Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:59 AM GMT

PDB ID	:	2F4B
Title	:	Crystal structure of the ligand binding domain of human PPAR-gamma in complex with an agonist
Authors	:	Lu, I.L.; Peng, Y.H.; Mahindroo, N.; Hsieh, H.P.; Wu, S.Y.
Deposited on	:	2005-11-23
Resolution	:	2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

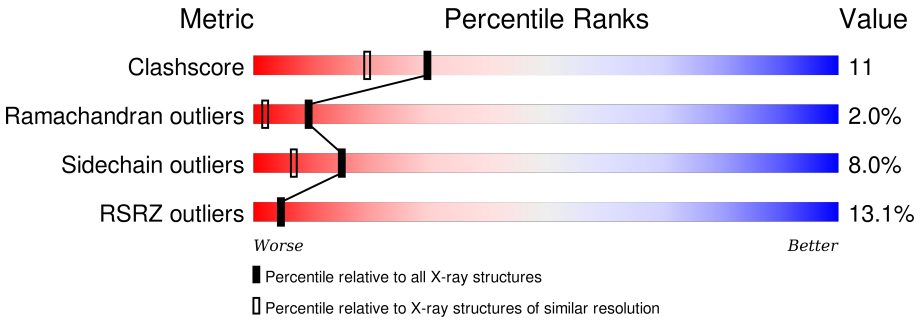
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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))
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	271	10% 71% 25%
1	B	271	16% 75% 21%

2 Entry composition

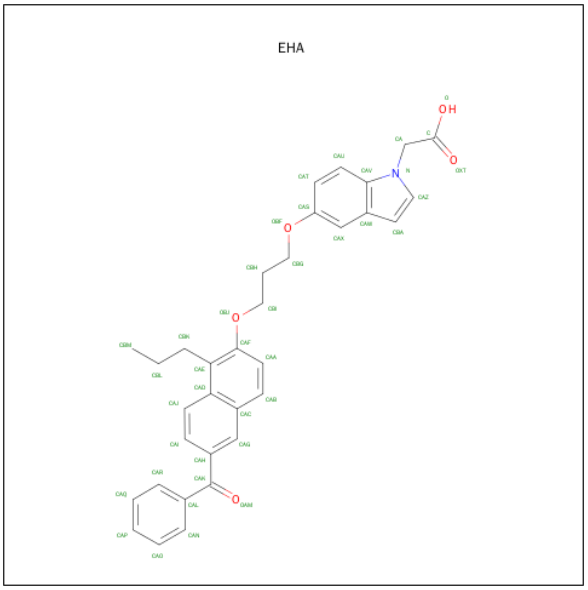
There are 3 unique types of molecules in this entry. The entry contains 4535 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2178	1406	355	407	10			
1	B	271	Total	C	N	O	S	0	0	0
			2178	1406	355	407	10			

- Molecule 2 is (5-{3-[(6-BENZOYL-1-PROPYL-2-NAPHTHYL)OXY]PROPOXY}-1H-INDOL-1-YL)ACETIC ACID (three-letter code: EHA) (formula: $C_{33}H_{31}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			39	33	1	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	59	Total	O	0	0
			59	59		

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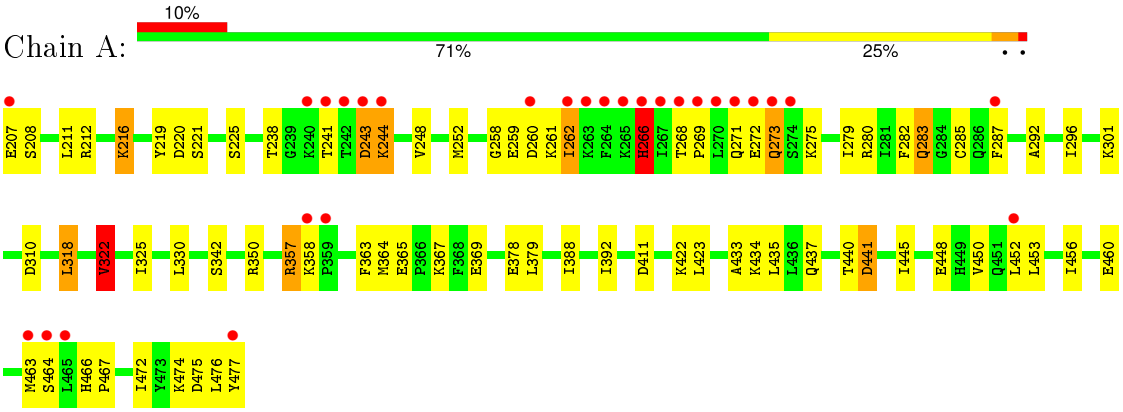
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	81	Total	O	0	0
			81	81		

3 Residue-property plots (i)

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.

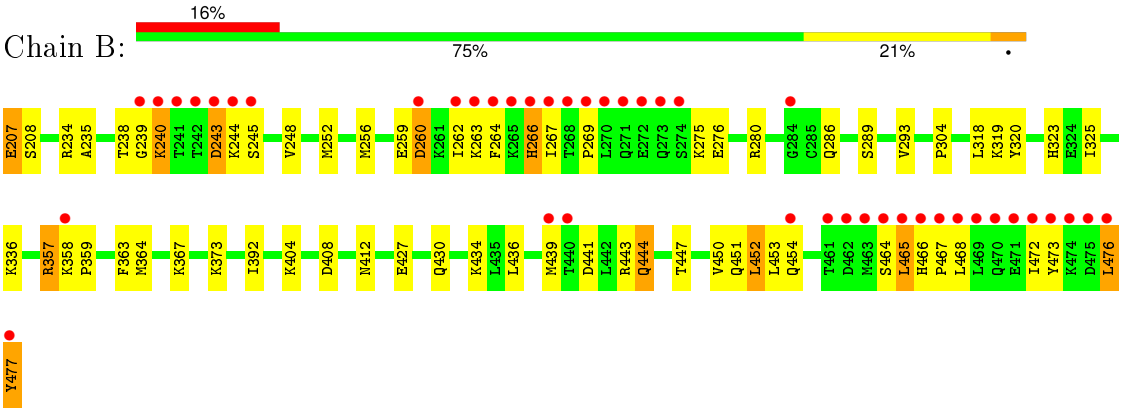
- Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain A:



- Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.97Å 88.64Å 57.88Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	30.00 – 2.07 26.69 – 2.07	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-2.07) 93.3 (26.69-2.07)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.56 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.219 , 0.288 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.9	EDS
Estimated twinning fraction	0.000 for l,k,-h 0.031 for h,-k,-l 0.022 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 33485 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4535	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: EHA

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	0.97	1/2216 (0.0%)	0.90	3/2985 (0.1%)
1	B	1.00	2/2216 (0.1%)	0.94	3/2985 (0.1%)
All	All	0.98	3/4432 (0.1%)	0.92	6/5970 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	THR	C-O	6.08	1.34	1.23
1	B	207	GLU	CD-OE1	5.87	1.32	1.25
1	A	369	GLU	CG-CD	5.07	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	266	HIS	O-C-N	-7.47	110.75	122.70
1	A	266	HIS	CA-C-O	-6.29	106.89	120.10
1	B	234	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	A	322	VAL	CG1-CB-CG2	5.84	120.24	110.90
1	B	452	LEU	CA-CB-CG	5.17	127.20	115.30
1	B	207	GLU	CG-CD-OE2	-5.15	108.00	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	HIS	Mainchain
1	A	357	ARG	Peptide
1	B	245	SER	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2178	0	2241	56	0
1	B	2178	0	2241	45	0
2	A	39	0	30	5	0
3	A	59	0	0	3	0
3	B	81	0	0	11	0
All	All	4535	0	4512	100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (100) 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:B:444:GLN:HB3	3:B:98:HOH:O	1.47	1.11
1:B:412:ASN:HB3	3:B:3:HOH:O	1.60	1.01
1:A:275:LYS:HD3	1:A:279:ILE:HG21	1.52	0.90
1:A:216:LYS:NZ	1:A:219:TYR:CD2	2.44	0.85
1:A:243:ASP:HB2	1:A:244:LYS:HG2	1.58	0.84
1:A:216:LYS:NZ	1:A:219:TYR:HD2	1.76	0.83
1:B:256:MET:HG2	3:B:129:HOH:O	1.79	0.81
1:B:243:ASP:CG	1:B:244:LYS:N	2.37	0.78
1:A:330:LEU:HD21	2:A:201:EHA:HBG1	1.63	0.78
1:A:273:GLN:HB3	1:A:280:ARG:CD	2.13	0.77
1:B:243:ASP:OD1	1:B:244:LYS:N	2.19	0.74
1:A:273:GLN:CB	1:A:280:ARG:HD3	2.18	0.73
1:A:216:LYS:HZ2	1:A:219:TYR:HD2	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.72	0.69
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.73	0.69
1:A:279:ILE:O	1:A:283:GLN:HG3	1.93	0.69
1:A:448:GLU:O	1:A:452:LEU:HD13	1.92	0.68
1:B:259:GLU:OE1	1:B:280:ARG:NH2	2.26	0.68
1:A:422:LYS:HG3	3:A:95:HOH:O	1.93	0.68
1:A:301:LYS:HD2	1:B:468:LEU:HD13	1.76	0.67
1:A:411:ASP:HB2	3:A:77:HOH:O	1.97	0.65
1:B:319:LYS:NZ	1:B:472:ILE:O	2.30	0.64
1:A:325:ILE:HG12	1:A:388:ILE:HG23	1.79	0.64
1:B:235:ALA:HA	1:B:240:LYS:HE3	1.82	0.62
1:A:279:ILE:O	1:A:283:GLN:CG	2.48	0.62
1:B:439:MET:O	1:B:443:ARG:HG3	1.99	0.62
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.31	0.60
1:A:272:GLU:O	1:A:280:ARG:HD2	2.02	0.59
1:A:441:ASP:O	1:A:445:ILE:HG12	2.02	0.59
1:B:364:MET:O	1:B:367:LYS:HB2	2.02	0.59
1:B:319:LYS:HE3	1:B:320:TYR:CZ	2.38	0.58
1:A:273:GLN:HB3	1:A:280:ARG:HD2	1.83	0.58
1:A:330:LEU:CD2	2:A:201:EHA:HBG1	2.31	0.58
1:A:262:ILE:HG23	1:A:266:HIS:HA	1.86	0.58
1:B:286:GLN:HE22	1:B:465:LEU:HB3	1.67	0.58
1:A:463:MET:HG3	1:A:464:SER:H	1.67	0.57
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.86	0.56
1:B:260:ASP:O	1:B:264:PHE:HB2	2.06	0.55
1:A:216:LYS:HE3	1:A:216:LYS:O	2.06	0.55
1:B:263:LYS:HD3	1:B:263:LYS:O	2.07	0.54
1:A:273:GLN:CB	1:A:280:ARG:CD	2.79	0.54
1:A:241:THR:OG1	1:A:243:ASP:OD1	2.25	0.54
1:B:430:GLN:O	1:B:434:LYS:HG3	2.08	0.54
1:A:280:ARG:HA	1:A:283:GLN:HG3	1.89	0.54
1:A:357:ARG:NH2	1:A:460:GLU:OE1	2.41	0.53
1:B:357:ARG:HG3	1:B:359:PRO:HD2	1.91	0.53
1:A:287:PHE:C	1:A:287:PHE:CD2	2.82	0.53
1:B:262:ILE:HB	3:B:85:HOH:O	2.08	0.53
1:B:275:LYS:HG3	1:B:276:GLU:H	1.74	0.52
1:B:427:GLU:HG2	3:B:38:HOH:O	2.09	0.51
1:B:363:PHE:CE2	1:B:364:MET:HG2	2.47	0.50
1:B:404:LYS:HE2	1:B:408:ASP:OD1	2.12	0.50
1:B:450:VAL:HG21	1:B:476:LEU:HD22	1.94	0.50
1:B:263:LYS:HA	1:B:266:HIS:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ASP:OD1	1:B:244:LYS:HG2	2.13	0.49
1:A:434:LYS:HA	1:A:437:GLN:HE21	1.78	0.49
1:A:261:LYS:O	1:A:262:ILE:C	2.51	0.48
1:B:275:LYS:HG3	1:B:276:GLU:N	2.28	0.48
1:A:357:ARG:HH22	1:A:460:GLU:CD	2.16	0.48
1:A:318:LEU:O	1:A:322:VAL:HB	2.14	0.48
1:A:330:LEU:HD21	2:A:201:EHA:CBG	2.39	0.48
1:B:451:GLN:HG3	1:B:477:TYR:OXT	2.13	0.47
1:B:451:GLN:O	1:B:454:GLN:HB2	2.14	0.47
1:A:363:PHE:HE2	1:A:456:ILE:HD11	1.79	0.47
1:B:434:LYS:HE3	3:B:140:HOH:O	2.16	0.45
1:B:275:LYS:NZ	3:B:88:HOH:O	2.50	0.45
1:A:259:GLU:C	1:A:261:LYS:H	2.20	0.44
1:A:466:HIS:CG	1:A:467:PRO:HD2	2.52	0.44
1:A:272:GLU:O	1:A:273:GLN:HB3	2.17	0.44
1:B:289:SER:O	1:B:293:VAL:HG23	2.17	0.44
1:B:466:HIS:HA	1:B:467:PRO:HD3	1.89	0.44
1:A:258:GLY:O	1:A:261:LYS:HB2	2.18	0.44
1:B:467:PRO:HD3	3:B:127:HOH:O	2.16	0.44
1:A:364:MET:SD	2:A:201:EHA:HBH1	2.58	0.43
1:A:433:ALA:O	1:A:437:GLN:HG3	2.19	0.43
1:B:235:ALA:HB3	3:B:125:HOH:O	2.18	0.43
3:A:50:HOH:O	1:B:466:HIS:CE1	2.71	0.43
1:A:216:LYS:CE	1:A:216:LYS:O	2.67	0.43
1:A:279:ILE:O	1:A:283:GLN:HG2	2.19	0.43
1:A:350:ARG:NH2	1:A:365:GLU:OE2	2.41	0.43
1:A:325:ILE:HG12	1:A:388:ILE:HD12	2.01	0.42
2:A:201:EHA:HBI1	2:A:201:EHA:HAA	1.76	0.42
1:B:373:LYS:HB2	3:B:68:HOH:O	2.19	0.42
1:A:310:ASP:OD2	1:B:269:PRO:HD2	2.20	0.42
1:B:262:ILE:HD12	3:B:72:HOH:O	2.19	0.42
1:B:476:LEU:HD23	1:B:477:TYR:H	1.84	0.42
1:A:266:HIS:N	1:A:266:HIS:CD2	2.87	0.42
1:B:266:HIS:HB3	1:B:267:ILE:H	1.59	0.42
1:A:474:LYS:O	1:A:475:ASP:C	2.58	0.42
1:A:207:GLU:O	1:A:211:LEU:HG	2.20	0.42
1:B:436:LEU:O	1:B:439:MET:HB2	2.20	0.41
1:A:273:GLN:HB2	1:A:280:ARG:HD3	1.99	0.41
1:A:450:VAL:O	1:A:453:LEU:HB2	2.20	0.41
1:A:212:ARG:HD3	1:A:423:LEU:HD11	2.03	0.41
1:B:319:LYS:HG3	1:B:472:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ILE:O	1:A:476:LEU:HD13	2.20	0.41
1:A:282:PHE:O	1:A:285:CYS:HB2	2.21	0.41
1:A:325:ILE:HG23	1:A:388:ILE:HD12	2.03	0.40
1:A:292:ALA:O	1:A:296:ILE:HG13	2.22	0.40
1:B:444:GLN:HA	1:B:447:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	269/271 (99%)	249 (93%)	13 (5%)	7 (3%)	7 1
1	B	269/271 (99%)	254 (94%)	11 (4%)	4 (2%)	13 4
All	All	538/542 (99%)	503 (94%)	24 (4%)	11 (2%)	9 2

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	ILE
1	B	266	HIS
1	A	260	ASP
1	B	473	TYR
1	A	271	GLN
1	B	239	GLY
1	A	358	LYS
1	B	243	ASP
1	A	244	LYS
1	A	269	PRO
1	A	273	GLN

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	244/244 (100%)	225 (92%)	19 (8%)	16 7
1	B	244/244 (100%)	224 (92%)	20 (8%)	14 6
All	All	488/488 (100%)	449 (92%)	39 (8%)	15 7

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	SER
1	A	216	LYS
1	A	220	ASP
1	A	221	SER
1	A	225	SER
1	A	238	THR
1	A	243	ASP
1	A	248	VAL
1	A	252	MET
1	A	268	THR
1	A	283	GLN
1	A	318	LEU
1	A	322	VAL
1	A	342	SER
1	A	367	LYS
1	A	378	GLU
1	A	440	THR
1	A	441	ASP
1	A	477	TYR
1	B	207	GLU
1	B	208	SER
1	B	240	LYS
1	B	248	VAL
1	B	252	MET
1	B	260	ASP
1	B	304	PRO
1	B	318	LEU

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Mol	Chain	Res	Type
1	B	323	HIS
1	B	336	LYS
1	B	357	ARG
1	B	358	LYS
1	B	441	ASP
1	B	444	GLN
1	B	452	LEU
1	B	453	LEU
1	B	464	SER
1	B	465	LEU
1	B	476	LEU
1	B	477	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	A	294	GLN
1	A	437	GLN
1	A	451	GLN
1	B	273	GLN
1	B	283	GLN
1	B	286	GLN
1	B	466	HIS
1	B	470	GLN

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 (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EHA	A	201	-	40,43,43	1.57	5 (12%)	51,59,59	0.97	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EHA	A	201	-	-	0/21/23/23	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	EHA	CAV-N	-4.42	1.34	1.39
2	A	201	EHA	CAZ-N	-3.06	1.34	1.38
2	A	201	EHA	CAF-CAE	2.59	1.41	1.38
2	A	201	EHA	CAH-CAK	3.37	1.55	1.49
2	A	201	EHA	CAL-CAK	4.19	1.56	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	EHA	CAJ-CAD-CAE	-2.30	119.86	122.72
2	A	201	EHA	OBF-CBG-CBH	2.23	117.04	108.39
2	A	201	EHA	CBA-CAW-CAV	2.31	108.17	106.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	EHA	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	271/271 (100%)	0.68	28 (10%)	9 9	17, 33, 69, 99	0
1	B	271/271 (100%)	1.12	43 (15%)	3 2	15, 31, 99, 130	0
All	All	542/542 (100%)	0.90	71 (13%)	5 5	15, 32, 94, 130	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	476	LEU	16.1
1	B	477	TYR	13.2
1	A	264	PHE	12.7
1	A	270	LEU	12.3
1	A	269	PRO	12.2
1	A	267	ILE	12.1
1	B	465	LEU	11.6
1	B	472	ILE	11.1
1	B	468	LEU	9.9
1	B	473	TYR	9.8
1	A	262	ILE	9.7
1	B	241	THR	9.3
1	B	264	PHE	9.1
1	A	266	HIS	8.9
1	B	475	ASP	8.8
1	B	267	ILE	8.3
1	B	474	LYS	8.2
1	B	268	THR	7.4
1	B	463	MET	7.1
1	A	242	THR	7.0
1	A	265	LYS	6.9
1	B	266	HIS	6.8
1	B	469	LEU	6.5
1	B	274	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	270	LEU	6.1
1	B	467	PRO	6.1
1	B	471	GLU	5.8
1	B	273	GLN	5.8
1	A	272	GLU	5.7
1	B	260	ASP	5.5
1	B	269	PRO	5.5
1	B	242	THR	5.4
1	B	470	GLN	5.4
1	B	265	LYS	5.4
1	B	243	ASP	5.4
1	B	239	GLY	5.3
1	A	271	GLN	4.7
1	B	272	GLU	4.7
1	A	274	SER	4.7
1	B	262	ILE	4.6
1	B	466	HIS	4.5
1	A	244	LYS	4.4
1	A	263	LYS	4.2
1	A	477	TYR	4.2
1	B	461	THR	4.2
1	B	240	LYS	4.1
1	A	241	THR	4.0
1	B	454	GLN	3.7
1	A	260	ASP	3.5
1	B	358	LYS	3.4
1	B	244	LYS	3.3
1	A	273	GLN	3.2
1	A	465	LEU	3.1
1	A	243	ASP	3.1
1	B	464	SER	3.0
1	A	268	THR	2.9
1	A	463	MET	2.8
1	A	464	SER	2.8
1	A	358	LYS	2.8
1	A	452	LEU	2.7
1	B	440	THR	2.6
1	A	207	GLU	2.5
1	B	462	ASP	2.5
1	B	263	LYS	2.5
1	A	287	PHE	2.4
1	B	271	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	240	LYS	2.3
1	A	359	PRO	2.2
1	B	245	SER	2.1
1	B	284	GLY	2.1
1	B	439	MET	2.1

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	EHA	A	201	39/39	0.73	0.23	0.58	58,62,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.