Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 03:37 PM GMT

PDB ID : 1R20
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)

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.285
Clashscore		45
Ramachandran outliers		5.2%
Sidechain outliers		14.5%
RSRZ outliers		0

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
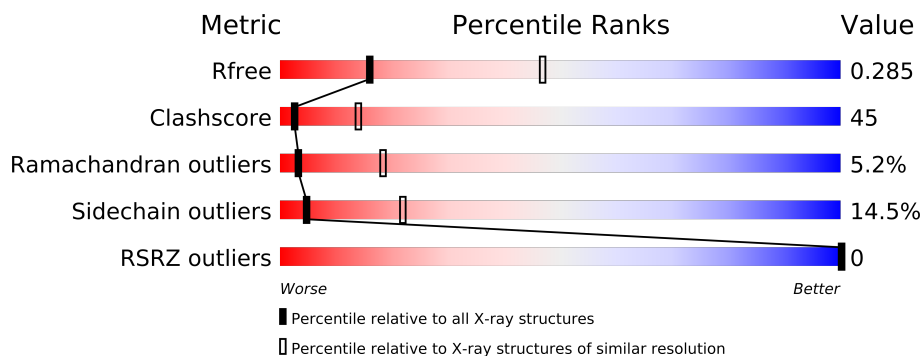
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	263	
2	D	265	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 3806 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	239	Total 1897	C 1216	N 332	O 337	S 12	0	0	0

- Molecule 2 is a protein called ECDYSONE RECEPTOR.

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

- Molecule 3 is N-(TERT-BUTYL)-3,5-DIMETHYL-N'-[(5-METHYL-2,3-DIHYDRO-1,4-BENZODIOXIN-6-YL)CARBONYL]BENZOHYDRAZIDE (three-letter code: HWG) (formula: $C_{23}H_{28}N_2O_4$).
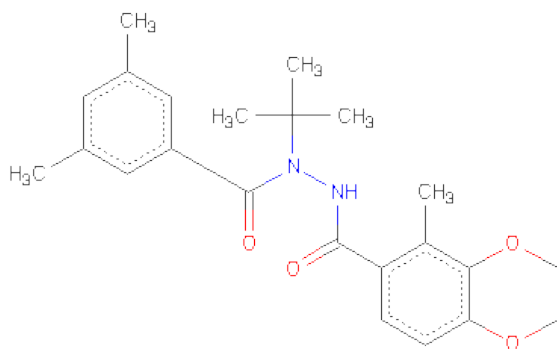
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total 29	C 23	N 2	O 4	0	0

- Molecule 4 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PH OSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: $C_{39}H_{68}NO_8P$).
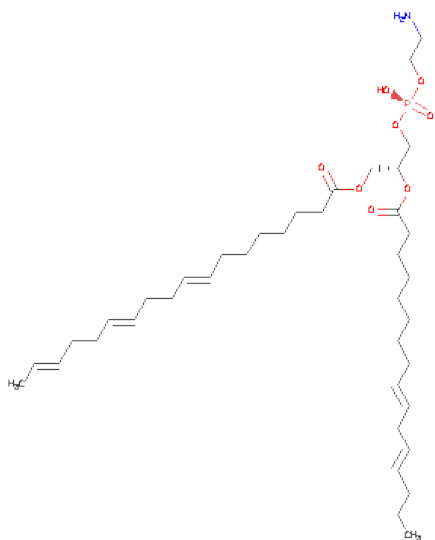
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	49	39	1	8	1	0	0

- Molecule 5 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ULTRASPIRACLE PROTEIN

Chain A:
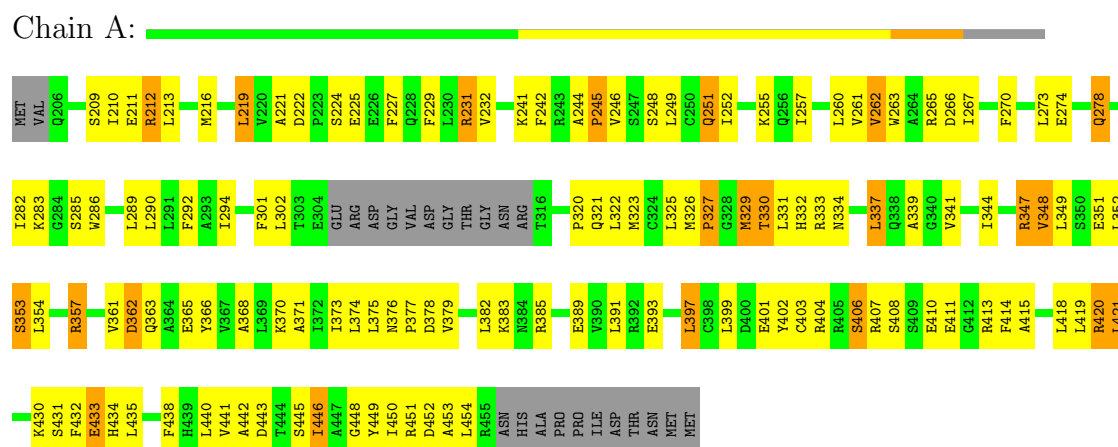
- Molecule 2: ECDYSONE RECEPTOR

Chain D:
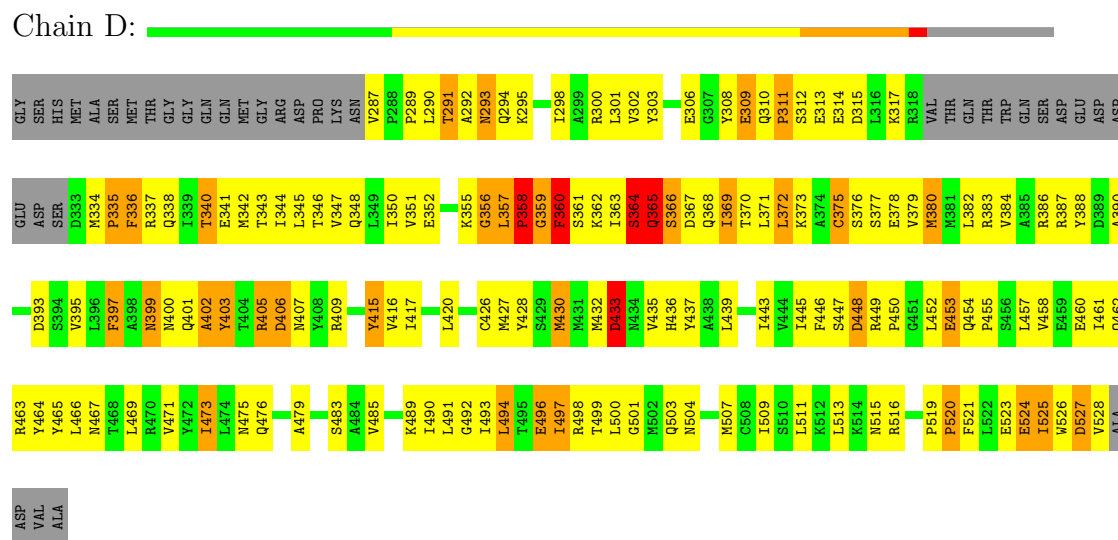
4　Data and refinement statistics (i)

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 14.84　–　3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.00) 95.5 (14.84-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.48 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244　,　0.289 0.248　,　0.285	Depositor DCC
R_{free} test set	1532 reflections (10.14%)	DCC
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 , 32.4	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Outliers	0 of 15108 reflections	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.*

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[1]Intensities estimated from amplitudes.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HWG, 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	A	0.79	1/1932 (0.1%)	0.91	0/2606
2	D	0.83	5/1852 (0.3%)	0.90	1/2505 (0.0%)
All	All	0.81	6/3784 (0.2%)	0.91	1/5111 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	360	PHE	CE1-CZ	7.10	1.50	1.37
2	D	426	CYS	CB-SG	-6.20	1.71	1.82
1	A	329	MET	SD-CE	6.17	2.12	1.77
2	D	360	PHE	CD2-CE2	5.29	1.49	1.39
2	D	364	SER	CB-OG	5.15	1.49	1.42
2	D	360	PHE	CE2-CZ	5.03	1.47	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	364	SER	CB-CA-C	-5.90	98.89	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2   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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1897	0	1933	145	1
2	D	1820	0	1837	196	0
3	D	29	0	28	10	0
4	A	49	0	67	5	0
5	A	1	0	0	0	0
5	D	10	0	0	3	0
All	All	3806	0	3865	342	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 45.

All (342) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:213:LEU:HA	1:A:216:MET:HE2	1.53	0.91
2:D:523:GLU:O	2:D:527:ASP:HA	1.71	0.91
2:D:430:MET:HE1	2:D:489:LYS:HB3	1.53	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
2:D:504:ASN:HA	3:D:2000:HWG:H343	1.55	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
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
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
2:D:375:CYS:O	2:D:379:VAL:HG12	1.80	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:262:VAL:HG22	1:A:265:ARG:NH2	1.96	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:365:GLN:NE2	2:D:365:GLN:HA	1.97	0.76
1:A:435:LEU:HB3	1:A:441:VAL:HG23	1.68	0.76
2:D:384:VAL:HG22	2:D:397:PHE:CE2	2.21	0.76
1:A:354:LEU:O	1:A:357:ARG:HB3	1.85	0.76
2:D:473:ILE:CD1	2:D:483:SER:HB2	2.16	0.75
1:A:216:MET:HA	1:A:219:LEU:CD2	2.17	0.75
2:D:291:THR:HG22	2:D:292:ALA:N	1.98	0.74
1:A:435:LEU:HD22	1:A:441:VAL:HG23	1.68	0.74
1:A:413:ARG:HH11	1:A:413:ARG:HG2	1.51	0.74
1:A:210:ILE:HD11	1:A:368:ALA:HB2	1.69	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:H	2:D:415:TYR:HD1	1.33	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
1:A:415:ALA:O	1:A:419:LEU:HG	1.89	0.73
2:D:360:PHE:O	2:D:361:SER:C	2.28	0.72
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:400:ASN:C	2:D:402:ALA:H	1.92	0.72
2:D:351:VAL:HG13	2:D:372:LEU:CD2	2.19	0.72
2:D:336:PHE:HE2	2:D:511:LEU:HD13	1.55	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:HD12	2:D:513:LEU:O	1.92	0.70
2:D:306:GLU:O	2:D:309:GLU:HB2	1.92	0.70
2:D:420:LEU:HD13	3: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:355:LYS:C	2:D:357:LEU:H	1.94	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
1:A:349:LEU:HA	1:A:353:SER:CB	2.25	0.67
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
2:D:401:GLN:H	2:D:401:GLN:NE2	1.94	0.65
2:D:345:LEU:O	2:D:348:GLN:HB2	1.96	0.65
1:A:325:LEU:HD11	1:A:331:LEU:HG	1.79	0.65
2:D:365:GLN:NE2	2:D:365:GLN:CA	2.58	0.65
2:D:397:PHE:CD2	2:D:403:TYR:HE1	2.15	0.65
2:D:504:ASN:O	2:D:507:MET:N	2.30	0.64
1:A:389:GLU:O	1:A:393:GLU:HG3	1.98	0.64
1:A:301:PHE:HB3	1:A:322:LEU:HD12	1.78	0.64
2:D:504:ASN:ND2	3: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:415:TYR:CD1	2:D:415:TYR:N	2.66	0.63
2:D:473:ILE:C	2:D:473:ILE:HD12	2.18	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
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:359:GLY:O	2:D:362:LYS:HB2	2.00	0.62
2:D:308:TYR:CE2	2:D:352:GLU:HB3	2.34	0.62
2:D:401:GLN:N	2:D:401:GLN:NE2	2.47	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	3:D:2000:HWG:H142	1.82	0.62
2:D:308:TYR:HE2	2:D:352:GLU:HB3	1.64	0.62
1:A:435:LEU:HD22	1:A:441:VAL:CG2	2.29	0.62
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
2:D:452:LEU:O	2:D:455:PRO:HD3	2.01	0.60
1:A:212:ARG:HG3	1:A:212:ARG:HH11	1.67	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:415:TYR:N	2:D:415:TYR:HD1	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
2:D:346:THR:O	2:D:350:ILE:HG13	2.02	0.59
1:A:349:LEU:O	1:A:354:LEU:N	2.29	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
1:A:231:ARG:C	1:A:231:ARG:HD3	2.24	0.58
2:D:433:ASP:N	2:D:436:HIS:HD2	2.00	0.58
2:D:287:VAL:HG23	2:D:287:VAL:O	2.02	0.57
2:D:386:ARG:NH2	2:D:433:ASP:O	2.37	0.57
2:D:400:ASN:C	2:D:402:ALA:N	2.57	0.57
2:D:334:MET:C	2:D:336:PHE:H	2.06	0.57
1:A:213:LEU:HD23	1:A:216:MET:HE1	1.86	0.57
1:A:231:ARG:O	1:A:231:ARG:HD3	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:375:CYS:SG	2:D:445:ILE:HG13	2.46	0.56
2:D:344:ILE:HG22	2:D:348:GLN:HE21	1.70	0.56
1:A:373:ILE:HG22	1:A:373:ILE:O	2.05	0.56
1:A:407:ARG:CA	1:A:407:ARG:NE	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:448:ASP:O	2:D:448:ASP:OD1	2.24	0.55
2:D:310:GLN:CG	2:D:383:ARG:HH11	2.20	0.55
2:D:433:ASP:HB2	2:D:436:HIS:CD2	2.42	0.54
2:D:290:LEU:HB2	2:D:295:LYS:HG3	1.89	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
2:D:364:SER:HG	2:D:367:ASP:H	1.56	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:302:LEU:CD1	1:A:321:GLN:N	2.71	0.54
1:A:265:ARG:NH1	1:A:454:LEU:O	2.41	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:D:336:PHE:HD2	2:D:516:ARG:HH21	1.52	0.53
1:A:441:VAL:HG12	1:A:442:ALA:N	2.22	0.53
2:D:430:MET:CE	2:D:489:LYS:HB3	2.35	0.53
1:A:438:PHE:CE1	4:A:4000:EPH:H51	2.44	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:380:MET:HB3	3:D:2000:HWG:H261	1.91	0.52
4:A:4000:EPH:H361	4:A:4000:EPH:H232	1.91	0.52
1:A:212:ARG:HG3	1:A:212:ARG:NH1	2.25	0.52
2:D:446:PHE:CB	2:D:462:GLN:HB2	2.40	0.51
1:A:341:VAL:HG12	1:A:434:HIS:CE1	2.46	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
2:D:343:THR:O	2:D:347:VAL:HG23	2.11	0.51
2:D:504:ASN:HA	3:D:2000:HWG:C34	2.33	0.51
1:A:373:ILE:O	1:A:373:ILE:CG2	2.59	0.51
1:A:401:GLU:O	1:A:402:TYR:C	2.48	0.51
2:D:294:GLN:HE22	2:D:471:VAL:HG21	1.76	0.51
2:D:466:LEU:HD21	2:D:491:LEU:HD21	1.91	0.51
2:D:449:ARG:HB3	2:D:450:PRO:HD2	1.93	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
2:D:336:PHE:CE2	2:D:511:LEU:HD13	2.43	0.50
2:D:313:GLU:N	2:D:313:GLU:OE2	2.44	0.50
1:A:448:GLY:O	1:A:451:ARG:HB3	2.11	0.50
1:A:333:ARG:HH12	1:A:337:LEU:HD23	1.76	0.50
2:D:397:PHE:C	2:D:399:ASN:N	2.62	0.50
1:A:413:ARG:NH1	1:A:413:ARG:HG2	2.23	0.50
2:D:313:GLU:C	2:D:315:ASP:H	2.13	0.50
2:D:433:ASP:N	2:D:436:HIS:CD2	2.65	0.50
1:A:246:VAL:HG11	1:A:440:LEU:HD21	1.93	0.50
1:A:371:ALA:O	1:A:375:LEU:HG	2.12	0.49
1:A:266:ASP:O	1:A:267:ILE:C	2.50	0.49
1:A:407:ARG:O	1:A:410:GLU:HB2	2.12	0.49
2:D:503:GLN:HB3	3:D:2000:HWG:C15	2.42	0.49
1:A:278:GLN:HB3	1:A:454:LEU:HD11	1.94	0.49
2:D:336:PHE:CD1	2:D:336:PHE:C	2.86	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:D:365:GLN:O	2:D:368:GLN:HG2	2.12	0.49
1:A:325:LEU:HD11	1:A:331:LEU:CG	2.42	0.49
2:D:335:PRO:C	2:D:337:ARG:N	2.65	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:260:LEU:CD2	1:A:289:LEU:HB3	2.42	0.49
1:A:453:ALA:O	1:A:454:LEU:C	2.49	0.49
1:A:302:LEU:CD1	1:A:322:LEU:N	2.65	0.48
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
1:A:326:MET:O	1:A:327:PRO:C	2.52	0.48
1:A:432:PHE:O	1:A:433:GLU:C	2.51	0.48
2:D:334:MET:O	2:D:336:PHE:N	2.44	0.48
2:D:290:LEU:C	2:D:291:THR:O	2.50	0.48
1:A:401:GLU:O	1:A:404:ARG:HG2	2.13	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:407:ARG:CA	1:A:407:ARG:HE	2.27	0.48
1:A:347:ARG:O	1:A:351:GLU:HB2	2.14	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:433:ASP:HB2	2:D:436:HIS:CG	2.49	0.47
1:A:407:ARG:HA	1:A:407:ARG:HE	1.77	0.47
1:A:273:LEU:O	1:A:274:GLU:C	2.51	0.47
2:D:308:TYR:O	2:D:310:GLN:N	2.47	0.47
2:D:341:GLU:O	2:D:342:MET:C	2.52	0.47
2:D:380:MET:HB3	3:D:2000:HWG:C26	2.44	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:461:ILE:O	2:D:464:TYR:N	2.42	0.47
2:D:356:GLY:O	2:D:358:PRO:HD3	2.15	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:401:GLN:H	2:D:401:GLN:HE21	1.63	0.46
2:D:388:TYR:OH	2:D:393:ASP:OD1	2.23	0.46
2:D:293:ASN:N	2:D:293:ASN:OD1	2.46	0.46
4:A:4000:EPH:H102	4:A:4000:EPH:H25	1.98	0.46
1:A:283:LYS:HG3	1:A:446:ILE:CG2	2.44	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:402:TYR:CD2	1:A:402:TYR:C	2.88	0.46
2:D:509:ILE:HD12	2:D:528:VAL:CB	2.45	0.46
2:D:313:GLU:C	2:D:315:ASP:N	2.69	0.46
1:A:323:MET:HE1	4:A:4000:EPH:H171	1.96	0.46
1:A:418:LEU:HD23	1:A:418:LEU:HA	1.66	0.46
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
1:A:283:LYS:HG3	1:A:446:ILE:HG22	1.97	0.46
1:A:413:ARG:CG	1:A:413:ARG:HH11	2.22	0.45
1:A:441:VAL:CG1	1:A:442:ALA:N	2.79	0.45
1:A:323:MET:HE1	1:A:331:LEU:HD12	1.99	0.45
2:D:430:MET:HB3	5:D:1010:HOH:O	2.16	0.45
1:A:362:ASP:OD1	1:A:363:GLN:N	2.49	0.45
1:A:370:LYS:O	1:A:371:ALA:C	2.55	0.45
2:D:406:ASP:O	2:D:407:ASN:C	2.52	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
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:443:ASP:HA	1:A:446:ILE:HG12	2.00	0.44
1:A:430:LYS:O	1:A:433:GLU:HB2	2.17	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
2:D:490:ILE:O	2:D:491:LEU:C	2.54	0.44
2:D:363:ILE:HG22	2:D:364:SER:N	2.32	0.44
1:A:413:ARG:CG	1:A:413:ARG:NH1	2.80	0.44
1:A:257:ILE:O	1:A:261:VAL:HG23	2.18	0.44
1:A:333:ARG:NH1	1:A:333:ARG:HG2	2.33	0.44
2:D:338:GLN:HE21	2:D:338:GLN:HB3	1.62	0.43
1:A:323:MET:CE	4:A:4000:EPH:H171	2.48	0.43
1:A:411:GLU:HA	1:A:411:GLU:OE2	2.18	0.43
2:D:309:GLU:O	2:D:310:GLN:C	2.57	0.43
1:A:365:GLU:OE2	1:A:413:ARG:CZ	2.67	0.43
1:A:362:ASP:OD2	1:A:402:TYR:OH	2.28	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:285:SER:O	1:A:286:TRP:C	2.55	0.43
2:D:376:SER:OG	2:D:377:SER:N	2.51	0.43
1:A:231:ARG:C	1:A:231:ARG:CD	2.85	0.43
2:D:519:PRO:C	2:D:521:PHE:H	2.21	0.43
1:A:301:PHE:CE1	1:A:330:THR:HB	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:370:LYS:O	1:A:373:ILE:N	2.52	0.43
2:D:335:PRO:C	2:D:337:ARG:H	2.22	0.43
1:A:302:LEU:HD13	1:A:320:PRO:HA	1.99	0.43
2:D:360:PHE:CE2	2:D:372:LEU:HD11	2.54	0.43
1:A:337:LEU:O	1:A:339:ALA:N	2.52	0.43
2:D:409:ARG:HB3	2:D:409:ARG:NH1	2.33	0.43
2:D:290:LEU:HD13	2:D:298:ILE:HD12	2.00	0.42
1:A:292:PHE:CE2	1:A:366:TYR:CD1	3.07	0.42
2:D:360:PHE:O	2:D:362:LYS:N	2.53	0.42
2:D:290:LEU:O	2:D:291:THR:O	2.37	0.42
2:D:464:TYR:O	2:D:465:TYR:C	2.56	0.42
1:A:282:ILE:HG22	1:A:450:ILE:HD13	2.01	0.42
2:D:523:GLU:HG3	2:D:524:GLU:N	2.34	0.42
2:D:503:GLN:CD	3:D:2000:HWG:H151	2.40	0.42
2:D:504:ASN:O	2:D:507:MET:HB3	2.20	0.42
2:D:473:ILE:CD1	2:D:483:SER:CB	2.91	0.42
2:D:369:ILE:HG13	2:D:369:ILE:O	2.18	0.42
2:D:369:ILE:CG1	2:D:369:ILE:O	2.68	0.42
2:D:463:ARG:HG2	2:D:463:ARG:O	2.18	0.42
1:A:337:LEU:C	1:A:339:ALA:N	2.72	0.42
1:A:399:LEU:HD23	1:A:414:PHE:CE1	2.55	0.42
1:A:420:ARG:HD3	1:A:420:ARG:HA	1.69	0.42
2:D:355:LYS:C	2:D:357:LEU:N	2.63	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: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
2:D:519:PRO:HA	2:D:520:PRO:HD3	1.92	0.41
1:A:344:ILE:HD11	1:A:431:SER:OG	2.20	0.41
2:D:399:ASN:C	2:D:400:ASN:O	2.57	0.41
1:A:379:VAL:O	1:A:382:LEU:HG	2.19	0.41
2:D:298:ILE:O	2:D:302:VAL:CG2	2.63	0.41
1:A:241:LYS:HE2	1:A:242:PHE:HE1	1.85	0.41
2:D:507:MET:CE	2:D:507:MET:HA	2.50	0.41
1:A:278:GLN:HB3	1:A:454:LEU:CD1	2.50	0.41
2:D:490:ILE:C	2:D:492:GLY:N	2.72	0.41
2:D:340:THR:O	2:D:344:ILE:CG1	2.62	0.41
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.85	0.41
1:A:333:ARG:NH1	1:A:337:LEU:HD23	2.34	0.41
1:A:241:LYS:HE2	1:A:242:PHE:CE1	2.56	0.41
1:A:241:LYS:HG3	1:A:242:PHE:CD1	2.55	0.41
1:A:229:PHE:HD2	1:A:446:ILE:HD12	1.81	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:231:ARG:O	1:A:231:ARG:CD	2.69	0.41
2:D:493:ILE:O	2:D:496:GLU:N	2.53	0.41
1:A:375:LEU:HD13	1:A:391:LEU:CB	2.48	0.41
2:D:340:THR:HG22	2:D:341:GLU:N	2.35	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
1:A:260:LEU:HD23	1:A:289:LEU:CD1	2.49	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:503:GLN:HB3	3:D:2000:HWG:H151	2.04	0.40
2:D:473:ILE:O	2:D:473:ILE:HD12	2.20	0.40
2:D:400:ASN:HB2	2:D:402:ALA:HB2	2.04	0.40
1:A:349:LEU:HA	1:A:353:SER:HB3	2.03	0.40
1:A:445:SER:O	1:A:446:ILE:C	2.60	0.40
2:D:494:LEU:HG	5:D:1003:HOH:O	2.20	0.40
2:D:367:ASP:CG	2:D:453:GLU:HB2	2.41	0.40
2:D:346:THR:HG21	2:D:380:MET:HE3	2.03	0.40
2:D:416:VAL:O	2:D:417:ILE:C	2.57	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	Distance(Å)	Clash(Å)
1:A:329:MET:SD	1:A:329:MET:SD[4_556]	2.05	0.15

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	14	54
2	D	224/265 (84%)	147 (66%)	57 (25%)	20 (9%)	1	5
All	All	459/528 (87%)	346 (75%)	89 (19%)	24 (5%)	3	18

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/232 (89%)	182 (88%)	24 (12%)	8	31
2	D	201/235 (86%)	166 (83%)	35 (17%)	3	14
All	All	407/467 (87%)	348 (86%)	59 (14%)	5	22

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	ARG
1	A	219	LEU

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Mol	Chain	Res	Type
1	A	231	ARG
1	A	232	VAL
1	A	245	PRO
1	A	251	GLN
1	A	262	VAL
1	A	278	GLN
1	A	330	THR
1	A	337	LEU
1	A	347	ARG
1	A	353	SER
1	A	357	ARG
1	A	361	VAL
1	A	362	ASP
1	A	374	LEU
1	A	385	ARG
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	452	ASP
2	D	293	ASN
2	D	300	ARG
2	D	301	LEU
2	D	303	TYR
2	D	336	PHE
2	D	340	THR
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	372	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

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Mol	Chain	Res	Type
2	D	415	TYR
2	D	427	MET
2	D	430	MET
2	D	433	ASP
2	D	447	SER
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	332	HIS
1	A	343	GLN
1	A	363	GLN
1	A	376	ASN
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	504	ASN

5.3.3　RNA ⓘ

There are no RNA chains 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	1.90	14 (29%)	53,53,53	1.87	9 (16%)
3	HWG	D	2000	-	31,31,31	3.68	10 (32%)	46,46,46	2.67	15 (32%)

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	HWG	D	2000	-	-	0/22/29/29	0/1/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2000	HWG	C12-C11	15.50	1.56	1.40
3	D	2000	HWG	C9-C10	5.75	1.52	1.40
3	D	2000	HWG	C2-C3	5.42	1.47	1.39
3	D	2000	HWG	C3-C38	5.17	1.58	1.50
4	A	4000	EPH	C25-C24	4.36	1.55	1.31
4	A	4000	EPH	C16-C15	4.35	1.55	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2000	HWG	C45-N40	4.34	1.57	1.52
4	A	4000	EPH	C1-C2	-4.28	1.38	1.50
4	A	4000	EPH	C29-C28	3.92	1.53	1.31
3	D	2000	HWG	C4-C3	3.83	1.45	1.39
4	A	4000	EPH	C13-C12	3.82	1.52	1.31
4	A	4000	EPH	C32-C33	3.76	1.56	1.29
3	D	2000	HWG	N41-N40	-3.75	1.36	1.39
4	A	4000	EPH	C22-C23	-3.28	1.40	1.52
4	A	4000	EPH	P1-O8	-2.88	1.46	1.59
3	D	2000	HWG	C39-N41	2.82	1.39	1.35
3	D	2000	HWG	C4-C5	2.73	1.44	1.38
3	D	2000	HWG	C38-N40	2.68	1.44	1.37
4	A	4000	EPH	C21-C20	-2.56	1.35	1.51
4	A	4000	EPH	C20-C19	-2.55	1.35	1.51
4	A	4000	EPH	O8-C38	2.18	1.54	1.44
4	A	4000	EPH	C18-C4	2.10	1.57	1.50
4	A	4000	EPH	C37-C2	2.08	1.56	1.50
4	A	4000	EPH	P1-O6	-2.07	1.45	1.55

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2000	HWG	O16-C10-C11	8.47	124.85	115.46
3	D	2000	HWG	O13-C9-C10	-7.35	117.02	121.91
4	A	4000	EPH	O8-P1-O5	6.59	123.47	104.68
3	D	2000	HWG	C46-C45-N40	6.38	114.59	108.85
4	A	4000	EPH	O8-P1-O7	-5.08	89.48	109.37
4	A	4000	EPH	O5-P1-O7	-4.54	91.60	109.37
3	D	2000	HWG	C11-C12-C39	4.36	123.78	120.55
4	A	4000	EPH	O6-P1-O7	-4.28	88.33	112.21
3	D	2000	HWG	C9-C10-C11	-4.16	116.61	120.82
3	D	2000	HWG	C45-N40-N41	3.92	125.05	119.37
3	D	2000	HWG	C54-C45-N40	3.87	112.33	108.85
3	D	2000	HWG	C12-C39-N41	3.67	122.01	115.46
3	D	2000	HWG	C12-C11-C10	3.67	119.68	117.35
4	A	4000	EPH	O6-P1-O8	3.57	126.50	108.51
3	D	2000	HWG	C14-O13-C9	3.45	120.72	114.18
3	D	2000	HWG	C4-C3-C2	-2.69	116.30	119.64
4	A	4000	EPH	C11-C12-C13	-2.58	110.80	125.43
4	A	4000	EPH	C1-O2-C4	2.53	124.53	117.13
3	D	2000	HWG	O13-C9-C8	2.41	120.79	116.74
4	A	4000	EPH	C17-C16-C15	-2.22	112.83	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2000	HWG	C34-C11-C10	-2.22	117.42	121.09
4	A	4000	EPH	C14-C13-C12	-2.13	111.74	124.86
3	D	2000	HWG	C7-C12-C11	-2.07	119.48	120.77
3	D	2000	HWG	O43-C39-N41	-2.03	119.25	122.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	239/263 (90%)	-0.27	0	100	100	34, 62, 105, 123	0
2	D	228/265 (86%)	-0.21	0	100	100	40, 74, 128, 139	0
All	All	467/528 (88%)	-0.24	0	100	100	34, 68, 109, 139	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å²)	Q<0.9
4	EPH	A	4000	49/49	0.23	1.19	79,82,100,101	0
3	HWG	D	2000	29/29	0.19	-0.05	63,69,76,77	0

6.5 Other polymers (i)

There are no such residues in this entry.