A	601	P8S	O1-S1-C1	2.42	109.40	102.17
2	A	601	P8S	O2-S1-C1	2.45	111.80	104.99
2	A	602	P8S	O1-S1-C1	3.34	112.13	102.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	P8S	11	0
2	A	602	P8S	3	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	554/585 (94%)	0.76	56 (10%) 8 11	38, 58, 85, 97	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	VAL	5.0
1	A	171	ALA	4.3
1	A	60	GLU	4.2
1	A	569	ALA	4.0
1	A	214[A]	TRP	3.7
1	A	297	GLU	3.6
1	A	5	SER	3.5
1	A	568	PHE	3.5
1	A	443	ALA	3.5
1	A	49	PHE	3.4
1	A	367	HIS	3.4
1	A	92	ALA	3.3
1	A	134	PHE	3.3
1	A	532	LEU	3.2
1	A	178	LEU	3.2
1	A	115	LEU	3.0
1	A	172	ALA	3.0
1	A	452	TYR	3.0
1	A	74	LEU	3.0
1	A	55	ALA	3.0
1	A	493	VAL	2.9
1	A	511	ALA	2.9
1	A	280	GLU	2.9
1	A	562	ASP	2.9
1	A	560	LYS	2.8
1	A	185	LEU	2.8
1	A	168	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	395	PHE	2.7
1	A	104	GLN	2.7
1	A	564	LYS	2.6
1	A	565	GLU	2.6
1	A	463	LEU	2.6
1	A	548	MET	2.6
1	A	388	ILE	2.6
1	A	300	ALA	2.6
1	A	453	LEU	2.5
1	A	317	LYS	2.4
1	A	455	VAL	2.3
1	A	167	GLU	2.3
1	A	327	LEU	2.3
1	A	473	VAL	2.3
1	A	72	ASP	2.3
1	A	59	ALA	2.3
1	A	553	ALA	2.3
1	A	510	HIS	2.2
1	A	166	THR	2.2
1	A	347	LEU	2.2
1	A	398	LEU	2.2
1	A	69	LEU	2.2
1	A	561	ALA	2.1
1	A	170	GLN	2.1
1	A	401	TYR	2.1
1	A	370	TYR	2.1
1	A	164	ALA	2.0
1	A	187	ASP	2.0
1	A	229	ALA	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 [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. 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	P8S	A	602	29/29	0.84	0.24	1.52	53,63,72,75	29
2	P8S	A	601	29/29	0.94	0.13	-0.96	55,65,73,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.