



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:29 AM UTC

PDB ID : 1R1K / pdb_00001r1k
Title : Crystal structure of the ligand-binding domains of the heterodimer EcR/USP bound to ponasterone A
Authors : Billas, I.M.L.; Iwema, T.; Garnier, J.-M.; Mitschler, A.; Rochel, N.; Moras, D.; Structural Proteomics in Europe (SPINE)
Deposited on : 2003-09-24
Resolution : 2.90 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

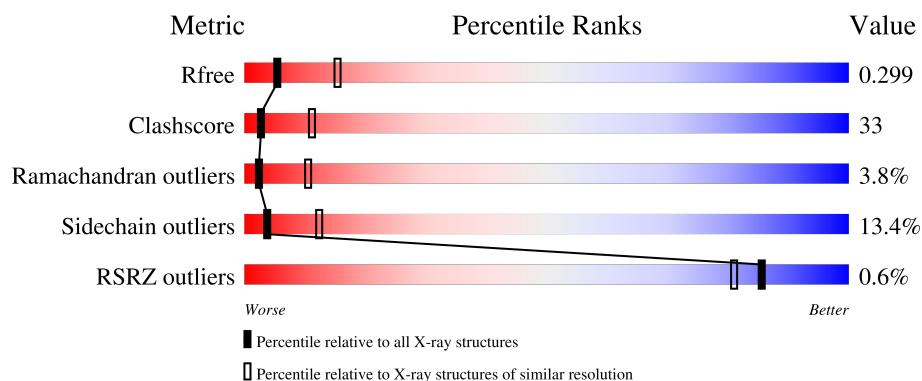
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	D	266	38% 43% 8% 11%
2	A	263	36% 44% 11% 8%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3887 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.

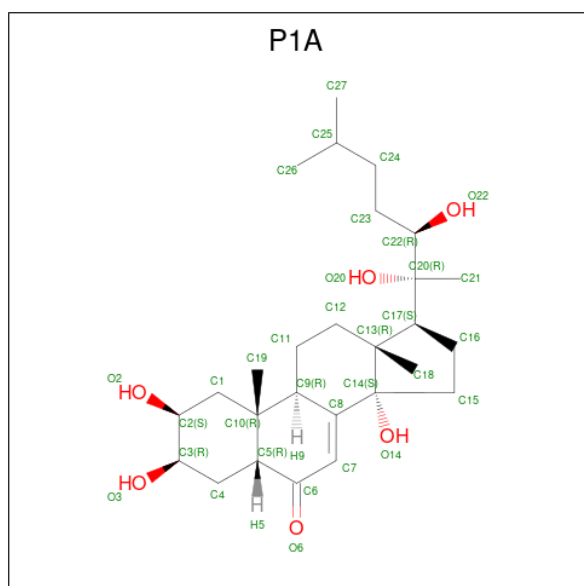
- Molecule 1 is a protein called Ecdysone receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	236	Total	C	N	O	S	0	0	0
			1872	1194	316	346	16			

- Molecule 2 is a protein called ULTRASPIRACLE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	241	Total	C	N	O	S	0	0	0
			1925	1233	335	345	12			

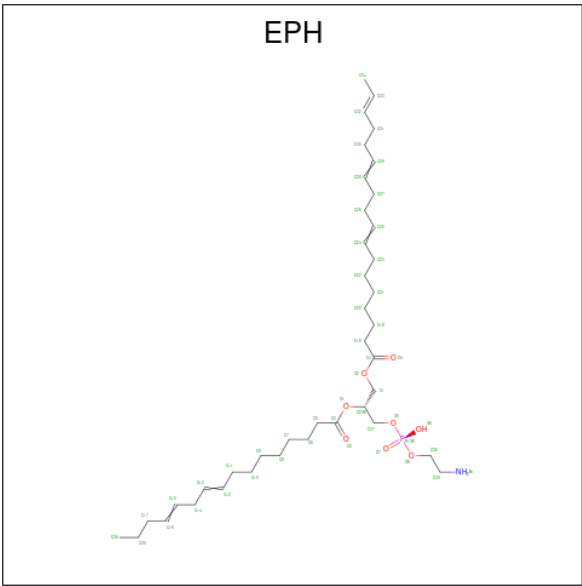
- Molecule 3 is 2,3,14,20,22-PENTAHYDROXYCHOLEST-7-EN-6-ONE (CCD ID: P1A) (formula: $C_{27}H_{44}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			33	27	6		

- Molecule 4 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PH

OSPHATIDYLETHANOLAMINE (CCD ID: EPH) (formula: C₃₉H₆₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	3	Total O	0	0
			3 3		
5	A	5	Total O	0	0
			5 5		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	57.40Å 57.40Å 302.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.90) 99.2 (20.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.88Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.304 0.241 , 0.299	Depositor DCC
R_{free} test set	1388 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3887	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPH, P1A

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	D	0.69	0/1905	1.09	7/2579 (0.3%)
2	A	0.65	0/1960	1.11	15/2646 (0.6%)
All	All	0.67	0/3865	1.10	22/5225 (0.4%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	417	ILE	N-CA-C	13.38	123.10	110.53
2	A	406	SER	N-CA-C	8.51	123.48	113.18
1	D	512	LYS	N-CA-C	-7.75	102.91	111.36
2	A	267	ILE	CA-C-N	7.05	128.65	119.84
2	A	267	ILE	C-N-CA	7.05	128.65	119.84
2	A	263	TRP	N-CA-C	-7.03	104.34	113.12
2	A	376	ASN	CA-C-N	6.94	126.65	119.64
2	A	376	ASN	C-N-CA	6.94	126.65	119.64
2	A	229	PHE	N-CA-C	-6.75	103.73	112.23
1	D	335	PRO	N-CA-C	-6.25	104.84	113.53
2	A	446	ILE	N-CA-C	6.15	116.31	110.53
1	D	382	LEU	N-CA-C	-6.09	104.64	111.28
2	A	345	PHE	N-CA-C	-6.05	104.60	111.07
1	D	518	LEU	N-CA-C	-5.76	101.23	109.24
2	A	252	ILE	N-CA-C	-5.61	105.03	110.42
2	A	368	ALA	N-CA-C	-5.37	105.08	111.03
1	D	288	PRO	N-CA-C	5.36	117.24	110.70
2	A	286	TRP	N-CA-C	5.34	117.52	111.11
2	A	420	ARG	N-CA-C	-5.32	105.93	112.90
1	D	461	ILE	N-CA-C	-5.21	103.98	111.17
2	A	287	ASN	N-CA-C	-5.21	105.30	110.97
2	A	336	ALA	N-CA-C	-5.20	105.61	111.28

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	D	1872	0	1880	138	0
2	A	1925	0	1970	128	1
3	D	33	0	43	4	0
4	A	49	0	67	6	0
5	A	5	0	0	1	0
5	D	3	0	0	0	0
All	All	3887	0	3960	261	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (261) 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:D:502:MET:HE2	2:A:429:LEU:HB3	1.23	1.12
1:D:480:SER:HB2	1:D:481:PRO:HD2	1.51	0.93
1:D:453:GLU:C	1:D:455:PRO:HD3	1.95	0.91
1:D:403:TYR:HA	1:D:407:ASN:HD22	1.35	0.89
1:D:478:SER:O	1:D:480:SER:N	2.08	0.87
2:A:262:VAL:HG23	2:A:265:ARG:NH2	1.92	0.85
1:D:346:THR:O	1:D:350:ILE:HG13	1.78	0.82
2:A:376:ASN:HD22	2:A:379:VAL:HG23	1.43	0.82
2:A:451:ARG:HD2	2:A:452:ASP:N	1.96	0.81
1:D:365:GLN:O	1:D:369:ILE:HG22	1.81	0.80
1:D:335:PRO:HB2	1:D:411:ALA:HB2	1.65	0.79
2:A:431:SER:HB2	4:A:4000:EPH:H142	1.64	0.79
1:D:452:LEU:HB3	1:D:455:PRO:HG3	1.68	0.76
1:D:480:SER:CB	1:D:481:PRO:HD2	2.14	0.76
1:D:403:TYR:HA	1:D:407:ASN:ND2	2.01	0.75
2:A:406:SER:O	2:A:407:ARG:HG3	1.89	0.73
2:A:334:ASN:O	2:A:338:GLN:HG2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:GLU:CD	1:D:313:GLU:H	1.99	0.71
1:D:290:LEU:HB2	1:D:294:GLN:HE21	1.56	0.70
2:A:262:VAL:HG23	2:A:265:ARG:HH21	1.54	0.69
2:A:363:GLN:O	2:A:367:VAL:HG13	1.92	0.69
2:A:341:VAL:HG12	2:A:434:HIS:ND1	2.08	0.69
2:A:376:ASN:ND2	2:A:379:VAL:HG23	2.08	0.69
1:D:499:THR:HA	2:A:429:LEU:HD21	1.75	0.69
2:A:389:GLU:O	2:A:393:GLU:HG3	1.93	0.68
2:A:216:MET:HE3	2:A:266:ASP:O	1.93	0.68
2:A:275:MET:HA	2:A:278:GLN:HB2	1.75	0.68
1:D:346:THR:HG22	1:D:350:ILE:HD11	1.76	0.68
1:D:447:SER:HA	1:D:462:GLN:HE22	1.59	0.68
1:D:474:LEU:HD23	1:D:483:CYS:SG	2.34	0.67
1:D:378:GLU:HB3	1:D:497:ILE:CG2	2.25	0.67
1:D:399:ASN:HD21	1:D:401:GLN:HG3	1.58	0.67
1:D:298:ILE:O	1:D:302:VAL:HG23	1.95	0.66
2:A:263:TRP:CZ2	2:A:370:LYS:HE2	2.31	0.65
1:D:444:VAL:O	1:D:447:SER:HB2	1.96	0.65
1:D:499:THR:O	1:D:503:GLN:HG3	1.95	0.65
2:A:206:GLN:NE2	2:A:212:ARG:HD3	2.11	0.65
2:A:213:LEU:HA	2:A:216:MET:SD	2.37	0.65
2:A:270:PHE:CE2	2:A:278:GLN:HG2	2.31	0.65
2:A:222:ASP:O	2:A:224:SER:N	2.30	0.65
1:D:290:LEU:CD1	1:D:295:LYS:HB2	2.26	0.64
1:D:357:LEU:HD11	1:D:445:ILE:HD13	1.77	0.64
1:D:447:SER:HA	1:D:462:GLN:NE2	2.13	0.64
2:A:434:HIS:HB3	4:A:4000:EPH:H112	1.79	0.64
2:A:286:TRP:O	2:A:290:LEU:HB2	1.99	0.62
2:A:369:LEU:O	2:A:373:ILE:HG13	1.99	0.62
2:A:287:ASN:ND2	2:A:428:SER:HB2	2.14	0.62
2:A:344:ILE:HD11	2:A:431:SER:HB3	1.82	0.62
1:D:381:MET:HB3	1:D:497:ILE:HD12	1.82	0.61
1:D:399:ASN:HD21	1:D:401:GLN:CG	2.13	0.61
1:D:409:ARG:HA	1:D:414:ALA:HB2	1.82	0.60
1:D:369:ILE:HD11	1:D:373:LYS:NZ	2.17	0.60
1:D:297:LEU:CD1	1:D:358:PRO:HG2	2.32	0.60
2:A:268:PRO:O	2:A:269:HIS:HB2	1.99	0.60
2:A:214:LEU:HD12	2:A:367:VAL:HG21	1.81	0.60
2:A:213:LEU:O	2:A:216:MET:N	2.31	0.60
1:D:423:PHE:CZ	1:D:497:ILE:HD11	2.37	0.59
1:D:363:ILE:CG2	1:D:367:ASP:HB2	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:VAL:N	1:D:288:PRO:CD	2.65	0.59
2:A:360:ARG:O	2:A:360:ARG:HG2	2.03	0.58
1:D:499:THR:OG1	2:A:425:ARG:HD2	2.02	0.58
1:D:469:LEU:HG	1:D:473:ILE:HD11	1.85	0.58
1:D:290:LEU:HD12	1:D:290:LEU:O	2.04	0.58
2:A:395:MET:HA	2:A:395:MET:HE3	1.86	0.58
2:A:270:PHE:O	2:A:278:GLN:NE2	2.37	0.58
2:A:275:MET:O	2:A:276:GLU:C	2.47	0.58
1:D:404:THR:H	1:D:407:ASN:ND2	2.01	0.58
1:D:509:ILE:C	1:D:511:LEU:H	2.12	0.57
1:D:290:LEU:HB2	1:D:294:GLN:NE2	2.17	0.57
1:D:369:ILE:HD11	1:D:373:LYS:HZ2	1.70	0.57
2:A:244:ALA:N	2:A:245:PRO:HD2	2.19	0.57
2:A:299:MET:HG2	2:A:357:ARG:HD3	1.87	0.57
1:D:409:ARG:HD2	1:D:414:ALA:HB2	1.85	0.57
1:D:453:GLU:O	1:D:455:PRO:HD3	2.04	0.57
2:A:238:VAL:HG13	4:A:4000:EPH:H62	1.86	0.57
1:D:313:GLU:CD	1:D:313:GLU:N	2.63	0.56
1:D:290:LEU:HD13	1:D:295:LYS:HB2	1.87	0.56
2:A:300:GLU:C	2:A:302:LEU:H	2.13	0.56
1:D:476:GLN:HE21	1:D:476:GLN:HA	1.70	0.56
1:D:480:SER:O	1:D:483:CYS:HB2	2.06	0.56
1:D:518:LEU:O	1:D:519:PRO:C	2.45	0.56
1:D:511:LEU:HB2	1:D:518:LEU:HD21	1.89	0.55
1:D:511:LEU:CB	1:D:518:LEU:HD21	2.37	0.55
1:D:290:LEU:HD11	1:D:295:LYS:HB2	1.88	0.55
1:D:320:THR:HG23	1:D:320:THR:O	2.07	0.55
1:D:399:ASN:ND2	1:D:401:GLN:CG	2.70	0.55
2:A:287:ASN:HD22	2:A:428:SER:HB2	1.73	0.54
2:A:288:GLU:HG2	2:A:424:LEU:HG	1.90	0.54
2:A:331:LEU:HD13	4:A:4000:EPH:H363	1.88	0.54
1:D:290:LEU:HD21	1:D:295:LYS:HD3	1.90	0.54
1:D:355:LYS:C	1:D:357:LEU:H	2.16	0.54
2:A:326:MET:HE2	2:A:329:MET:HB3	1.90	0.54
1:D:297:LEU:HD13	1:D:358:PRO:HG2	1.90	0.53
1:D:379:VAL:C	1:D:381:MET:N	2.65	0.53
2:A:326:MET:O	2:A:327:PRO:C	2.48	0.53
2:A:448:GLY:O	2:A:452:ASP:N	2.38	0.53
2:A:404:ARG:O	2:A:408:SER:HB2	2.09	0.53
1:D:478:SER:C	1:D:480:SER:N	2.66	0.53
1:D:399:ASN:ND2	1:D:401:GLN:HG2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:241:LYS:HE3	2:A:242:PHE:CE1	2.44	0.53
1:D:435:VAL:HG21	1:D:472:TYR:CE1	2.43	0.53
2:A:296:TRP:CE3	2:A:299:MET:HE1	2.43	0.52
2:A:300:GLU:O	2:A:302:LEU:N	2.42	0.52
2:A:392:ARG:HG2	2:A:396:PHE:CE2	2.43	0.52
2:A:332:HIS:CD2	2:A:334:ASN:H	2.27	0.52
2:A:269:HIS:HA	2:A:272:GLN:HG2	1.92	0.52
1:D:290:LEU:CB	1:D:294:GLN:NE2	2.73	0.52
2:A:361:VAL:HA	2:A:365:GLU:OE2	2.09	0.52
2:A:294:ILE:HG21	2:A:323:MET:HE3	1.91	0.52
1:D:367:ASP:O	1:D:370:THR:HB	2.09	0.52
2:A:323:MET:HE1	4:A:4000:EPH:H351	1.92	0.52
1:D:499:THR:HA	2:A:429:LEU:CD2	2.40	0.51
2:A:406:SER:C	2:A:407:ARG:HG3	2.35	0.51
1:D:502:MET:HE2	2:A:429:LEU:CB	2.16	0.51
2:A:242:PHE:C	2:A:245:PRO:HD2	2.36	0.51
2:A:269:HIS:HB2	2:A:391:LEU:HD21	1.93	0.51
1:D:480:SER:CB	1:D:481:PRO:CD	2.85	0.50
2:A:208:LEU:CD2	2:A:395:MET:SD	3.00	0.50
1:D:290:LEU:CB	1:D:294:GLN:HE21	2.24	0.50
2:A:265:ARG:HA	2:A:270:PHE:CD2	2.46	0.50
1:D:449:ARG:H	1:D:452:LEU:HD22	1.76	0.50
2:A:225:GLU:OE2	2:A:225:GLU:HA	2.11	0.50
2:A:296:TRP:O	2:A:299:MET:HB2	2.12	0.50
1:D:413:MET:HE1	3:D:3000:P1A:H263	1.93	0.50
1:D:379:VAL:C	1:D:381:MET:H	2.19	0.50
1:D:378:GLU:O	1:D:381:MET:HB2	2.11	0.49
1:D:381:MET:HB3	1:D:497:ILE:CD1	2.42	0.49
1:D:460:GLU:C	1:D:462:GLN:N	2.68	0.49
1:D:344:ILE:HG12	1:D:522:LEU:HD22	1.93	0.49
2:A:208:LEU:HB2	2:A:268:PRO:HB2	1.94	0.49
2:A:407:ARG:O	2:A:410:GLU:HG2	2.12	0.49
2:A:447:ALA:O	2:A:450:ILE:HB	2.12	0.49
1:D:454:GLN:O	1:D:457:LEU:HB3	2.13	0.49
1:D:476:GLN:HE21	1:D:476:GLN:CA	2.25	0.49
2:A:418:LEU:HA	2:A:421:LEU:HD22	1.95	0.49
2:A:208:LEU:HD21	2:A:395:MET:SD	2.52	0.49
1:D:297:LEU:HD22	1:D:464:TYR:HE2	1.77	0.49
2:A:262:VAL:HG22	2:A:262:VAL:O	2.12	0.49
2:A:268:PRO:O	2:A:269:HIS:CB	2.60	0.49
1:D:476:GLN:HA	1:D:476:GLN:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:356:MET:O	2:A:357:ARG:C	2.55	0.49
1:D:363:ILE:HG22	1:D:367:ASP:HB2	1.94	0.49
2:A:210:ILE:O	2:A:214:LEU:HD13	2.13	0.48
1:D:443:ILE:HD13	1:D:466:LEU:HD23	1.96	0.48
1:D:511:LEU:HD23	1:D:514:LYS:HE2	1.95	0.48
1:D:442:ALA:HA	1:D:445:ILE:HD12	1.96	0.48
1:D:287:VAL:N	1:D:288:PRO:HD3	2.29	0.47
2:A:395:MET:HE3	2:A:395:MET:CA	2.43	0.47
2:A:339:ALA:HB2	4:A:4000:EPH:H202	1.95	0.47
1:D:435:VAL:HG21	1:D:472:TYR:CZ	2.49	0.47
1:D:497:ILE:HD13	1:D:497:ILE:HA	1.69	0.47
2:A:368:ALA:O	2:A:369:LEU:C	2.57	0.47
1:D:339:ILE:HG21	1:D:413:MET:HE3	1.97	0.47
1:D:343:THR:O	1:D:347:VAL:HG23	2.15	0.47
1:D:409:ARG:O	1:D:410:LYS:C	2.56	0.47
1:D:454:GLN:N	1:D:455:PRO:HD3	2.30	0.47
2:A:341:VAL:HG12	2:A:434:HIS:CE1	2.50	0.47
2:A:400:ASP:O	2:A:404:ARG:HG3	2.15	0.47
1:D:509:ILE:C	1:D:511:LEU:N	2.73	0.47
2:A:415:ALA:O	2:A:419:LEU:HB2	2.14	0.47
2:A:413:ARG:HG3	2:A:413:ARG:HH11	1.80	0.47
1:D:369:ILE:O	1:D:373:LYS:HB2	2.16	0.46
2:A:213:LEU:HD23	2:A:216:MET:SD	2.55	0.46
2:A:274:GLU:O	2:A:277:ASP:HB2	2.16	0.46
2:A:413:ARG:HG3	2:A:413:ARG:NH1	2.30	0.46
2:A:236:SER:HB2	2:A:238:VAL:HG23	1.97	0.46
2:A:254:ASN:O	2:A:255:LYS:C	2.58	0.46
2:A:341:VAL:HG12	2:A:434:HIS:HD1	1.80	0.46
1:D:508:CYS:O	1:D:518:LEU:HD11	2.15	0.46
2:A:227:PHE:HB3	2:A:229:PHE:CE1	2.50	0.46
2:A:301:PHE:CD2	2:A:322:LEU:HD22	2.50	0.46
1:D:384:VAL:HG23	1:D:395:VAL:HG11	1.98	0.46
1:D:432:MET:HB2	1:D:437:TYR:CE1	2.51	0.46
1:D:409:ARG:O	1:D:412:GLY:N	2.35	0.46
1:D:339:ILE:HG23	3:D:3000:P1A:C16	2.47	0.45
1:D:481:PRO:O	1:D:483:CYS:N	2.49	0.45
1:D:466:LEU:HD21	1:D:491:LEU:HD21	1.99	0.45
2:A:265:ARG:HA	2:A:270:PHE:HD2	1.80	0.45
2:A:216:MET:HA	2:A:219:LEU:HD12	1.98	0.45
2:A:439:HIS:HB3	5:A:1009:HOH:O	2.16	0.45
2:A:401:GLU:HG3	2:A:402:TYR:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:296:TRP:CZ3	2:A:361:VAL:HG22	2.51	0.45
2:A:348:VAL:O	2:A:352:LEU:HB2	2.16	0.45
2:A:376:ASN:HA	2:A:377:PRO:HD3	1.69	0.45
1:D:366:SER:O	1:D:369:ILE:HG23	2.17	0.45
1:D:381:MET:SD	1:D:420:LEU:HD11	2.57	0.45
1:D:507:MET:O	1:D:511:LEU:HG	2.17	0.45
1:D:509:ILE:O	1:D:511:LEU:N	2.50	0.45
1:D:344:ILE:HD11	1:D:519:PRO:CG	2.47	0.45
1:D:336:PHE:CZ	1:D:516:ARG:HG3	2.52	0.44
2:A:238:VAL:O	2:A:239:PRO:C	2.60	0.44
1:D:343:THR:CG2	1:D:380:MET:HE1	2.48	0.44
2:A:393:GLU:O	2:A:397:LEU:HD22	2.18	0.44
2:A:401:GLU:O	2:A:404:ARG:HB2	2.18	0.44
2:A:407:ARG:HB3	2:A:410:GLU:HG2	1.99	0.44
2:A:300:GLU:C	2:A:302:LEU:N	2.74	0.44
1:D:339:ILE:HG23	3:D:3000:P1A:H162	2.00	0.44
1:D:354:ALA:CB	1:D:372:LEU:HD21	2.47	0.44
1:D:453:GLU:HB3	1:D:454:GLN:NE2	2.33	0.44
2:A:299:MET:O	2:A:302:LEU:HB2	2.18	0.44
2:A:446:ILE:O	2:A:450:ILE:HG13	2.17	0.44
2:A:240:PRO:HA	2:A:243:ARG:HG2	1.99	0.44
2:A:397:LEU:O	2:A:398:CYS:C	2.61	0.44
2:A:455:ARG:HA	2:A:455:ARG:HD3	1.84	0.44
2:A:216:MET:HE1	2:A:267:ILE:HA	2.00	0.43
1:D:375:CYS:O	1:D:376:SER:C	2.59	0.43
1:D:378:GLU:OE1	1:D:498:ARG:HD2	2.17	0.43
1:D:484:ALA:O	1:D:487:PHE:N	2.50	0.43
1:D:354:ALA:HA	1:D:357:LEU:HD12	1.99	0.43
1:D:369:ILE:O	1:D:373:LYS:HG3	2.18	0.43
2:A:272:GLN:NE2	2:A:272:GLN:HA	2.33	0.43
1:D:469:LEU:O	1:D:473:ILE:HG13	2.19	0.43
2:A:208:LEU:CB	2:A:268:PRO:HB2	2.48	0.43
2:A:446:ILE:O	2:A:447:ALA:C	2.61	0.43
1:D:313:GLU:O	1:D:317:LYS:HB2	2.19	0.43
1:D:381:MET:CB	1:D:497:ILE:HD12	2.47	0.43
2:A:252:ILE:O	2:A:253:GLY:C	2.62	0.43
1:D:344:ILE:HG23	1:D:521:PHE:CD2	2.53	0.43
1:D:484:ALA:O	1:D:485:VAL:C	2.61	0.43
1:D:510:SER:O	1:D:514:LYS:HG3	2.19	0.43
2:A:205:VAL:HG22	2:A:206:GLN:N	2.33	0.43
2:A:216:MET:HE1	2:A:267:ILE:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:257:ILE:O	2:A:261:VAL:HG23	2.19	0.42
1:D:449:ARG:HA	1:D:450:PRO:HD3	1.86	0.42
1:D:513:LEU:C	1:D:515:ASN:H	2.26	0.42
2:A:251:GLN:HE21	2:A:251:GLN:HB3	1.54	0.42
2:A:299:MET:HE2	2:A:356:MET:HB2	2.01	0.42
2:A:401:GLU:O	2:A:405:ARG:N	2.49	0.42
2:A:418:LEU:HA	2:A:418:LEU:HD23	1.87	0.42
2:A:212:ARG:O	2:A:215:GLU:HB2	2.19	0.42
1:D:301:LEU:HB3	1:D:438:ALA:HB1	2.02	0.42
2:A:207:GLU:HA	2:A:207:GLU:OE2	2.20	0.42
1:D:423:PHE:O	1:D:427:MET:HG2	2.19	0.42
1:D:388:TYR:CG	1:D:424:CYS:HB3	2.55	0.42
2:A:303:THR:O	2:A:304:GLU:O	2.37	0.42
1:D:460:GLU:O	1:D:461:ILE:C	2.63	0.41
2:A:208:LEU:HD12	2:A:391:LEU:HD22	2.01	0.41
1:D:295:LYS:HD2	1:D:295:LYS:HA	1.82	0.41
1:D:441:THR:O	1:D:442:ALA:C	2.63	0.41
2:A:441:VAL:C	2:A:443:ASP:H	2.28	0.41
1:D:373:LYS:HD2	1:D:525:ILE:O	2.20	0.41
1:D:292:ALA:O	1:D:293:ASN:C	2.63	0.41
1:D:481:PRO:C	1:D:483:CYS:N	2.78	0.41
2:A:440:LEU:HD12	2:A:440:LEU:HA	1.92	0.41
2:A:451:ARG:NH1	2:A:452:ASP:OD1	2.53	0.41
2:A:436:PHE:HE2	2:A:441:VAL:HB	1.85	0.41
1:D:346:THR:OG1	3:D:3000:P1A:H9	2.21	0.41
1:D:357:LEU:CD1	1:D:445:ILE:HD13	2.50	0.41
2:A:244:ALA:N	2:A:245:PRO:CD	2.82	0.41
2:A:407:ARG:O	2:A:409:SER:N	2.54	0.41
1:D:354:ALA:HB1	1:D:372:LEU:HD21	2.02	0.41
1:D:357:LEU:HA	1:D:358:PRO:HD3	1.89	0.41
1:D:516:ARG:HA	1:D:516:ARG:HD2	1.72	0.40
1:D:521:PHE:CD2	1:D:522:LEU:HD13	2.57	0.40
1:D:432:MET:HE3	1:D:437:TYR:CE1	2.57	0.40
2:A:451:ARG:HD2	2:A:452:ASP:CA	2.51	0.40
1:D:367:ASP:O	1:D:370:THR:N	2.55	0.40
2:A:322:LEU:O	2:A:349:LEU:HD11	2.22	0.40
2:A:239:PRO:HA	2:A:240:PRO:HD3	1.87	0.40
1:D:301:LEU:HD21	1:D:357:LEU:HD23	2.04	0.40
1:D:474:LEU:HD23	1:D:474:LEU:HA	1.91	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:329:MET:SD	2:A:329:MET:SD[4_557]	2.08	0.12

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	D	232/266 (87%)	193 (83%)	29 (12%)	10 (4%)	2	8
2	A	237/263 (90%)	197 (83%)	32 (14%)	8 (3%)	3	12
All	All	469/529 (89%)	390 (83%)	61 (13%)	18 (4%)	2	10

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	322	THR
1	D	479	ALA
2	A	301	PHE
1	D	482	ARG
2	A	408	SER
2	A	443	ASP
1	D	289	PRO
1	D	291	THR
1	D	510	SER
1	D	409	ARG
2	A	268	PRO
2	A	451	ARG
1	D	410	LYS
1	D	436	HIS
2	A	269	HIS
2	A	223	PRO
2	A	422	PRO
1	D	485	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	D	205/235 (87%)	179 (87%)	26 (13%)	4	14
2	A	212/232 (91%)	182 (86%)	30 (14%)	3	11
All	All	417/467 (89%)	361 (87%)	56 (13%)	4	12

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	306	GLU
1	D	313	GLU
1	D	316	LEU
1	D	320	THR
1	D	349	LEU
1	D	369	ILE
1	D	373	LYS
1	D	381	MET
1	D	396	LEU
1	D	405	ARG
1	D	416	VAL
1	D	419	ASP
1	D	421	LEU
1	D	430	MET
1	D	439	LEU
1	D	447	SER
1	D	452	LEU
1	D	463	ARG
1	D	466	LEU
1	D	476	GLN
1	D	477	ASN
1	D	483	CYS
1	D	495	THR
1	D	502	MET
1	D	505	SER
1	D	522	LEU
2	A	208	LEU

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Mol	Chain	Res	Type
2	A	243	ARG
2	A	248	SER
2	A	251	GLN
2	A	260	LEU
2	A	263	TRP
2	A	278	GLN
2	A	288	GLU
2	A	290	LEU
2	A	291	LEU
2	A	322	LEU
2	A	326	MET
2	A	329	MET
2	A	330	THR
2	A	337	LEU
2	A	355	LYS
2	A	359	LEU
2	A	361	VAL
2	A	367	VAL
2	A	374	LEU
2	A	380	LYS
2	A	383	LYS
2	A	384	ASN
2	A	386	GLN
2	A	397	LEU
2	A	411	GLU
2	A	421	LEU
2	A	429	LEU
2	A	430	LYS
2	A	440	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	293	ASN
1	D	294	GLN
1	D	348	GLN
1	D	368	GLN
1	D	407	ASN
1	D	454	GLN
1	D	462	GLN
1	D	475	ASN
1	D	476	GLN

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Mol	Chain	Res	Type
2	A	206	GLN
2	A	228	GLN
2	A	251	GLN
2	A	256	GLN
2	A	272	GLN
2	A	278	GLN
2	A	338	GLN
2	A	343	GLN
2	A	363	GLN
2	A	376	ASN
2	A	384	ASN
2	A	386	GLN
2	A	439	HIS

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	$\# Z > 2$
3	P1A	D	3000	-	36,36,36	3.72	17 (47%)	60,60,60	2.33	19 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EPH	A	4000	-	48,48,48	1.65	8 (16%)	51,53,53	1.61	7 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P1A	D	3000	-	-	2/17/87/87	0/4/4/4
4	EPH	A	4000	-	-	17/52/52/52	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3000	P1A	C20-C22	8.99	1.68	1.55
3	D	3000	P1A	C9-C8	7.31	1.65	1.52
3	D	3000	P1A	C1-C10	6.97	1.64	1.54
3	D	3000	P1A	C21-C20	6.48	1.63	1.52
3	D	3000	P1A	O3-C3	-6.18	1.30	1.43
3	D	3000	P1A	C23-C22	5.92	1.60	1.52
3	D	3000	P1A	C5-C6	5.47	1.59	1.51
3	D	3000	P1A	C3-C2	5.29	1.60	1.52
3	D	3000	P1A	C10-C9	5.13	1.64	1.56
3	D	3000	P1A	C19-C10	5.08	1.62	1.54
3	D	3000	P1A	C12-C13	4.52	1.62	1.54
4	A	4000	EPH	C25-C24	4.33	1.56	1.31
4	A	4000	EPH	C16-C15	4.24	1.55	1.31
4	A	4000	EPH	C29-C28	4.11	1.55	1.31
4	A	4000	EPH	P1-O8	-3.78	1.44	1.59
4	A	4000	EPH	C13-C12	3.62	1.52	1.31
4	A	4000	EPH	C32-C33	3.44	1.54	1.29
3	D	3000	P1A	C11-C9	3.40	1.59	1.53
3	D	3000	P1A	O20-C20	-3.40	1.38	1.44
3	D	3000	P1A	C7-C6	2.97	1.51	1.46
3	D	3000	P1A	O6-C6	-2.80	1.18	1.22
3	D	3000	P1A	C16-C17	2.48	1.58	1.54
4	A	4000	EPH	O8-C38	2.45	1.54	1.44
4	A	4000	EPH	P1-O6	-2.44	1.44	1.55
3	D	3000	P1A	C18-C13	2.38	1.58	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3000	P1A	C21-C20-C22	7.98	114.95	110.29
3	D	3000	P1A	C20-C17-C13	6.25	126.58	120.43
3	D	3000	P1A	C24-C23-C22	-4.99	106.50	112.86
4	A	4000	EPH	O8-P1-O7	-4.79	89.97	108.94
4	A	4000	EPH	O5-P1-O7	-4.75	90.12	108.94
4	A	4000	EPH	O6-P1-O7	-4.70	90.57	112.44
3	D	3000	P1A	C18-C13-C14	4.65	114.91	109.11
3	D	3000	P1A	O14-C14-C8	-4.26	98.67	106.13
4	A	4000	EPH	O6-P1-O8	3.86	125.08	107.57
3	D	3000	P1A	C19-C10-C9	3.62	115.96	109.89
3	D	3000	P1A	O14-C14-C13	3.42	115.65	108.01
3	D	3000	P1A	O14-C14-C15	-3.21	102.42	110.26
3	D	3000	P1A	C4-C5-C10	3.10	116.93	112.75
3	D	3000	P1A	C10-C1-C2	-3.04	109.17	114.17
3	D	3000	P1A	O6-C6-C7	-3.03	116.44	121.46
3	D	3000	P1A	C19-C10-C5	-2.88	105.05	109.89
4	A	4000	EPH	P1-O8-C38	-2.51	109.32	121.26
4	A	4000	EPH	C31-C30-C29	2.50	119.01	112.73
3	D	3000	P1A	C12-C13-C14	-2.47	104.42	107.79
3	D	3000	P1A	C4-C3-C2	2.41	113.36	110.38
3	D	3000	P1A	O20-C20-C17	-2.37	105.26	108.77
4	A	4000	EPH	C1-O2-C4	2.34	125.67	117.12
3	D	3000	P1A	C10-C9-C8	-2.22	109.16	112.54
3	D	3000	P1A	O22-C22-C23	-2.09	105.12	108.98
3	D	3000	P1A	C19-C10-C1	-2.06	105.97	108.99
3	D	3000	P1A	C11-C9-C10	-2.04	110.52	113.92

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4000	EPH	C29-C30-C31-C32
4	A	4000	EPH	C38-O8-P1-O5
4	A	4000	EPH	C27-C28-C29-C30
4	A	4000	EPH	C14-C15-C16-C17
4	A	4000	EPH	C11-C12-C13-C14
4	A	4000	EPH	C20-C21-C22-C23
4	A	4000	EPH	C5-C6-C7-C8
4	A	4000	EPH	C9-C10-C11-C12
4	A	4000	EPH	C28-C29-C30-C31
4	A	4000	EPH	C25-C26-C27-C28
4	A	4000	EPH	C7-C8-C9-C10
4	A	4000	EPH	C37-O5-P1-O7

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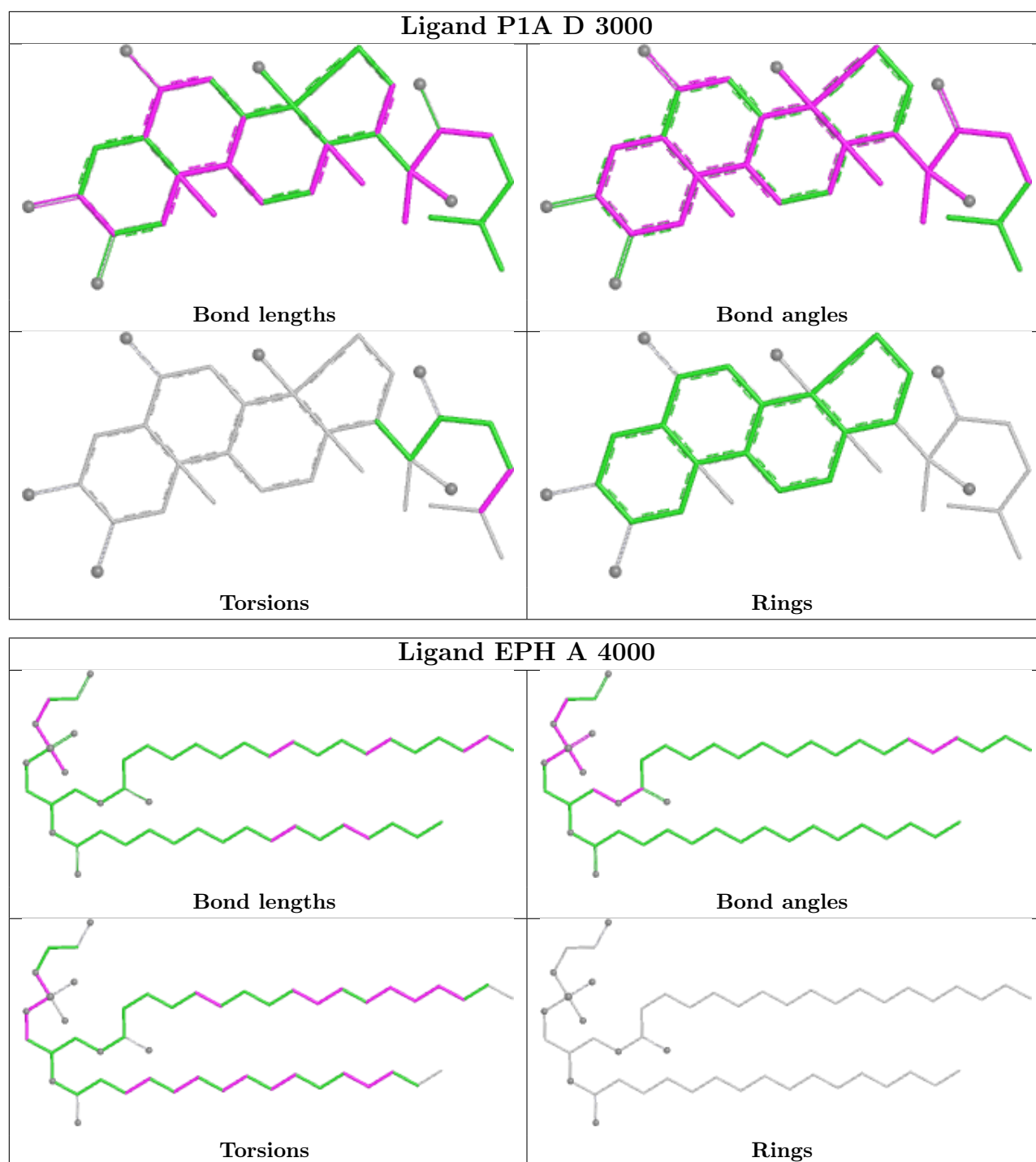
Mol	Chain	Res	Type	Atoms
4	A	4000	EPH	C37-O5-P1-O8
3	D	3000	P1A	C23-C24-C25-C27
3	D	3000	P1A	C23-C24-C25-C26
4	A	4000	EPH	C15-C16-C17-C35
4	A	4000	EPH	C24-C25-C26-C27
4	A	4000	EPH	C2-C37-O5-P1
4	A	4000	EPH	C30-C31-C32-C33

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3000	P1A	4	0
4	A	4000	EPH	6	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	D	236/266 (88%)	-0.29	3 (1%) 75 67	40, 71, 98, 113	0
2	A	241/263 (91%)	-0.31	0 100 100	42, 70, 107, 122	0
All	All	477/529 (90%)	-0.30	3 (0%) 85 81	40, 70, 104, 122	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	431	MET	2.6
1	D	321	GLN	2.6
1	D	287	VAL	2.5

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](#)

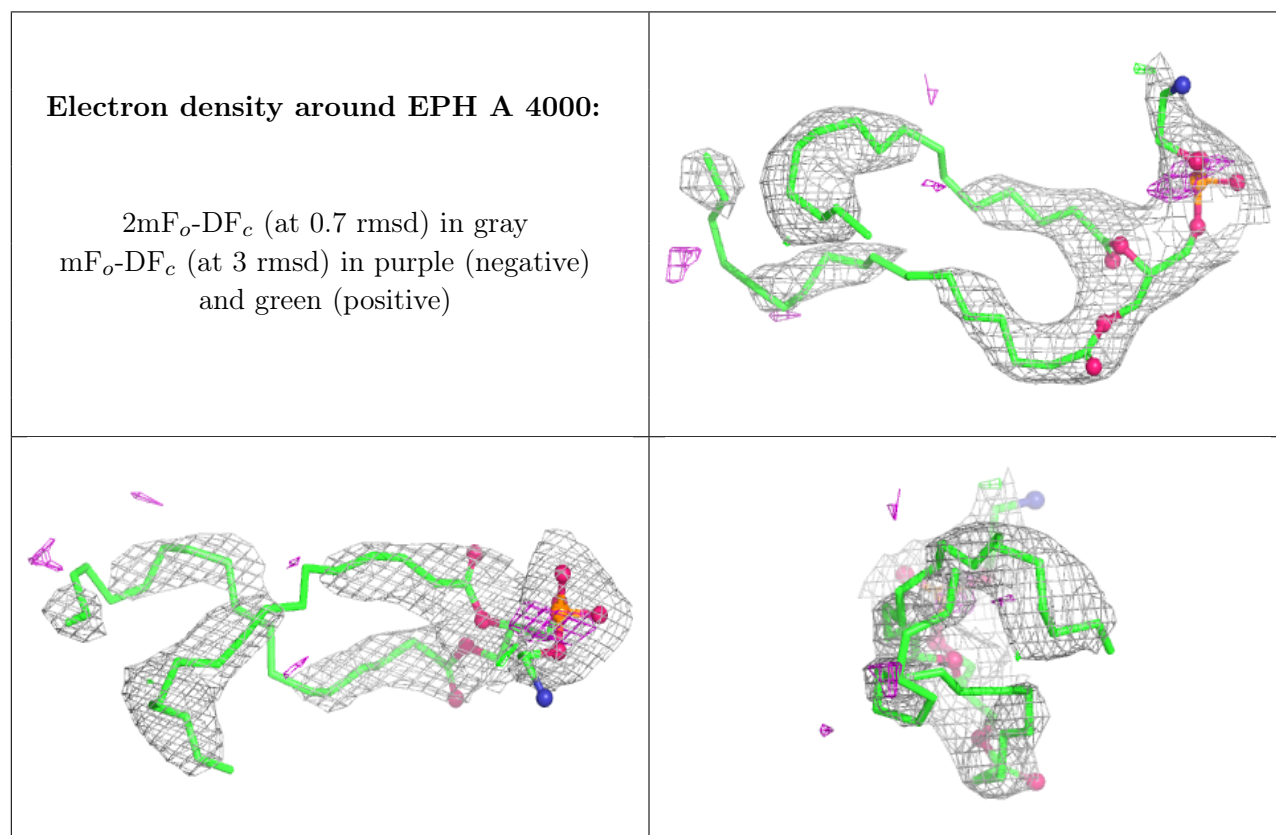
There are no oligosaccharides in this entry.

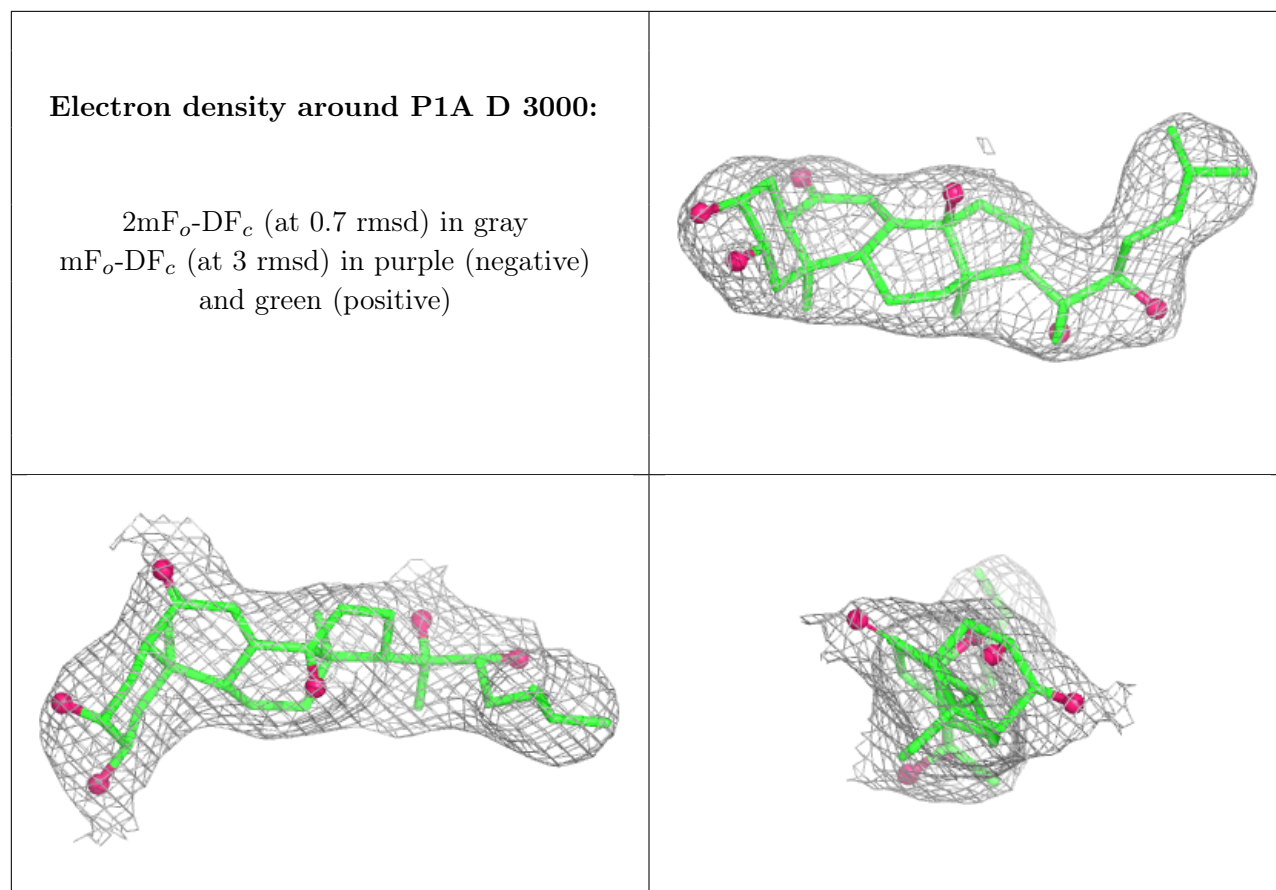
6.4 Ligands [i](#)

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
4	EPH	A	4000	49/49	0.87	0.15	86,92,111,111	0
3	P1A	D	3000	33/33	0.93	0.10	43,46,55,56	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.