



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:24 AM EDT

PDB ID : 1R20 / pdb_00001r20
Title : Crystal structure of the ligand-binding domains of the heterodimer EcR/USP bound to the synthetic agonist BYI06830
Authors : Billas, I.M.L.; Iwema, T.; Garnier, J.M.; Mitschler, A.; Rochel, N.; Moras, D.; Structural Proteomics in Europe (SPINE)
Deposited on : 2003-09-25
Resolution : 3.00 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

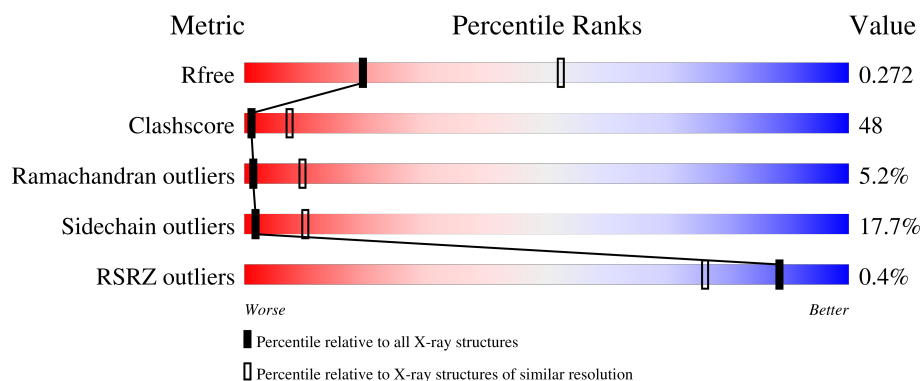
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	263	
2	D	265	

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
4	HWG	D	2000	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3806 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.

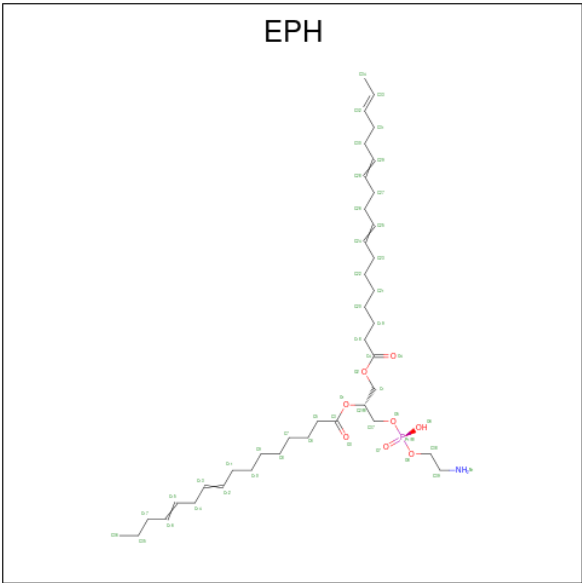
- Molecule 1 is a protein called ULTRASPIRACLE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	239	1897	1216	332	337	12	0	0	0

- Molecule 2 is a protein called ECDYSONE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	228	1820	1162	307	336	15	0	0	0

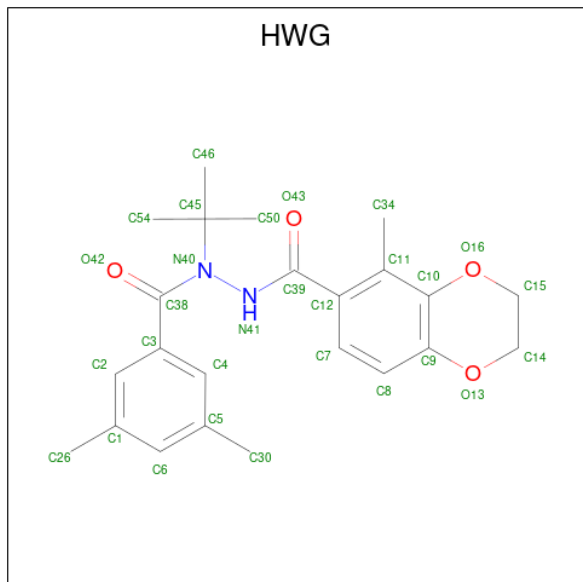
- Molecule 3 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (CCD ID: EPH) (formula: C₃₉H₆₈NO₈P).



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

- Molecule 4 is N-(TERT-BUTYL)-3,5-DIMETHYL-N'-[(5-METHYL-2,3-DIHYDRO-1,4

-BENZODIOXIN-6-YL)CARBONYL]BENZOHYDRAZIDE (CCD ID: HWG) (formula: $C_{23}H_{28}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			29	23	2	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	D	10	Total	O	0	0
			10	10		

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.43Å 149.43Å 61.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.00) 94.5 (15.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.48 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.289 0.228 , 0.272	Depositor DCC
R_{free} test set	1532 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	72.5	Xtriage
Anisotropy	0.790	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3806	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, HWG

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	1.07	5/1932 (0.3%)	1.35	24/2606 (0.9%)
2	D	1.03	3/1852 (0.2%)	1.35	25/2505 (1.0%)
All	All	1.05	8/3784 (0.2%)	1.35	49/5111 (1.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	MET	SD-CE	13.14	2.12	1.79
2	D	427	MET	SD-CE	8.41	2.00	1.79
2	D	502	MET	SD-CE	8.39	2.00	1.79
2	D	363	ILE	CA-CB	7.20	1.61	1.54
1	A	421	LEU	C-O	-6.28	1.18	1.24
1	A	326	MET	SD-CE	5.48	1.93	1.79
1	A	329	MET	CG-SD	5.23	1.93	1.80
1	A	282	ILE	CA-CB	-5.13	1.47	1.54

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ALA	N-CA-C	-12.36	97.89	111.36
2	D	434	ASN	N-CA-C	-10.36	100.94	114.31
1	A	421	LEU	CA-C-N	-9.11	108.45	119.84
1	A	421	LEU	C-N-CA	-9.11	108.45	119.84
2	D	416	VAL	N-CA-C	8.72	118.61	110.42
2	D	514	LYS	N-CA-C	-8.59	99.57	112.54
1	A	420	ARG	N-CA-C	-7.60	102.94	112.90
2	D	518	LEU	CA-C-N	7.55	128.16	120.38
2	D	518	LEU	C-N-CA	7.55	128.16	120.38
2	D	508	CYS	N-CA-C	-7.47	101.90	111.02
2	D	398	ALA	N-CA-C	-7.44	102.07	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	376	SER	N-CA-C	7.28	118.86	111.07
1	A	349	LEU	N-CA-C	7.00	120.71	111.75
2	D	292	ALA	N-CA-C	-6.98	103.76	112.90
2	D	353	PHE	N-CA-C	-6.72	103.88	111.07
1	A	364	ALA	N-CA-C	-6.68	103.62	111.03
2	D	340	THR	N-CA-C	6.48	118.00	111.07
2	D	401	GLN	N-CA-C	-6.45	104.47	113.37
2	D	370	THR	N-CA-C	-6.44	103.54	111.40
1	A	236	SER	N-CA-C	-6.40	101.31	110.59
2	D	447	SER	N-CA-C	-6.34	101.04	110.23
2	D	308	TYR	N-CA-C	-6.32	106.28	112.97
1	A	302	LEU	N-CA-C	6.31	118.74	108.26
1	A	283	LYS	N-CA-C	-6.25	104.47	111.28
2	D	448	ASP	N-CA-C	6.23	118.12	109.15
1	A	274	GLU	N-CA-C	-6.07	101.32	110.24
1	A	303	THR	N-CA-C	-5.98	104.36	112.26
1	A	255	LYS	N-CA-C	-5.97	104.69	111.07
1	A	413	ARG	N-CA-C	-5.89	104.49	111.03
2	D	475	ASN	N-CA-C	-5.85	104.82	111.14
2	D	364	SER	CB-CA-C	-5.79	98.89	110.42
1	A	329	MET	N-CA-C	-5.78	98.48	110.80
1	A	249	LEU	N-CA-C	-5.75	105.10	111.36
1	A	343	GLN	N-CA-C	5.71	119.43	112.23
1	A	381	GLY	N-CA-C	5.71	123.52	115.30
1	A	441	VAL	CB-CA-C	-5.70	103.76	111.63
2	D	425	ARG	N-CA-C	-5.67	105.00	111.07
2	D	348	GLN	N-CA-C	5.63	117.41	111.28
1	A	229	PHE	N-CA-C	-5.61	105.17	112.23
2	D	363	ILE	CB-CA-C	-5.60	102.85	111.08
2	D	391	ALA	N-CA-C	5.49	117.70	111.11
2	D	334	MET	N-CA-C	-5.37	102.72	110.40
2	D	503	GLN	N-CA-C	-5.20	105.73	111.71
1	A	426	SER	N-CA-C	-5.17	105.53	111.07
2	D	422	HIS	N-CA-C	-5.16	105.30	111.03
1	A	396	PHE	N-CA-C	-5.07	105.45	111.69
1	A	356	MET	N-CA-C	-5.03	106.31	112.90
1	A	376	ASN	CA-C-N	-5.03	114.61	120.04
1	A	376	ASN	C-N-CA	-5.03	114.61	120.04

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1897	0	1933	154	1
2	D	1820	0	1837	216	0
3	A	49	0	67	4	0
4	D	29	0	28	12	0
5	A	1	0	0	0	0
5	D	10	0	0	3	0
All	All	3806	0	3865	371	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 48.

All (371) 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:329:MET:SD	1:A:329:MET:CE	2.12	1.38
2:D:405:ARG:HH11	2:D:405:ARG:HB2	1.03	1.12
1:A:302:LEU:HD12	1:A:322:LEU:H	1.11	1.11
2:D:365:GLN:HE21	2:D:365:GLN:HA	1.14	1.05
2:D:291:THR:HG22	2:D:292:ALA:H	1.21	1.04
2:D:338:GLN:HE22	2:D:401:GLN:HB2	1.20	1.04
2:D:433:ASP:H	2:D:436:HIS:CD2	1.82	0.98
2:D:405:ARG:HB2	2:D:405:ARG:NH1	1.78	0.97
2:D:287:VAL:HG12	2:D:479:ALA:HB2	1.46	0.97
1:A:244:ALA:HB3	1:A:245:PRO:HD3	1.49	0.94
2:D:371:LEU:O	2:D:375:CYS:HB3	1.70	0.92
2:D:523:GLU:O	2:D:527:ASP:HA	1.71	0.91
2:D:351:VAL:HG13	2:D:372:LEU:HD22	1.53	0.90
2:D:338:GLN:NE2	2:D:401:GLN:HB2	1.86	0.90
1:A:213:LEU:HA	1:A:216:MET:HE2	1.53	0.89
2:D:405:ARG:HH11	2:D:405:ARG:CB	1.86	0.88
2:D:365:GLN:HE21	2:D:365:GLN:CA	1.89	0.86
2:D:452:LEU:HB2	2:D:455:PRO:HG3	1.58	0.86
1:A:302:LEU:HD12	1:A:322:LEU:N	1.93	0.84
2:D:289:PRO:HA	2:D:475:ASN:HD21	1.41	0.84
2:D:310:GLN:HG3	2:D:383:ARG:HB3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:CD1	1:A:322:LEU:H	1.91	0.83
2:D:310:GLN:NE2	2:D:346:THR:HG23	1.94	0.82
2:D:467:ASN:O	2:D:471:VAL:HG23	1.80	0.82
2:D:383:ARG:HD3	2:D:437:TYR:OH	1.80	0.81
1:A:323:MET:HE1	3:A:4000:EPH:H171	1.63	0.81
2:D:390:ALA:HB2	2:D:428:TYR:CE2	2.15	0.81
2:D:469:LEU:O	2:D:473:ILE:HG23	1.81	0.80
1:A:262:VAL:HG22	1:A:265:ARG:NH2	1.96	0.80
2:D:375:CYS:O	2:D:379:VAL:HG12	1.80	0.80
2:D:340:THR:O	2:D:344:ILE:HG13	1.80	0.80
1:A:344:ILE:O	1:A:348:VAL:HG23	1.82	0.80
2:D:520:PRO:HA	2:D:523:GLU:HG2	1.65	0.79
2:D:369:ILE:O	2:D:373:LYS:HG3	1.82	0.79
2:D:433:ASP:H	2:D:436:HIS:HD2	1.29	0.79
1:A:407:ARG:HA	1:A:407:ARG:NE	1.99	0.78
2:D:298:ILE:O	2:D:302:VAL:HG23	1.83	0.78
1:A:227:PHE:HB3	1:A:449:TYR:CD1	2.19	0.78
2:D:360:PHE:O	2:D:361:SER:C	2.28	0.77
2:D:365:GLN:HA	2:D:365:GLN:NE2	1.97	0.76
1:A:435:LEU:HB3	1:A:441:VAL:HG23	1.68	0.76
1:A:354:LEU:O	1:A:357:ARG:HB3	1.85	0.76
2:D:384:VAL:HG22	2:D:397:PHE:CE2	2.21	0.76
2:D:473:ILE:CD1	2:D:483:SER:HB2	2.16	0.75
2:D:346:THR:HG21	2:D:380:MET:HE3	1.69	0.75
1:A:216:MET:HA	1:A:219:LEU:CD2	2.17	0.75
1:A:435:LEU:HD22	1:A:441:VAL:HG23	1.68	0.74
2:D:291:THR:HG22	2:D:292:ALA:N	1.98	0.74
2:D:400:ASN:C	2:D:402:ALA:H	1.92	0.74
1:A:210:ILE:HD11	1:A:368:ALA:HB2	1.69	0.74
1:A:413:ARG:HG2	1:A:413:ARG:HH11	1.51	0.74
2:D:439:LEU:O	2:D:443:ILE:HG13	1.88	0.74
1:A:349:LEU:HA	1:A:353:SER:HB2	1.68	0.73
1:A:376:ASN:HD21	1:A:378:ASP:HB2	1.52	0.73
2:D:415:TYR:HD1	2:D:415:TYR:H	1.33	0.73
2:D:507:MET:HE3	2:D:507:MET:HA	1.68	0.73
1:A:415:ALA:O	1:A:419:LEU:HG	1.89	0.73
2:D:357:LEU:O	2:D:359:GLY:N	2.22	0.73
2:D:371:LEU:HD21	2:D:452:LEU:HD11	1.71	0.73
2:D:355:LYS:O	2:D:357:LEU:N	2.22	0.72
1:A:270:PHE:CE2	1:A:278:GLN:HG2	2.25	0.72
2:D:355:LYS:C	2:D:357:LEU:H	1.94	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:336:PHE:HE2	2:D:511:LEU:HD13	1.55	0.72
2:D:351:VAL:HG13	2:D:372:LEU:CD2	2.19	0.72
2:D:310:GLN:HG2	2:D:383:ARG:HH11	1.56	0.70
1:A:213:LEU:HD23	1:A:216:MET:CE	2.21	0.70
2:D:513:LEU:O	2:D:513:LEU:HD12	1.92	0.70
2:D:306:GLU:O	2:D:309:GLU:HB2	1.92	0.70
2:D:420:LEU:HD13	4:D:2000:HWG:H8	1.74	0.69
2:D:366:SER:HA	2:D:369:ILE:CG2	2.22	0.69
2:D:289:PRO:HA	2:D:475:ASN:ND2	2.07	0.69
1:A:435:LEU:HD23	1:A:440:LEU:HB2	1.72	0.69
2:D:287:VAL:CG1	2:D:479:ALA:HB2	2.22	0.68
2:D:298:ILE:HG23	2:D:435:VAL:HG13	1.76	0.68
1:A:227:PHE:HD2	1:A:449:TYR:HD1	1.40	0.68
1:A:260:LEU:HD23	1:A:289:LEU:HD13	1.76	0.68
2:D:473:ILE:C	2:D:473:ILE:HD12	2.18	0.68
1:A:349:LEU:HA	1:A:353:SER:CB	2.25	0.67
2:D:380:MET:HB3	4:D:2000:HWG:H262	1.77	0.66
1:A:375:LEU:HD13	1:A:391:LEU:HB3	1.78	0.65
2:D:473:ILE:HD11	2:D:483:SER:HB2	1.78	0.65
1:A:325:LEU:HD11	1:A:331:LEU:HG	1.79	0.65
2:D:345:LEU:O	2:D:348:GLN:HB2	1.96	0.65
2:D:401:GLN:H	2:D:401:GLN:NE2	1.94	0.65
2:D:365:GLN:CA	2:D:365:GLN:NE2	2.58	0.65
2:D:397:PHE:CD2	2:D:403:TYR:HE1	2.15	0.65
1:A:389:GLU:O	1:A:393:GLU:HG3	1.98	0.64
2:D:504:ASN:O	2:D:507:MET:N	2.30	0.64
1:A:301:PHE:HB3	1:A:322:LEU:HD12	1.78	0.64
2:D:504:ASN:ND2	4:D:2000:HWG:O43	2.31	0.64
2:D:501:GLY:O	2:D:504:ASN:HB3	1.97	0.63
2:D:525:ILE:HG22	2:D:526:TRP:CD1	2.33	0.63
2:D:347:VAL:O	2:D:351:VAL:HG23	1.98	0.63
2:D:334:MET:C	2:D:336:PHE:H	2.06	0.63
2:D:415:TYR:CD1	2:D:415:TYR:N	2.66	0.63
1:A:274:GLU:HG2	1:A:383:LYS:HD3	1.80	0.63
1:A:260:LEU:HD21	1:A:289:LEU:HB3	1.80	0.63
1:A:231:ARG:HD3	1:A:231:ARG:C	2.24	0.62
2:D:310:GLN:HG3	2:D:383:ARG:CB	2.28	0.62
1:A:229:PHE:CD2	1:A:446:ILE:HD12	2.35	0.62
2:D:308:TYR:CE2	2:D:352:GLU:HB3	2.34	0.62
2:D:359:GLY:O	2:D:362:LYS:HB2	2.00	0.62
2:D:400:ASN:C	2:D:402:ALA:N	2.57	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:GLN:NE2	2:D:401:GLN:N	2.47	0.62
2:D:381:MET:HE3	2:D:500:LEU:HB3	1.81	0.62
2:D:460:GLU:HA	2:D:463:ARG:NH1	2.14	0.62
1:A:365:GLU:OE2	1:A:413:ARG:NH1	2.32	0.62
2:D:500:LEU:HG	4:D:2000:HWG:H142	1.82	0.62
1:A:435:LEU:HD22	1:A:441:VAL:CG2	2.29	0.62
2:D:308:TYR:HE2	2:D:352:GLU:HB3	1.64	0.62
2:D:430:MET:HE2	2:D:489:LYS:HE3	1.82	0.61
2:D:452:LEU:CB	2:D:455:PRO:HG3	2.29	0.61
1:A:227:PHE:CD2	1:A:449:TYR:HD1	2.19	0.61
2:D:384:VAL:HG22	2:D:397:PHE:HE2	1.66	0.61
2:D:521:PHE:O	2:D:524:GLU:HB3	2.01	0.60
1:A:213:LEU:HA	1:A:216:MET:CE	2.30	0.60
1:A:212:ARG:HG3	1:A:212:ARG:HH11	1.67	0.60
2:D:452:LEU:O	2:D:455:PRO:HD3	2.01	0.60
2:D:344:ILE:HD11	2:D:519:PRO:HG2	1.83	0.60
2:D:344:ILE:HG23	2:D:521:PHE:HD2	1.65	0.60
2:D:287:VAL:HG12	2:D:479:ALA:CB	2.28	0.60
2:D:415:TYR:HD1	2:D:415:TYR:N	1.99	0.60
2:D:366:SER:O	2:D:369:ILE:HG23	2.01	0.60
1:A:435:LEU:HB3	1:A:441:VAL:CG2	2.32	0.59
1:A:349:LEU:O	1:A:354:LEU:N	2.29	0.59
2:D:346:THR:O	2:D:350:ILE:HG13	2.02	0.59
2:D:310:GLN:O	2:D:312:SER:N	2.36	0.59
2:D:384:VAL:HG13	2:D:395:VAL:HG11	1.84	0.59
2:D:291:THR:CG2	2:D:292:ALA:H	2.05	0.58
2:D:310:GLN:HE22	2:D:346:THR:HG23	1.67	0.58
1:A:377:PRO:HG3	1:A:389:GLU:HG2	1.85	0.58
1:A:263:TRP:CZ2	1:A:267:ILE:HD11	2.39	0.58
2:D:504:ASN:HA	4:D:2000:HWG:C34	2.33	0.58
2:D:433:ASP:N	2:D:436:HIS:HD2	2.00	0.58
2:D:287:VAL:O	2:D:287:VAL:HG23	2.02	0.57
2:D:386:ARG:NH2	2:D:433:ASP:O	2.37	0.57
2:D:430:MET:HE2	2:D:489:LYS:HB3	1.87	0.57
2:D:430:MET:CE	2:D:489:LYS:HB3	2.35	0.57
1:A:231:ARG:HD3	1:A:231:ARG:O	2.05	0.56
1:A:251:GLN:OE1	1:A:255:LYS:HE3	2.05	0.56
1:A:332:HIS:CD2	1:A:334:ASN:H	2.24	0.56
2:D:372:LEU:O	2:D:376:SER:HB3	2.05	0.56
2:D:384:VAL:HG21	4:D:2000:HWG:H301	1.88	0.56
2:D:375:CYS:SG	2:D:445:ILE:HG13	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:344:ILE:HG22	2:D:348:GLN:HE21	1.70	0.56
2:D:355:LYS:C	2:D:357:LEU:N	2.63	0.56
1:A:373:ILE:HG22	1:A:373:ILE:O	2.05	0.56
1:A:407:ARG:NE	1:A:407:ARG:CA	2.69	0.55
2:D:364:SER:OG	2:D:365:GLN:N	2.34	0.55
2:D:313:GLU:O	2:D:315:ASP:N	2.39	0.55
2:D:289:PRO:CA	2:D:475:ASN:HD21	2.14	0.55
2:D:313:GLU:C	2:D:315:ASP:H	2.13	0.55
2:D:448:ASP:OD1	2:D:448:ASP:O	2.24	0.55
2:D:310:GLN:CG	2:D:383:ARG:HH11	2.20	0.55
2:D:397:PHE:C	2:D:399:ASN:N	2.62	0.55
2:D:432:MET:HE1	2:D:440:LEU:HD22	1.87	0.54
2:D:433:ASP:HB2	2:D:436:HIS:CD2	2.42	0.54
1:A:266:ASP:O	1:A:267:ILE:C	2.50	0.54
2:D:290:LEU:HB2	2:D:295:LYS:HG3	1.89	0.54
1:A:213:LEU:HD23	1:A:216:MET:HE1	1.88	0.54
2:D:336:PHE:CD1	2:D:336:PHE:C	2.86	0.54
2:D:360:PHE:O	2:D:363:ILE:N	2.40	0.54
2:D:446:PHE:HB3	2:D:462:GLN:HB2	1.90	0.54
1:A:262:VAL:HG22	1:A:265:ARG:HH21	1.72	0.54
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.72	0.54
1:A:401:GLU:O	1:A:402:TYR:C	2.48	0.54
1:A:265:ARG:NH1	1:A:454:LEU:O	2.41	0.54
1:A:302:LEU:CD1	1:A:321:GLN:N	2.71	0.54
2:D:378:GLU:OE1	2:D:498:ARG:HD3	2.08	0.54
2:D:485:VAL:O	2:D:489:LYS:HG3	2.09	0.53
1:A:453:ALA:O	1:A:454:LEU:C	2.49	0.53
2:D:310:GLN:HE22	2:D:346:THR:HA	1.73	0.53
1:A:222:ASP:O	1:A:224:SER:N	2.40	0.53
1:A:326:MET:O	1:A:327:PRO:C	2.52	0.53
2:D:336:PHE:HD2	2:D:516:ARG:HH21	1.52	0.53
1:A:432:PHE:O	1:A:433:GLU:C	2.51	0.53
1:A:441:VAL:HG12	1:A:442:ALA:N	2.22	0.53
1:A:438:PHE:CE1	3:A:4000:EPH:H51	2.44	0.53
2:D:290:LEU:C	2:D:291:THR:O	2.50	0.53
1:A:397:LEU:HD12	2:D:485:VAL:HG23	1.90	0.53
1:A:244:ALA:HB3	1:A:245:PRO:CD	2.31	0.52
2:D:520:PRO:HA	2:D:523:GLU:CG	2.37	0.52
2:D:335:PRO:C	2:D:337:ARG:N	2.65	0.52
1:A:273:LEU:O	1:A:274:GLU:C	2.51	0.52
2:D:364:SER:HG	2:D:367:ASP:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4000:EPH:H361	3:A:4000:EPH:H232	1.91	0.52
2:D:341:GLU:O	2:D:342:MET:C	2.52	0.52
1:A:212:ARG:HG3	1:A:212:ARG:NH1	2.25	0.52
1:A:341:VAL:HG12	1:A:434:HIS:CE1	2.46	0.51
2:D:446:PHE:CB	2:D:462:GLN:HB2	2.40	0.51
1:A:402:TYR:C	1:A:402:TYR:CD2	2.88	0.51
1:A:406:SER:OG	1:A:407:ARG:N	2.40	0.51
2:D:382:LEU:HG	2:D:497:ILE:HD11	1.92	0.51
1:A:224:SER:OG	1:A:225:GLU:N	2.44	0.51
2:D:363:ILE:HG22	2:D:364:SER:O	2.10	0.51
1:A:373:ILE:O	1:A:373:ILE:CG2	2.59	0.51
2:D:343:THR:O	2:D:347:VAL:HG23	2.11	0.51
2:D:294:GLN:HE22	2:D:471:VAL:HG21	1.76	0.51
2:D:449:ARG:HB3	2:D:450:PRO:HD2	1.93	0.51
2:D:466:LEU:HD21	2:D:491:LEU:HD21	1.91	0.51
1:A:323:MET:HG3	1:A:349:LEU:HD21	1.92	0.50
1:A:216:MET:HA	1:A:219:LEU:HD22	1.92	0.50
1:A:448:GLY:O	1:A:451:ARG:HB3	2.11	0.50
2:D:313:GLU:C	2:D:315:ASP:N	2.69	0.50
2:D:313:GLU:OE2	2:D:313:GLU:N	2.44	0.50
2:D:336:PHE:CE2	2:D:511:LEU:HD13	2.43	0.50
1:A:333:ARG:HH12	1:A:337:LEU:HD23	1.76	0.50
1:A:413:ARG:HG2	1:A:413:ARG:NH1	2.23	0.50
1:A:246:VAL:HG11	1:A:440:LEU:HD21	1.93	0.50
2:D:433:ASP:N	2:D:436:HIS:CD2	2.65	0.50
1:A:371:ALA:O	1:A:375:LEU:HG	2.12	0.49
1:A:407:ARG:O	1:A:410:GLU:HB2	2.12	0.49
1:A:370:LYS:O	1:A:371:ALA:C	2.55	0.49
2:D:406:ASP:O	2:D:407:ASN:C	2.52	0.49
2:D:503:GLN:HB3	4:D:2000:HWG:C15	2.42	0.49
1:A:278:GLN:HB3	1:A:454:LEU:HD11	1.94	0.49
1:A:229:PHE:CD2	1:A:257:ILE:HG21	2.47	0.49
1:A:210:ILE:CD1	1:A:368:ALA:HB2	2.42	0.49
1:A:325:LEU:HD11	1:A:331:LEU:CG	2.42	0.49
2:D:365:GLN:O	2:D:368:GLN:HG2	2.12	0.49
1:A:245:PRO:O	1:A:249:LEU:HG	2.11	0.49
1:A:325:LEU:CD1	1:A:331:LEU:HG	2.43	0.49
1:A:329:MET:HE3	1:A:330:THR:N	2.28	0.49
1:A:260:LEU:CD2	1:A:289:LEU:HB3	2.42	0.49
1:A:231:ARG:C	1:A:231:ARG:CD	2.85	0.49
1:A:302:LEU:CD1	1:A:322:LEU:N	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:452:LEU:HD13	2:D:458:VAL:HG21	1.94	0.48
2:D:397:PHE:HD2	2:D:403:TYR:CE1	2.31	0.48
2:D:334:MET:O	2:D:336:PHE:N	2.44	0.48
1:A:401:GLU:O	1:A:404:ARG:HG2	2.13	0.48
2:D:504:ASN:HA	4:D:2000:HWG:H343	1.94	0.48
2:D:309:GLU:O	2:D:310:GLN:C	2.57	0.48
2:D:335:PRO:C	2:D:337:ARG:H	2.22	0.48
1:A:285:SER:O	1:A:286:TRP:C	2.55	0.48
2:D:397:PHE:CD2	2:D:403:TYR:CE1	2.99	0.48
2:D:432:MET:CE	2:D:490:ILE:HG23	2.44	0.48
1:A:347:ARG:O	1:A:351:GLU:HB2	2.14	0.48
1:A:407:ARG:CA	1:A:407:ARG:HE	2.27	0.48
2:D:519:PRO:C	2:D:521:PHE:H	2.21	0.48
1:A:376:ASN:HD22	1:A:379:VAL:HG23	1.78	0.48
1:A:209:SER:C	1:A:211:GLU:N	2.67	0.47
1:A:332:HIS:HD2	1:A:334:ASN:HB2	1.79	0.47
1:A:352:LEU:HD23	1:A:420:ARG:HG3	1.94	0.47
2:D:427:MET:HE3	2:D:432:MET:SD	2.54	0.47
2:D:433:ASP:HB2	2:D:436:HIS:CG	2.49	0.47
1:A:329:MET:HE3	1:A:330:THR:C	2.39	0.47
2:D:504:ASN:HA	4:D:2000:HWG:H341	1.96	0.47
1:A:407:ARG:HA	1:A:407:ARG:HE	1.77	0.47
2:D:464:TYR:O	2:D:465:TYR:C	2.56	0.47
2:D:308:TYR:O	2:D:310:GLN:N	2.47	0.47
2:D:390:ALA:HB2	2:D:428:TYR:HE2	1.75	0.47
2:D:406:ASP:O	2:D:409:ARG:N	2.47	0.47
2:D:503:GLN:CD	4:D:2000:HWG:H151	2.40	0.47
2:D:356:GLY:O	2:D:358:PRO:HD3	2.15	0.47
2:D:461:ILE:O	2:D:464:TYR:N	2.42	0.47
1:A:376:ASN:ND2	1:A:378:ASP:HB2	2.23	0.47
2:D:317:LYS:O	2:D:317:LYS:HG3	2.15	0.47
2:D:293:ASN:OD1	2:D:293:ASN:N	2.46	0.46
2:D:388:TYR:OH	2:D:393:ASP:OD1	2.23	0.46
2:D:401:GLN:H	2:D:401:GLN:HE21	1.63	0.46
1:A:283:LYS:HG3	1:A:446:ILE:CG2	2.44	0.46
3:A:4000:EPH:H25	3:A:4000:EPH:H102	1.98	0.46
2:D:509:ILE:HD12	2:D:528:VAL:CB	2.45	0.46
1:A:337:LEU:C	1:A:339:ALA:N	2.72	0.46
2:D:399:ASN:C	2:D:400:ASN:O	2.57	0.46
1:A:418:LEU:HA	1:A:418:LEU:HD23	1.66	0.46
1:A:283:LYS:HG3	1:A:446:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HD13	1:A:321:GLN:N	2.30	0.46
2:D:445:ILE:HG22	2:D:446:PHE:CD2	2.50	0.46
2:D:380:MET:HB3	4:D:2000:HWG:C26	2.44	0.45
1:A:413:ARG:HH11	1:A:413:ARG:CG	2.22	0.45
2:D:367:ASP:CG	2:D:453:GLU:HB2	2.41	0.45
1:A:441:VAL:CG1	1:A:442:ALA:N	2.79	0.45
2:D:430:MET:HB3	5:D:1010:HOH:O	2.16	0.45
1:A:445:SER:O	1:A:446:ILE:C	2.60	0.45
2:D:490:ILE:O	2:D:491:LEU:C	2.54	0.45
1:A:362:ASP:OD1	1:A:363:GLN:N	2.49	0.45
2:D:416:VAL:O	2:D:417:ILE:C	2.57	0.45
2:D:311:PRO:HD3	2:D:397:PHE:HE1	1.81	0.45
2:D:336:PHE:CD1	2:D:336:PHE:O	2.69	0.45
1:A:443:ASP:HA	1:A:446:ILE:HG12	2.00	0.44
2:D:346:THR:O	2:D:347:VAL:C	2.59	0.44
2:D:367:ASP:O	2:D:370:THR:HB	2.17	0.44
2:D:368:GLN:O	2:D:371:LEU:N	2.50	0.44
1:A:391:LEU:O	1:A:392:ARG:C	2.59	0.44
1:A:430:LYS:O	1:A:433:GLU:HB2	2.17	0.44
2:D:490:ILE:C	2:D:492:GLY:N	2.72	0.44
2:D:363:ILE:CG2	2:D:364:SER:N	2.81	0.44
2:D:489:LYS:HE2	5:D:1010:HOH:O	2.17	0.44
2:D:519:PRO:O	2:D:521:PHE:N	2.51	0.44
1:A:257:ILE:O	1:A:261:VAL:HG23	2.18	0.44
1:A:333:ARG:HG2	1:A:333:ARG:NH1	2.33	0.44
1:A:413:ARG:NH1	1:A:413:ARG:CG	2.80	0.44
2:D:363:ILE:HG22	2:D:364:SER:N	2.32	0.44
1:A:411:GLU:OE2	1:A:411:GLU:HA	2.18	0.43
2:D:338:GLN:HE21	2:D:338:GLN:HB3	1.62	0.43
1:A:248:SER:O	1:A:252:ILE:HG13	2.18	0.43
1:A:290:LEU:O	1:A:294:ILE:HG13	2.18	0.43
1:A:362:ASP:OD2	1:A:402:TYR:OH	2.28	0.43
1:A:365:GLU:OE2	1:A:413:ARG:CZ	2.67	0.43
2:D:310:GLN:O	2:D:311:PRO:C	2.59	0.43
2:D:308:TYR:O	2:D:309:GLU:C	2.59	0.43
2:D:376:SER:OG	2:D:377:SER:N	2.51	0.43
2:D:307:GLY:C	2:D:309:GLU:H	2.26	0.43
1:A:301:PHE:CE1	1:A:330:THR:HB	2.53	0.43
1:A:370:LYS:O	1:A:373:ILE:N	2.52	0.43
2:D:475:ASN:O	2:D:476:GLN:C	2.61	0.43
1:A:302:LEU:HD13	1:A:320:PRO:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:O	1:A:339:ALA:N	2.52	0.43
2:D:360:PHE:CE2	2:D:372:LEU:HD11	2.54	0.43
2:D:409:ARG:HB3	2:D:409:ARG:NH1	2.33	0.43
2:D:457:LEU:C	2:D:459:GLU:N	2.75	0.43
1:A:292:PHE:CE2	1:A:366:TYR:CD1	3.07	0.42
2:D:290:LEU:HD13	2:D:298:ILE:HD12	2.00	0.42
1:A:282:ILE:HG22	1:A:450:ILE:HD13	2.01	0.42
1:A:325:LEU:HD12	1:A:329:MET:HE2	2.01	0.42
2:D:290:LEU:O	2:D:291:THR:O	2.37	0.42
2:D:360:PHE:O	2:D:362:LYS:N	2.53	0.42
1:A:404:ARG:C	1:A:406:SER:H	2.28	0.42
2:D:334:MET:C	2:D:336:PHE:N	2.75	0.42
2:D:369:ILE:O	2:D:369:ILE:HG13	2.18	0.42
2:D:473:ILE:CD1	2:D:483:SER:CB	2.91	0.42
2:D:504:ASN:O	2:D:507:MET:HB3	2.20	0.42
2:D:522:LEU:O	2:D:523:GLU:C	2.61	0.42
2:D:523:GLU:HG3	2:D:524:GLU:N	2.34	0.42
1:A:254:ASN:O	1:A:255:LYS:C	2.62	0.42
1:A:399:LEU:HD23	1:A:414:PHE:CE1	2.55	0.42
2:D:463:ARG:O	2:D:463:ARG:HG2	2.18	0.42
1:A:420:ARG:HD3	1:A:420:ARG:HA	1.69	0.42
1:A:402:TYR:HD2	1:A:403:CYS:N	2.18	0.42
2:D:390:ALA:HB2	2:D:428:TYR:CZ	2.55	0.42
2:D:481:PRO:O	2:D:482:ARG:C	2.62	0.42
2:D:371:LEU:HD23	2:D:371:LEU:HA	1.79	0.42
1:A:242:PHE:HA	1:A:245:PRO:HD2	2.02	0.41
1:A:344:ILE:HD11	1:A:431:SER:OG	2.20	0.41
1:A:379:VAL:O	1:A:382:LEU:HG	2.19	0.41
2:D:519:PRO:HA	2:D:520:PRO:HD3	1.92	0.41
1:A:241:LYS:HE2	1:A:242:PHE:HE1	1.85	0.41
1:A:278:GLN:HB3	1:A:454:LEU:CD1	2.50	0.41
2:D:298:ILE:O	2:D:302:VAL:CG2	2.63	0.41
1:A:333:ARG:NH1	1:A:337:LEU:HD23	2.34	0.41
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.85	0.41
2:D:340:THR:O	2:D:344:ILE:CG1	2.62	0.41
1:A:241:LYS:HE2	1:A:242:PHE:CE1	2.56	0.41
1:A:229:PHE:HD2	1:A:446:ILE:HD12	1.81	0.41
1:A:231:ARG:O	1:A:231:ARG:CD	2.69	0.41
1:A:241:LYS:HG3	1:A:242:PHE:CD1	2.55	0.41
2:D:401:GLN:N	2:D:401:GLN:CD	2.78	0.41
2:D:493:ILE:O	2:D:496:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LEU:HD13	1:A:391:LEU:CB	2.48	0.41
1:A:286:TRP:CG	1:A:287:ASN:H	2.38	0.41
1:A:242:PHE:C	1:A:245:PRO:HD2	2.45	0.41
1:A:446:ILE:O	1:A:447:ALA:C	2.63	0.41
2:D:340:THR:HG22	2:D:341:GLU:N	2.35	0.41
2:D:522:LEU:C	2:D:524:GLU:N	2.79	0.41
1:A:275:MET:O	1:A:276:GLU:C	2.63	0.41
1:A:332:HIS:HD2	1:A:334:ASN:H	1.64	0.41
1:A:418:LEU:HD23	1:A:421:LEU:HD22	2.03	0.41
2:D:508:CYS:O	2:D:509:ILE:C	2.63	0.41
1:A:260:LEU:HD23	1:A:289:LEU:CD1	2.49	0.40
1:A:323:MET:HE2	1:A:331:LEU:HD12	2.03	0.40
2:D:463:ARG:HA	2:D:466:LEU:HB2	2.02	0.40
1:A:418:LEU:O	1:A:421:LEU:HB2	2.21	0.40
2:D:303:TYR:C	2:D:303:TYR:CD1	2.99	0.40
1:A:349:LEU:HA	1:A:353:SER:HB3	2.03	0.40
2:D:400:ASN:HB2	2:D:402:ALA:HB2	2.04	0.40
2:D:473:ILE:HD12	2:D:473:ILE:O	2.20	0.40
2:D:494:LEU:HG	5:D:1003:HOH:O	2.20	0.40
2:D:503:GLN:HB3	4:D:2000:HWG:H151	2.04	0.40
2:D:519:PRO:C	2:D:521:PHE:N	2.78	0.40
2:D:482:ARG:O	2:D:483:SER:C	2.64	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)
1:A:329:MET:SD	1:A:329:MET:SD[4_556]	2.05	0.15

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	235/263 (89%)	199 (85%)	32 (14%)	4 (2%)	7	32
2	D	224/265 (84%)	147 (66%)	57 (25%)	20 (9%)	0	3
All	All	459/528 (87%)	346 (75%)	89 (19%)	24 (5%)	1	9

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ALA
2	D	399	ASN
2	D	402	ALA
2	D	527	ASP
2	D	291	THR
2	D	314	GLU
2	D	356	GLY
2	D	358	PRO
2	D	360	PHE
2	D	365	GLN
2	D	433	ASP
2	D	515	ASN
2	D	335	PRO
2	D	359	GLY
2	D	309	GLU
2	D	366	SER
2	D	524	GLU
1	A	327	PRO
2	D	311	PRO
2	D	364	SER
2	D	525	ILE
1	A	348	VAL
2	D	520	PRO
1	A	446	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/232 (89%)	173 (84%)	33 (16%)	2	12
2	D	201/235 (86%)	162 (81%)	39 (19%)	1	8
All	All	407/467 (87%)	335 (82%)	72 (18%)	2	10

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	ILE
1	A	219	LEU
1	A	231	ARG
1	A	232	VAL
1	A	245	PRO
1	A	246	VAL
1	A	260	LEU
1	A	262	VAL
1	A	278	GLN
1	A	279	ILE
1	A	322	LEU
1	A	329	MET
1	A	330	THR
1	A	337	LEU
1	A	347	ARG
1	A	353	SER
1	A	357	ARG
1	A	358	THR
1	A	359	LEU
1	A	361	VAL
1	A	362	ASP
1	A	374	LEU
1	A	380	LYS
1	A	385	ARG
1	A	388	VAL
1	A	397	LEU
1	A	406	SER
1	A	408	SER
1	A	420	ARG
1	A	421	LEU
1	A	433	GLU
1	A	435	LEU
1	A	452	ASP
2	D	293	ASN
2	D	300	ARG

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Mol	Chain	Res	Type
2	D	301	LEU
2	D	302	VAL
2	D	303	TYR
2	D	336	PHE
2	D	340	THR
2	D	344	ILE
2	D	357	LEU
2	D	358	PRO
2	D	360	PHE
2	D	364	SER
2	D	365	GLN
2	D	369	ILE
2	D	371	LEU
2	D	375	CYS
2	D	380	MET
2	D	387	ARG
2	D	397	PHE
2	D	403	TYR
2	D	405	ARG
2	D	406	ASP
2	D	415	TYR
2	D	427	MET
2	D	430	MET
2	D	433	ASP
2	D	448	ASP
2	D	453	GLU
2	D	454	GLN
2	D	457	LEU
2	D	473	ILE
2	D	476	GLN
2	D	494	LEU
2	D	496	GLU
2	D	497	ILE
2	D	499	THR
2	D	500	LEU
2	D	507	MET
2	D	518	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	HIS

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Mol	Chain	Res	Type
1	A	343	GLN
1	A	363	GLN
1	A	376	ASN
1	A	384	ASN
1	A	434	HIS
2	D	338	GLN
2	D	348	GLN
2	D	365	GLN
2	D	368	GLN
2	D	400	ASN
2	D	401	GLN
2	D	436	HIS
2	D	462	GLN
2	D	475	ASN
2	D	476	GLN
2	D	477	ASN
2	D	504	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
3	EPH	A	4000	-	48,48,48	1.89	13 (27%)	51,53,53	1.64	6 (11%)
4	HWG	D	2000	-	30,31,31	3.36	11 (36%)	41,46,46	2.44	13 (31%)

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	EPH	A	4000	-	-	20/52/52/52	-
4	HWG	D	2000	-	-	2/22/29/29	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2000	HWG	C12-C11	12.67	1.56	1.40
4	D	2000	HWG	C9-C10	5.69	1.52	1.41
4	D	2000	HWG	C2-C3	5.41	1.47	1.39
4	D	2000	HWG	C3-C38	4.99	1.58	1.50
4	D	2000	HWG	C45-N40	4.36	1.57	1.51
3	A	4000	EPH	C25-C24	4.25	1.55	1.31
3	A	4000	EPH	C16-C15	4.23	1.55	1.31
3	A	4000	EPH	C1-C2	-3.84	1.38	1.50
3	A	4000	EPH	C29-C28	3.82	1.53	1.31
4	D	2000	HWG	C4-C3	3.80	1.45	1.39
3	A	4000	EPH	C13-C12	3.72	1.52	1.31
3	A	4000	EPH	C32-C33	3.69	1.56	1.29
3	A	4000	EPH	P1-O8	-3.38	1.46	1.59
4	D	2000	HWG	N41-N40	-3.25	1.36	1.39
3	A	4000	EPH	C21-C20	-3.21	1.35	1.51
4	D	2000	HWG	C4-C5	3.21	1.44	1.39
3	A	4000	EPH	C20-C19	-3.20	1.35	1.51
4	D	2000	HWG	C39-N41	2.85	1.39	1.35
3	A	4000	EPH	C22-C23	-2.83	1.40	1.52
3	A	4000	EPH	O8-C38	2.44	1.54	1.44
4	D	2000	HWG	O16-C10	2.40	1.41	1.37
3	A	4000	EPH	C18-C4	2.19	1.57	1.50
4	D	2000	HWG	C6-C5	2.13	1.42	1.39
3	A	4000	EPH	P1-O6	-2.07	1.45	1.55

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2000	HWG	C46-C45-N40	6.40	114.59	108.85
4	D	2000	HWG	O13-C9-C10	-6.30	117.02	121.78
4	D	2000	HWG	O16-C10-C11	6.28	124.85	115.67
3	A	4000	EPH	O6-P1-O7	-5.18	88.33	112.44
3	A	4000	EPH	O8-P1-O7	-4.91	89.48	108.94
3	A	4000	EPH	O5-P1-O7	-4.37	91.60	108.94
3	A	4000	EPH	O6-P1-O8	4.18	126.50	107.57
4	D	2000	HWG	C14-O13-C9	4.00	120.72	113.67
4	D	2000	HWG	C54-C45-N40	3.88	112.33	108.85
4	D	2000	HWG	C12-C39-N41	3.82	122.01	114.80
4	D	2000	HWG	C9-C10-C11	-3.65	116.61	121.18
4	D	2000	HWG	C4-C3-C2	-2.86	116.30	119.65
4	D	2000	HWG	O16-C10-C9	-2.64	118.54	121.82
4	D	2000	HWG	O13-C9-C8	2.45	120.79	116.89
4	D	2000	HWG	C34-C11-C10	-2.44	117.42	121.24
4	D	2000	HWG	C54-C45-C46	-2.19	104.59	109.48
3	A	4000	EPH	P1-O8-C38	-2.12	111.16	121.26
4	D	2000	HWG	O43-C39-N41	-2.10	119.25	122.42
3	A	4000	EPH	C1-O2-C4	2.03	124.53	117.12

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4000	EPH	C25-C26-C27-C28
3	A	4000	EPH	C37-O5-P1-O6
3	A	4000	EPH	C16-C17-C35-C36
3	A	4000	EPH	C38-O8-P1-O5
3	A	4000	EPH	O8-C38-C39-N1
3	A	4000	EPH	C27-C28-C29-C30
3	A	4000	EPH	C23-C24-C25-C26
3	A	4000	EPH	C14-C15-C16-C17
3	A	4000	EPH	C5-C6-C7-C8
3	A	4000	EPH	C31-C32-C33-C34
3	A	4000	EPH	C29-C30-C31-C32
3	A	4000	EPH	C39-C38-O8-P1
4	D	2000	HWG	C2-C3-C38-N40
3	A	4000	EPH	C38-O8-P1-O7
3	A	4000	EPH	C15-C16-C17-C35
4	D	2000	HWG	C4-C3-C38-N40
3	A	4000	EPH	C7-C8-C9-C10
3	A	4000	EPH	C11-C10-C9-C8
3	A	4000	EPH	C28-C29-C30-C31

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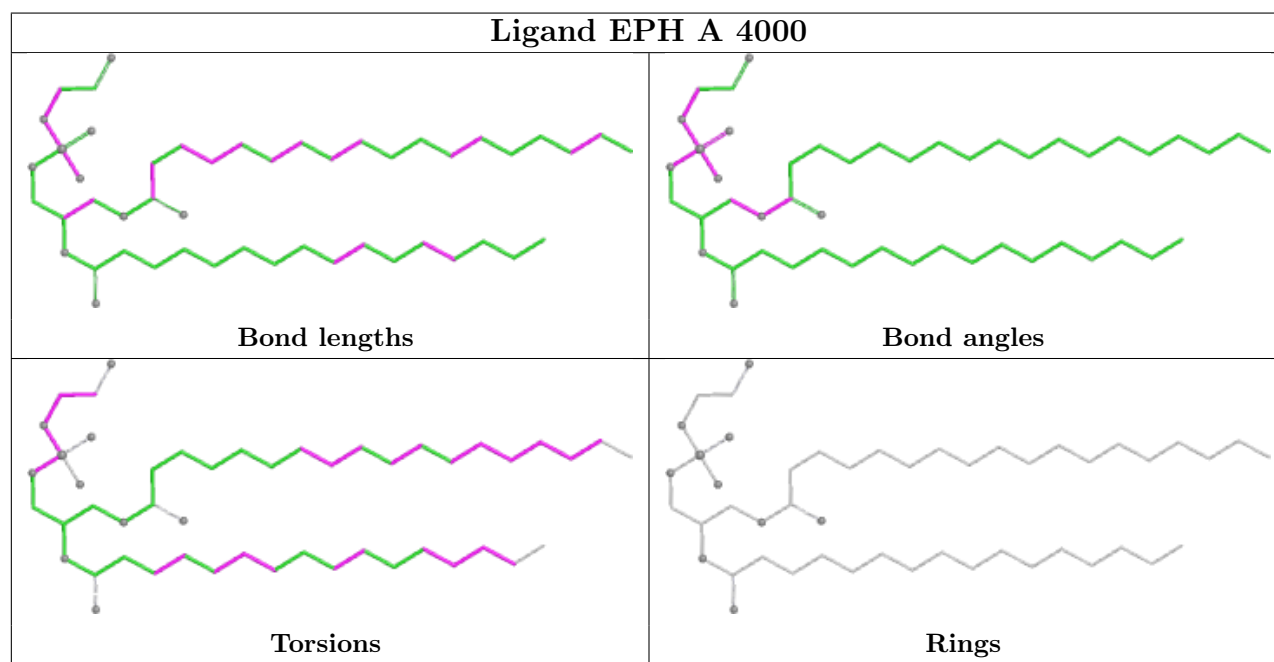
Mol	Chain	Res	Type	Atoms
3	A	4000	EPH	C22-C23-C24-C25
3	A	4000	EPH	C11-C12-C13-C14
3	A	4000	EPH	C30-C31-C32-C33

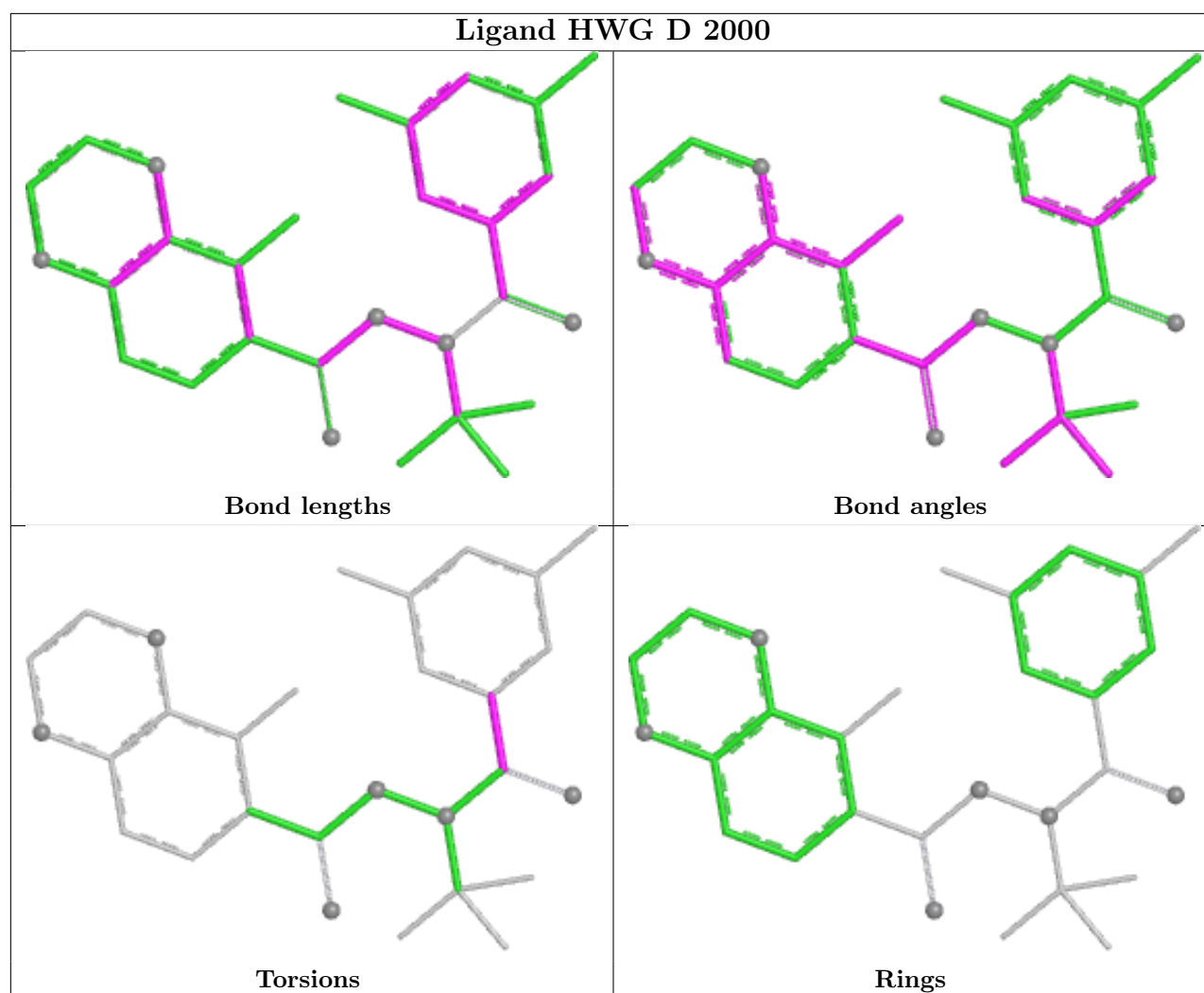
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4000	EPH	4	0
4	D	2000	HWG	12	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	239/263 (90%)	-0.36	0	100 100	34, 62, 105, 123	0
2	D	228/265 (86%)	-0.19	2 (0%)	81 61	40, 74, 128, 139	0
All	All	467/528 (88%)	-0.27	2 (0%)	88 76	34, 68, 109, 139	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	335	PRO	2.5
2	D	310	GLN	2.2

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](#)

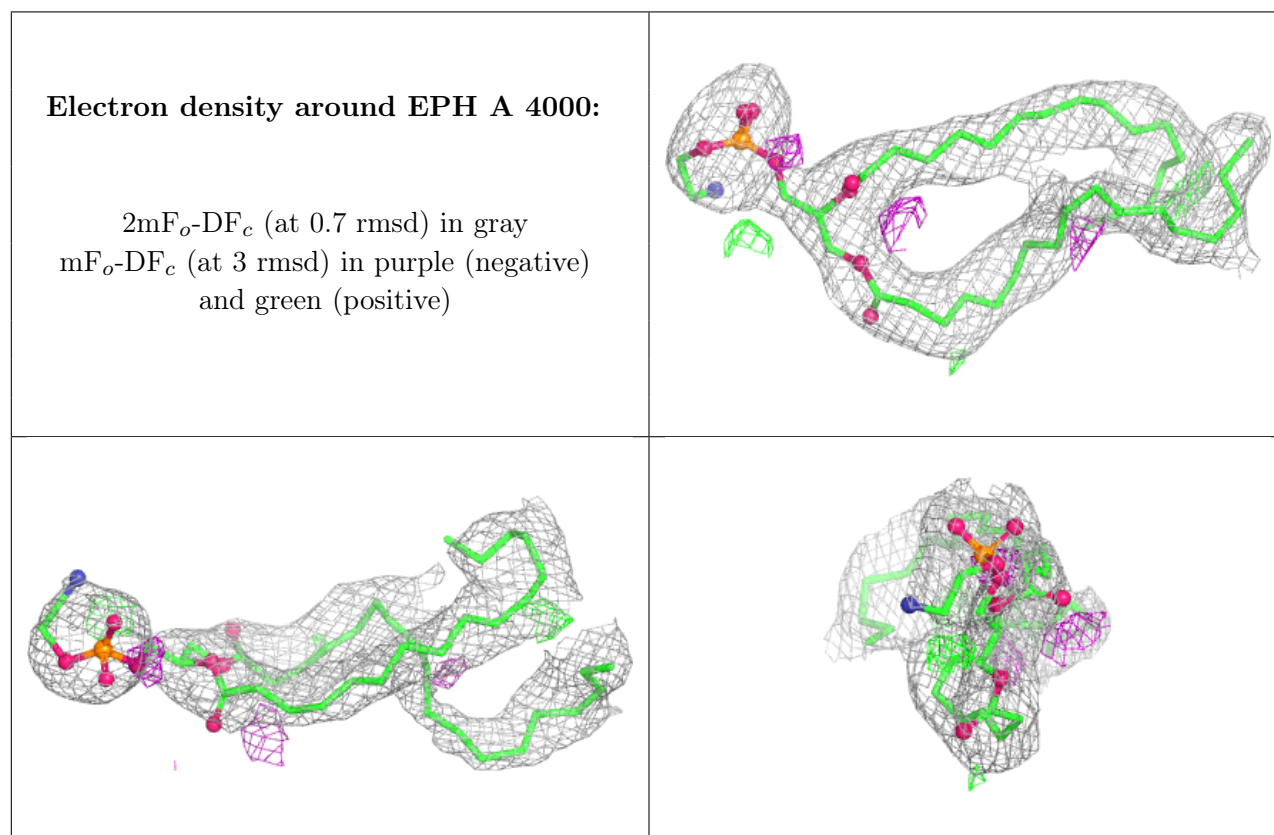
There are no oligosaccharides in this entry.

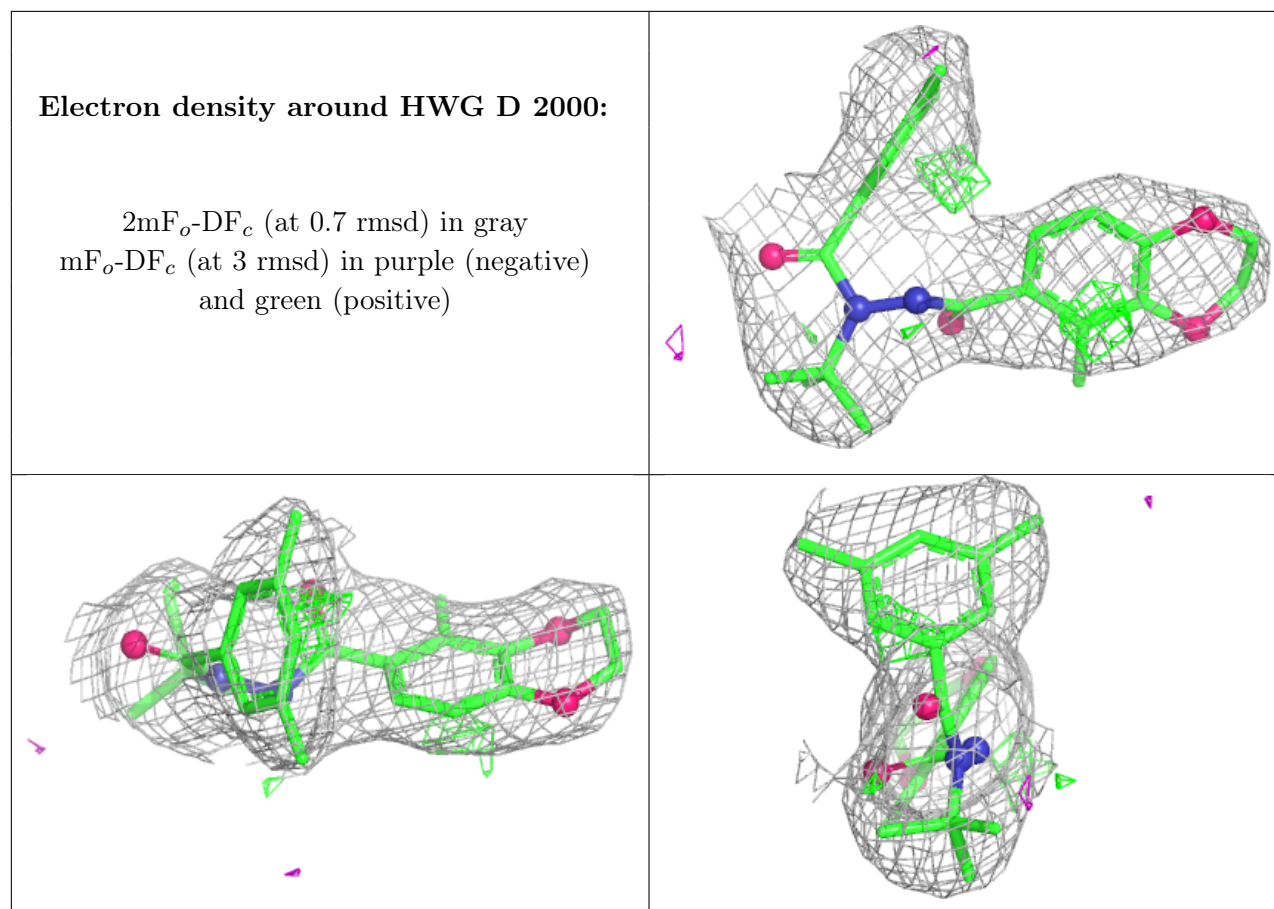
6.4 Ligands [i](#)

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
3	EPH	A	4000	49/49	0.82	0.12	79,82,100,101	0
4	HWG	D	2000	29/29	0.91	0.13	63,69,76,77	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 ⓘ

There are no such residues in this entry.