



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:00 pm GMT

PDB ID : 1R1K  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (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

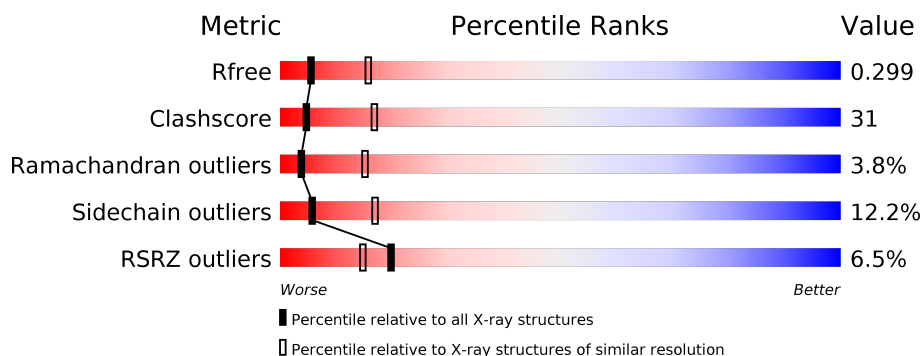
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	266	
2	A	263	

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
3	P1A	D	3000	-	-	-	X
4	EPH	A	4000	-	-	-	X

## 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.

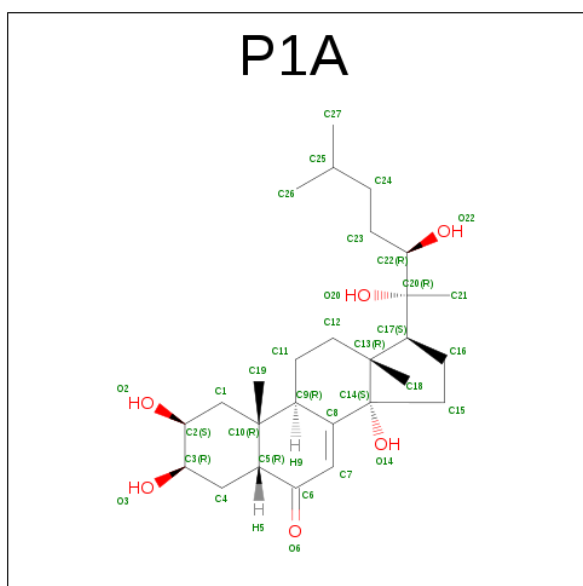
- Molecule 1 is a protein called Ecdysone receptor.

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			

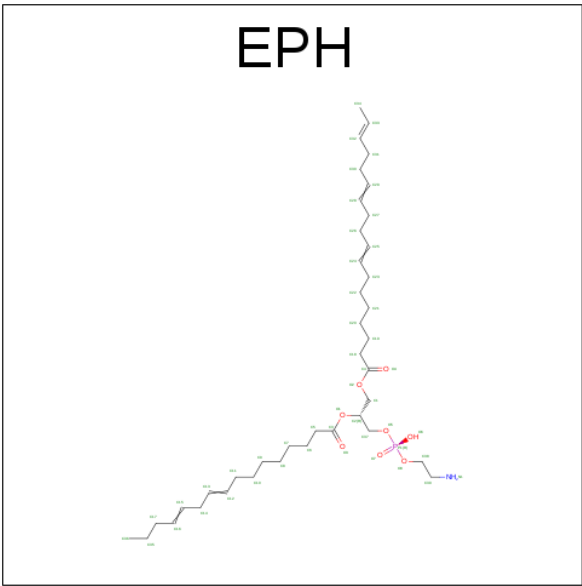
- Molecule 3 is 2,3,14,20,22-PENTAHYDROXYCHOLEST-7-EN-6-ONE (three-letter code: P1A) (formula:  $C_{27}H_{44}O_6$ ).



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 (three-letter code: EPH) (formula: C<sub>39</sub>H<sub>68</sub>NO<sub>8</sub>P).



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	A	5	Total	O	0	0
			5	5		
5	D	3	Total	O	0	0
			3	3		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.40Å 57.40Å 302.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.86 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.90) 99.6 (19.86-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (10.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.2	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 67.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: P1A, EPH

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	0.55	0/1905	0.72	0/2579
2	A	0.51	0/1960	0.70	0/2646
All	All	0.53	0/3865	0.71	0/5225

There are no bond length outliers.

There are no bond angle outliers.

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	D	1872	0	1880	130	0
2	A	1925	0	1970	119	1
3	D	33	0	43	3	0
4	A	49	0	67	5	0
5	A	5	0	0	1	0
5	D	3	0	0	0	0
All	All	3887	0	3960	242	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 31.

All (242) 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:480:SER:HB2	1:D:481:PRO:HD2	1.51	0.93
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
1:D:453:GLU:C	1:D:455:PRO:HD3	1.95	0.86
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
2:A:431:SER:HB2	4:A:4000:EPH:H142	1.64	0.79
1:D:335:PRO:HB2	1:D:411:ALA:HB2	1.65	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
1:D:502:MET:CE	2:A:429:LEU:HB3	2.17	0.74
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
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: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:313:GLU:CD	1:D:313:GLU:H	1.99	0.66
1:D:502:MET:HE1	2:A:429:LEU:HB3	1.75	0.66
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
2:A:206:GLN:NE2	2:A:212:ARG:HD3	2.11	0.65
1:D:499:THR:O	1:D:503:GLN:HG3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:344:ILE:HD11	2:A:431:SER:HB3	1.82	0.62
2:A:287:ASN:ND2	2:A:428:SER:HB2	2.14	0.62
2:A:268:PRO:O	2:A:269:HIS:HB2	1.99	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: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
2:A:216:MET:HE1	2:A:267:ILE:HA	1.85	0.59
1:D:363:ILE:CG2	1:D:367:ASP:HB2	2.31	0.59
1:D:287:VAL:N	1:D:288:PRO:CD	2.65	0.59
2:A:360:ARG:HG2	2:A:360:ARG:O	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:270:PHE:O	2:A:278:GLN:NE2	2.37	0.58
1:D:404:THR:H	1:D:407:ASN:ND2	2.01	0.58
1:D:290:LEU:HB2	1:D:294:GLN:NE2	2.17	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:290:LEU:HD13	1:D:295:LYS:HB2	1.87	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:502:MET:HE2	2:A:429:LEU:HB3	1.88	0.56
1:D:511:LEU:HB2	1:D:518:LEU:HD21	1.89	0.55
1:D:376:SER:HG	1:D:526:TRP:HE1	1.54	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:O	1:D:320:THR:HG23	2.07	0.55
1:D:399:ASN:ND2	1:D:401:GLN:CG	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:331:LEU:HD13	4:A:4000:EPH:H363	1.88	0.54
2:A:288:GLU:HG2	2:A:424:LEU:HG	1.90	0.54
2:A:287:ASN:HD22	2:A:428:SER:HB2	1.73	0.54
1:D:290:LEU:HD21	1:D:295:LYS:HD3	1.90	0.54
1:D:297:LEU:HD13	1:D:358:PRO:HG2	1.90	0.53
2:A:275:MET:O	2:A:276:GLU:C	2.47	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:399:ASN:ND2	1:D:401:GLN:HG2	2.23	0.53
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
1:D:369:ILE:HD11	1:D:373:LYS:HZ2	1.72	0.53
1:D:509:ILE:C	1:D:511:LEU:H	2.12	0.53
1:D:518:LEU:O	1:D:519:PRO:C	2.45	0.53
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
2:A:361:VAL:HA	2:A:365:GLU:OE2	2.09	0.52
1:D:290:LEU:CB	1:D:294:GLN:NE2	2.73	0.52
1:D:313:GLU:N	1:D:313:GLU:CD	2.63	0.52
2:A:300:GLU:C	2:A:302:LEU:H	2.13	0.52
1:D:367:ASP:O	1:D:370:THR:HB	2.09	0.52
1:D:499:THR:HA	2:A:429:LEU:CD2	2.40	0.51
2:A:269:HIS:HB2	2:A:391:LEU:HD21	1.93	0.51
2:A:208:LEU:CD2	2:A:395:MET:SD	3.00	0.50
1:D:480:SER:CB	1:D:481:PRO:CD	2.85	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
2:A:225:GLU:HA	2:A:225:GLU:OE2	2.11	0.50
2:A:296:TRP:O	2:A:299:MET:HB2	2.12	0.50
1:D:449:ARG:H	1:D:452:LEU:HD22	1.76	0.50
2:A:326:MET:O	2:A:327:PRO:C	2.48	0.49
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
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:344:ILE:HG12	1:D:522:LEU:HD22	1.93	0.49
2:A:418:LEU:HA	2:A:421:LEU:HD22	1.95	0.49
1:D:454:GLN:O	1:D:457:LEU:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:GLN:HE21	1:D:476:GLN:CA	2.25	0.49
2:A:208:LEU:HD21	2:A:395:MET:SD	2.52	0.49
1:D:355:LYS:C	1:D:357:LEU:H	2.16	0.49
1:D:297:LEU:HD22	1:D:464:TYR:HE2	1.77	0.49
2:A:262:VAL:O	2:A:262:VAL:HG22	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
2:A:395:MET:HE3	2:A:395:MET:HA	1.94	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:379:VAL:C	1:D:381:MET:N	2.65	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:478:SER:C	1:D:480:SER:N	2.66	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: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:HA	1:D:497:ILE:HD13	1.69	0.47
1:D:343:THR:O	1:D:347:VAL:HG23	2.15	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
2:A:415:ALA:O	2:A:419:LEU:HB2	2.14	0.47
2:A:406:SER:C	2:A:407:ARG:HG3	2.35	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:242:PHE:C	2:A:245:PRO:HD2	2.36	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:341:VAL:HG12	2:A:434:HIS:HD1	1.80	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:508:CYS:O	1:D:518:LEU:HD11	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:265:ARG:HA	2:A:270:PHE:HD2	1.80	0.45
1:D:466:LEU:HD21	1:D:491:LEU:HD21	1.99	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
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:379:VAL:C	1:D:381:MET:H	2.19	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:460:GLU:C	1:D:462:GLN:N	2.68	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: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:216:MET:CE	2:A:266:ASP:O	2.66	0.44
2:A:356:MET:O	2:A:357:ARG:C	2.55	0.44
1:D:339:ILE:HG23	3:D:3000:P1A:H162	2.00	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
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:240:PRO:HA	2:A:243:ARG:HG2	1.99	0.44
2:A:455:ARG:HA	2:A:455:ARG:HD3	1.84	0.44
2:A:205:VAL:HG22	2:A:206:GLN:N	2.33	0.43
2:A:216:MET:HE1	2:A:266:ASP:O	2.18	0.43
1:D:484:ALA:O	1:D:487:PHE:N	2.50	0.43
1:D:378:GLU:OE1	1:D:498:ARG:HD2	2.17	0.43
2:A:272:GLN:NE2	2:A:272:GLN:HA	2.33	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
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
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
1:D:344:ILE:HG23	1:D:521:PHE:CD2	2.53	0.43
1:D:510:SER:O	1:D:514:LYS:HG3	2.19	0.43

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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
2:A:368:ALA:O	2:A:369:LEU:C	2.57	0.42
1:D:449:ARG:HA	1:D:450:PRO:HD3	1.86	0.42
2:A:251:GLN:HB3	2:A:251:GLN:HE21	1.54	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
1:D:409:ARG:O	1:D:410:LYS:C	2.56	0.42
2:A:212:ARG:O	2:A:215:GLU:HB2	2.19	0.42
1:D:509:ILE:C	1:D:511:LEU:N	2.73	0.42
2:A:207:GLU:OE2	2:A:207:GLU:HA	2.20	0.42
1:D:301:LEU:HB3	1:D:438:ALA:HB1	2.02	0.42
1:D:423:PHE:O	1:D:427:MET:HG2	2.19	0.42
2:A:303:THR:O	2:A:304:GLU:O	2.37	0.42
1:D:388:TYR:CG	1:D:424:CYS:HB3	2.55	0.42
2:A:208:LEU:HD12	2:A:391:LEU:HD22	2.01	0.41
1:D:295:LYS:HA	1:D:295:LYS:HD2	1.82	0.41
1:D:373:LYS:HD2	1:D:525:ILE:O	2.20	0.41
2:A:254:ASN:O	2:A:255:LYS:C	2.58	0.41
2:A:440:LEU:HA	2:A:440:LEU:HD12	1.92	0.41
2:A:451:ARG:NH1	2:A:452:ASP:OD1	2.53	0.41
1:D:502:MET:HE1	2:A:429:LEU:CB	2.46	0.41
2:A:436:PHE:HE2	2:A:441:VAL:HB	1.85	0.41
2:A:407:ARG:O	2:A:409:SER:N	2.54	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
1:D:346:THR:OG1	3:D:3000:P1A:H9	2.21	0.41
1:D:357:LEU:HA	1:D:358:PRO:HD3	1.89	0.41
1:D:354:ALA:HB1	1:D:372:LEU:HD21	2.02	0.41
1:D:516:ARG:HD2	1:D:516:ARG:HA	1.72	0.40
1:D:521:PHE:CD2	1:D:522:LEU:HD13	2.57	0.40
2:A:451:ARG:HD2	2:A:452:ASP:CA	2.51	0.40
2:A:238:VAL:O	2:A:239:PRO:C	2.60	0.40
2:A:322:LEU:O	2:A:349:LEU:HD11	2.22	0.40
1:D:367:ASP:O	1:D:370:THR:N	2.55	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%)	3	12
2	A	237/263 (90%)	197 (83%)	32 (14%)	8 (3%)	4	18
All	All	469/529 (89%)	390 (83%)	61 (13%)	18 (4%)	4	15

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%)	180 (88%)	25 (12%)	6	17
2	A	212/232 (91%)	186 (88%)	26 (12%)	5	16
All	All	417/467 (89%)	366 (88%)	51 (12%)	6	17

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	290	LEU
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	381	MET
1	D	405	ARG
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	516	ARG
1	D	522	LEU
2	A	208	LEU
2	A	231	ARG

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Mol	Chain	Res	Type
2	A	243	ARG
2	A	248	SER
2	A	251	GLN
2	A	263	TRP
2	A	266	ASP
2	A	278	GLN
2	A	288	GLU
2	A	290	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	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	294	GLN
1	D	305	GLN
1	D	348	GLN
1	D	368	GLN
1	D	407	ASN
1	D	454	GLN
1	D	462	GLN
1	D	476	GLN
2	A	206	GLN
2	A	228	GLN
2	A	251	GLN
2	A	256	GLN
2	A	272	GLN
2	A	287	ASN

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Mol	Chain	Res	Type
2	A	338	GLN
2	A	343	GLN
2	A	363	GLN
2	A	376	ASN
2	A	386	GLN
2	A	439	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
4	EPH	A	4000	-	48,48,48	1.63	8 (16%)	50,53,53	1.61	8 (16%)
3	P1A	D	3000	-	36,36,36	3.51	17 (47%)	59,60,60	2.31	18 (30%)

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
4	EPH	A	4000	-	-	0/52/52/52	0/0/0/0
3	P1A	D	3000	-	-	0/17/87/87	0/4/4/4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3000	P1A	O3-C3	-5.90	1.30	1.43
4	A	4000	EPH	P1-O8	-3.42	1.44	1.59
3	D	3000	P1A	O20-C20	-3.32	1.38	1.44
3	D	3000	P1A	O6-C6	-2.58	1.18	1.22
4	A	4000	EPH	P1-O6	-2.21	1.44	1.55
3	D	3000	P1A	C18-C13	2.21	1.58	1.54
3	D	3000	P1A	C16-C17	2.25	1.58	1.54
4	A	4000	EPH	O8-C38	2.39	1.54	1.44
3	D	3000	P1A	C7-C6	2.84	1.51	1.45
4	A	4000	EPH	C32-C33	3.32	1.54	1.29
3	D	3000	P1A	C11-C9	3.34	1.59	1.53
4	A	4000	EPH	C13-C12	3.66	1.52	1.31
3	D	3000	P1A	C12-C13	4.11	1.62	1.54
4	A	4000	EPH	C29-C28	4.15	1.55	1.31
4	A	4000	EPH	C16-C15	4.29	1.55	1.31
4	A	4000	EPH	C25-C24	4.38	1.56	1.31
3	D	3000	P1A	C19-C10	4.64	1.62	1.54
3	D	3000	P1A	C10-C9	4.76	1.64	1.56
3	D	3000	P1A	C5-C6	5.24	1.59	1.51
3	D	3000	P1A	C23-C22	5.33	1.60	1.52
3	D	3000	P1A	C3-C2	5.67	1.60	1.52
3	D	3000	P1A	C21-C20	5.82	1.63	1.52
3	D	3000	P1A	C1-C10	6.31	1.64	1.54
3	D	3000	P1A	C9-C8	6.68	1.65	1.52
3	D	3000	P1A	C20-C22	8.81	1.68	1.55

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4000	EPH	O8-P1-O7	-4.78	89.97	109.25
3	D	3000	P1A	C24-C23-C22	-4.77	106.50	112.52
4	A	4000	EPH	O5-P1-O7	-4.74	90.12	109.25
4	A	4000	EPH	O6-P1-O7	-4.19	90.57	112.28
3	D	3000	P1A	O14-C14-C8	-4.13	98.67	106.04
3	D	3000	P1A	O14-C14-C15	-3.56	102.42	110.53
3	D	3000	P1A	C10-C1-C2	-3.04	109.17	114.04
3	D	3000	P1A	O6-C6-C7	-2.96	116.44	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3000	P1A	C19-C10-C5	-2.76	105.05	109.89
3	D	3000	P1A	C12-C13-C14	-2.36	104.42	107.76
4	A	4000	EPH	P1-O8-C38	-2.35	109.32	121.60
4	A	4000	EPH	C14-C13-C12	-2.27	111.50	124.90
3	D	3000	P1A	O20-C20-C17	-2.21	105.26	108.91
3	D	3000	P1A	O22-C22-C23	-2.16	105.12	109.14
3	D	3000	P1A	C10-C9-C8	-2.16	109.16	112.54
4	A	4000	EPH	C31-C30-C29	2.29	119.01	112.93
3	D	3000	P1A	C4-C3-C2	2.35	113.36	110.34
3	D	3000	P1A	C23-C24-C25	2.50	120.05	114.99
4	A	4000	EPH	C1-O2-C4	2.84	125.67	117.13
3	D	3000	P1A	C4-C5-C10	2.95	116.93	112.88
3	D	3000	P1A	C19-C10-C9	3.47	115.96	109.89
4	A	4000	EPH	O6-P1-O8	3.59	125.08	108.14
3	D	3000	P1A	O14-C14-C13	3.72	115.65	107.91
3	D	3000	P1A	C18-C13-C14	5.09	114.91	109.09
3	D	3000	P1A	C20-C17-C13	5.49	126.58	120.50
3	D	3000	P1A	C21-C20-C22	7.86	114.95	110.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4000	EPH	5	0
3	D	3000	P1A	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	D	236/266 (88%)	0.02	10 (4%) 37 32	40, 71, 98, 113	0
2	A	241/263 (91%)	0.16	21 (8%) 11 8	42, 70, 107, 122	0
All	All	477/529 (90%)	0.09	31 (6%) 20 15	40, 70, 104, 122	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	333	ASP	5.5
2	A	317	THR	4.7
2	A	316	THR	4.7
1	D	332	SER	4.5
2	A	205	VAL	4.4
2	A	225	GLU	4.0
2	A	224	SER	3.2
1	D	478	SER	3.1
2	A	315	ARG	3.0
2	A	226	GLU	2.9
1	D	431	MET	2.9
2	A	411	GLU	2.9
2	A	455	ARG	2.9
2	A	219	LEU	2.8
1	D	514	LYS	2.6
1	D	482	ARG	2.6
2	A	223	PRO	2.6
2	A	318	SER	2.6
2	A	303	THR	2.6
2	A	410	GLU	2.5
1	D	513	LEU	2.5
2	A	405	ARG	2.5
2	A	233	GLY	2.3
1	D	515	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	218	SER	2.3
1	D	323	TRP	2.3
2	A	304	GLU	2.2
2	A	228	GLN	2.2
2	A	444	THR	2.2
1	D	481	PRO	2.0
2	A	380	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	EPH	A	4000	49/49	0.79	0.36	3.96	86,92,111,111	0
3	P1A	D	3000	33/33	0.94	0.28	2.76	43,46,55,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.