



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:19 AM GMT

PDB ID : 3ADW  
Title : Human PPARgamma ligand-binding domain in complex with 5-methoxy-indole acetate and 15-oxo-eicosatetraenoic acid  
Authors : Waku, T.; Shiraki, T.; Oyama, T.; Morikawa, K.  
Deposited on : 2010-01-29  
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](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 (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

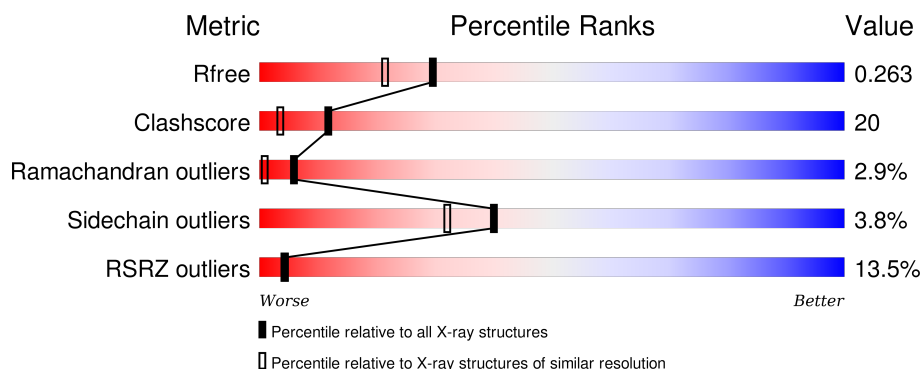
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1799 (2.08-2.04)
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  $\geq 3$ , 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	A	287	
1	B	287	

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
2	MYI	A	3	-	-	-	X
3	OCR	A	1	-	-	-	X
3	OCR	B	2	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4466 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.

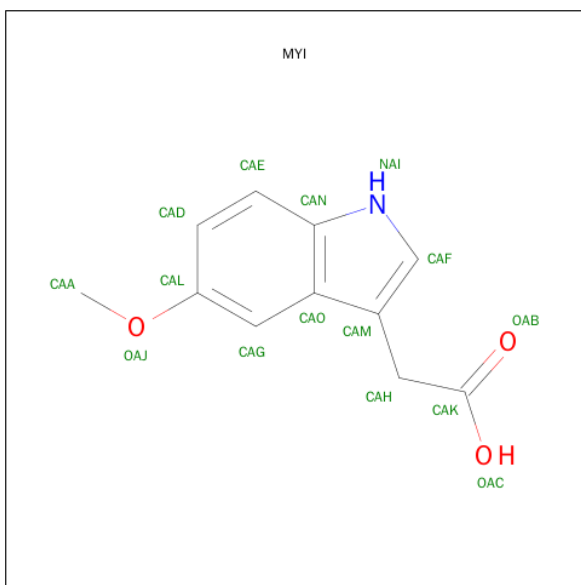
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2197	1417	360	410	10			
1	B	260	Total	C	N	O	S	0	0	0
			2088	1351	343	385	9			

There are 8 discrepancies between the modelled and reference sequences:

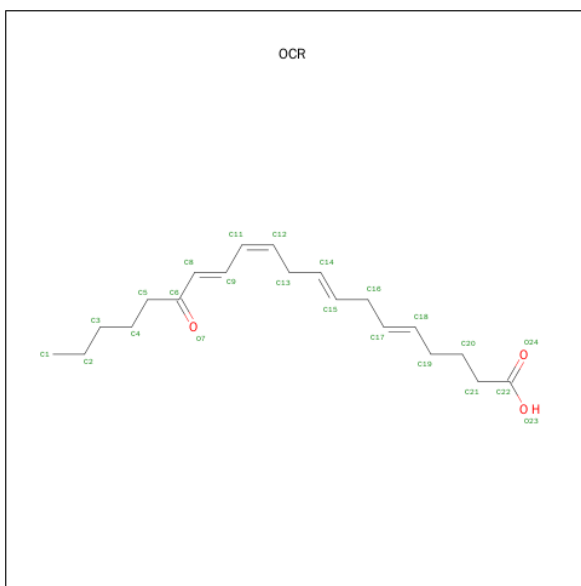
Chain	Residue	Modelled	Actual	Comment	Reference
A	191	GLY	-	EXPRESSION TAG	UNP P37231
A	192	SER	-	EXPRESSION TAG	UNP P37231
A	193	HIS	-	EXPRESSION TAG	UNP P37231
A	194	MET	-	EXPRESSION TAG	UNP P37231
B	191	GLY	-	EXPRESSION TAG	UNP P37231
B	192	SER	-	EXPRESSION TAG	UNP P37231
B	193	HIS	-	EXPRESSION TAG	UNP P37231
B	194	MET	-	EXPRESSION TAG	UNP P37231

- Molecule 2 is (5-METHOXY-1H-INDOL-3-YL)ACETIC ACID (three-letter code: MYI) (formula: C<sub>11</sub>H<sub>11</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	1	3		

- Molecule 3 is (5E,8E,11Z,13E)-15-OXOICOSA-5,8,11,13-TETRAENOIC ACID (three-letter code: OCR) (formula: C<sub>20</sub>H<sub>30</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	20	3		
3	B	1	Total	C	O	0	0
			23	20	3		

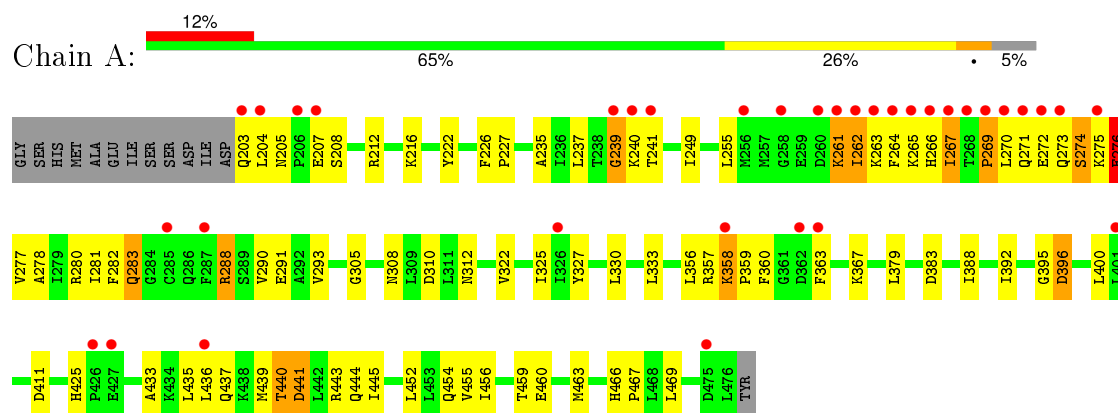
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total 59	O 59	0	0
4	B	61	Total 61	O 61	0	0

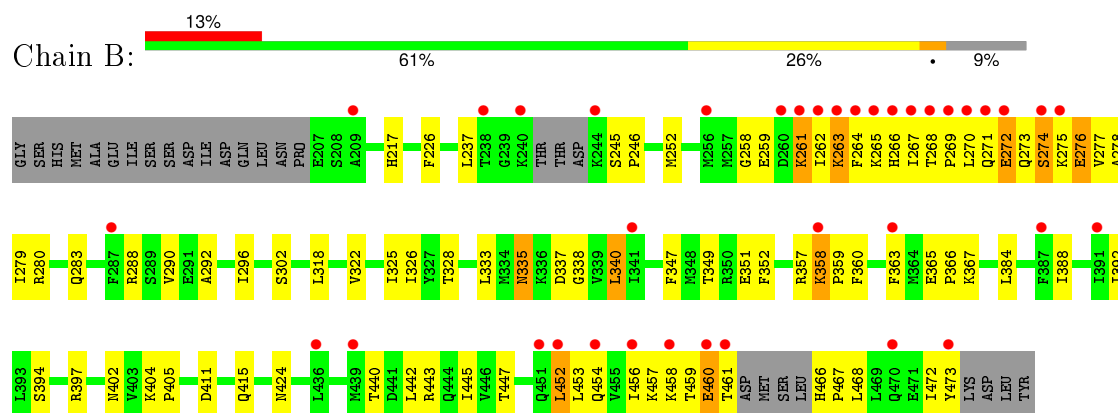
### 3 Residue-property plots

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: Peroxisome proliferator-activated receptor gamma



- Molecule 1: Peroxisome proliferator-activated receptor gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.03Å 61.18Å 118.47Å 90.00° 102.84° 90.00°	Depositor
Resolution (Å)	29.00 – 2.07 28.98 – 2.07	Depositor EDS
% Data completeness (in resolution range)	93.2 (29.00-2.07) 93.1 (28.98-2.07)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.06Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.230 , 0.265 0.228 , 0.263	Depositor DCC
$R_{free}$ test set	1850 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 38750 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MYI, OCR

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	0.37	0/2235	0.56	0/3013
1	B	0.36	0/2123	0.55	0/2857
All	All	0.37	0/4358	0.56	0/5870

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	TYR	Sidechain

### 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	2197	0	2263	85	0
1	B	2088	0	2154	96	0
2	A	15	0	10	1	0
3	A	23	0	28	5	0
3	B	23	0	28	6	0
4	A	59	0	0	1	0
4	B	61	0	0	1	0
All	All	4466	0	4483	178	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 20.

All (178) 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:358:LYS:HB3	1:B:359:PRO:HD2	1.34	1.08
1:B:358:LYS:HB3	1:B:359:PRO:CD	1.82	1.06
1:B:261:LYS:HA	1:B:261:LYS:HE3	1.39	1.05
1:B:349:THR:HG22	1:B:352:PHE:H	1.23	1.00
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.47	0.93
1:B:442:LEU:O	1:B:445:ILE:HG22	1.75	0.86
1:A:459:THR:HG23	1:A:460:GLU:HG2	1.57	0.85
1:B:335:ASN:C	1:B:335:ASN:HD22	1.81	0.82
1:A:240:LYS:HG3	1:A:241:THR:H	1.44	0.81
1:B:357:ARG:HH11	1:B:358:LYS:HB2	1.45	0.80
1:B:335:ASN:ND2	1:B:337:ASP:H	1.80	0.79
1:B:267:ILE:HD11	1:B:280:ARG:O	1.86	0.74
1:B:268:THR:OG1	1:B:269:PRO:HD3	1.87	0.73
1:B:357:ARG:HH11	1:B:358:LYS:CB	2.02	0.72
1:B:443:ARG:O	1:B:447:THR:HG23	1.88	0.72
1:A:212:ARG:O	1:A:216:LYS:HG2	1.90	0.70
1:A:437:GLN:O	1:A:440:THR:HG23	1.92	0.69
1:A:261:LYS:HD2	1:A:262:ILE:HG23	1.74	0.68
1:B:288:ARG:HE	3:B:2:OCR:C19	2.07	0.68
1:A:267:ILE:HD13	1:A:267:ILE:O	1.94	0.67
1:B:290:VAL:HG21	1:B:473:TYR:CD1	2.30	0.67
1:A:203:GLN:HG3	1:A:204:LEU:HD13	1.76	0.66
1:B:357:ARG:HD2	1:B:358:LYS:HB2	1.77	0.66
1:A:263:LYS:HE2	1:A:265:LYS:HE3	1.77	0.66
1:B:404:LYS:HB3	1:B:405:PRO:HD3	1.78	0.66
1:B:358:LYS:CB	1:B:359:PRO:CD	2.70	0.65
1:B:402:ASN:O	1:B:405:PRO:HD2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ASN:ND2	1:B:338:GLY:H	1.94	0.65
1:B:217:HIS:HE1	1:B:302:SER:O	1.79	0.65
1:B:349:THR:HG22	1:B:352:PHE:N	2.06	0.64
1:A:441:ASP:O	1:A:445:ILE:HG12	1.96	0.64
1:B:258:GLY:O	1:B:262:ILE:HG13	1.97	0.64
1:B:267:ILE:HD12	1:B:273:GLN:OE1	1.98	0.63
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.63	0.63
1:B:226:PHE:HE1	1:B:296:ILE:HD13	1.64	0.63
1:B:358:LYS:HD2	1:B:359:PRO:HD3	1.79	0.63
1:B:360:PHE:CE1	1:B:456:ILE:HD11	2.34	0.62
1:B:325:ILE:HG23	1:B:388:ILE:HD12	1.82	0.62
1:A:273:GLN:O	1:A:273:GLN:HG2	1.98	0.62
1:A:249:ILE:HD11	1:A:262:ILE:HD11	1.82	0.61
1:A:290:VAL:HG21	1:A:466:HIS:CD2	2.35	0.60
1:B:264:PHE:O	1:B:266:HIS:N	2.33	0.59
1:A:456:ILE:HA	1:A:459:THR:HG22	1.84	0.59
1:A:433:ALA:O	1:A:437:GLN:HG3	2.02	0.59
1:B:357:ARG:CD	1:B:358:LYS:HB2	2.31	0.59
1:B:367:LYS:HD3	1:B:445:ILE:HD11	1.84	0.59
1:A:443:ARG:HG3	1:B:440:THR:CG2	2.33	0.59
1:B:296:ILE:HD12	1:B:325:ILE:HG21	1.83	0.59
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.84	0.58
1:B:226:PHE:CE1	1:B:296:ILE:HD13	2.39	0.58
1:B:335:ASN:ND2	1:B:337:ASP:N	2.52	0.57
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.28	0.57
1:A:325:ILE:HD13	1:A:388:ILE:HG23	1.87	0.56
1:B:290:VAL:HG21	1:B:473:TYR:HD1	1.69	0.56
1:A:205:ASN:ND2	1:A:207:GLU:HB2	2.22	0.55
1:B:456:ILE:HG22	1:B:457:LYS:HD2	1.88	0.55
1:B:252:MET:SD	1:B:277:VAL:HG11	2.47	0.55
1:B:468:LEU:O	1:B:472:ILE:HG13	2.06	0.55
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.37	0.55
1:B:335:ASN:C	1:B:335:ASN:ND2	2.55	0.54
1:A:274:SER:HB3	1:A:280:ARG:HG3	1.90	0.54
1:B:359:PRO:HB2	1:B:452:LEU:HD21	1.90	0.54
1:B:453:LEU:O	1:B:456:ILE:HG22	2.08	0.54
1:A:240:LYS:HG3	1:A:241:THR:N	2.18	0.54
1:A:277:VAL:HG13	1:A:278:ALA:N	2.23	0.53
1:A:282:PHE:CZ	2:A:3:MYI:HAD	2.42	0.53
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.90	0.53
1:A:383:ASP:OD2	1:A:425:HIS:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.92	0.52
1:B:349:THR:CG2	1:B:352:PHE:H	2.08	0.52
1:A:208:SER:O	1:A:212:ARG:HG2	2.09	0.52
1:B:333:LEU:CD2	3:B:2:OCR:H20	2.40	0.52
1:B:277:VAL:HG23	1:B:278:ALA:N	2.25	0.52
1:A:264:PHE:O	1:A:266:HIS:N	2.39	0.52
1:A:237:LEU:C	1:A:239:GLY:H	2.11	0.52
1:B:453:LEU:C	1:B:457:LYS:HZ2	2.12	0.52
1:B:333:LEU:HD23	3:B:2:OCR:H20	1.90	0.52
1:B:328:THR:OG1	1:B:442:LEU:HD11	2.11	0.51
1:A:436:LEU:HA	1:A:439:MET:HE2	1.92	0.51
1:B:288:ARG:HE	3:B:2:OCR:H19	1.74	0.51
1:A:275:LYS:O	1:A:276:GLU:HB2	2.09	0.51
1:B:411:ASP:O	1:B:415:GLN:HG3	2.11	0.51
1:A:205:ASN:HD21	1:A:207:GLU:HB2	1.75	0.51
1:A:203:GLN:HG3	1:A:204:LEU:CD1	2.40	0.51
1:B:454:GLN:OE1	1:B:454:GLN:HA	2.11	0.50
1:B:360:PHE:O	1:B:363:PHE:HD1	1.94	0.50
1:B:288:ARG:HE	3:B:2:OCR:H19A	1.73	0.50
1:B:259:GLU:O	1:B:263:LYS:HA	2.11	0.50
1:A:203:GLN:HG3	1:A:204:LEU:N	2.26	0.50
1:A:273:GLN:C	1:A:275:LYS:H	2.15	0.50
1:B:367:LYS:HA	1:B:445:ILE:HD11	1.93	0.50
1:A:263:LYS:O	1:A:263:LYS:HD2	2.12	0.49
1:A:272:GLU:HG2	1:A:273:GLN:H	1.77	0.49
1:A:357:ARG:NH2	1:A:360:PHE:HE1	2.10	0.49
1:A:277:VAL:O	1:A:281:ILE:HG12	2.12	0.49
1:B:363:PHE:O	1:B:367:LYS:HE2	2.12	0.49
1:B:357:ARG:HH11	1:B:358:LYS:CG	2.24	0.49
1:B:453:LEU:HD22	1:B:457:LYS:HZ1	1.77	0.49
1:A:293:VAL:HG22	1:A:322:VAL:CG1	2.43	0.49
1:B:335:ASN:HD21	1:B:338:GLY:N	2.10	0.49
1:B:279:ILE:HG23	1:B:461:THR:HB	1.95	0.49
1:A:262:ILE:O	1:A:262:ILE:HG13	2.13	0.48
1:B:466:HIS:N	1:B:467:PRO:CD	2.75	0.48
1:A:455:VAL:O	1:A:459:THR:HG22	2.14	0.48
1:A:456:ILE:HG21	1:A:463:MET:HE1	1.95	0.48
1:B:335:ASN:ND2	1:B:338:GLY:N	2.61	0.48
1:B:237:LEU:HD21	1:B:340:LEU:HD13	1.96	0.48
1:B:367:LYS:CD	1:B:445:ILE:HD11	2.43	0.48
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:HG2	1:A:273:GLN:OE1	2.15	0.47
1:B:277:VAL:HG23	1:B:278:ALA:H	1.79	0.47
1:A:456:ILE:HA	1:A:459:THR:CG2	2.45	0.47
1:B:456:ILE:C	1:B:458:LYS:H	2.17	0.47
1:B:261:LYS:CE	1:B:261:LYS:HA	2.22	0.47
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.45	0.47
1:B:365:GLU:HB3	1:B:366:PRO:HD3	1.97	0.46
1:A:288:ARG:NH1	3:A:1:OCR:H20A	2.30	0.46
1:A:395:GLY:HA2	1:A:400:LEU:CD1	2.46	0.46
1:A:357:ARG:HG2	1:A:357:ARG:HH11	1.81	0.46
1:B:273:GLN:CG	1:B:283:GLN:HE22	2.29	0.46
1:A:443:ARG:HG3	1:B:440:THR:HG21	1.97	0.46
1:B:340:LEU:O	3:B:2:OCR:H21A	2.15	0.46
1:B:459:THR:O	1:B:460:GLU:HB2	2.15	0.45
1:B:394:SER:O	1:B:397:ARG:HG2	2.16	0.45
1:A:363:PHE:CZ	1:A:452:LEU:HB3	2.51	0.45
1:A:277:VAL:HG13	1:A:278:ALA:H	1.80	0.45
1:B:322:VAL:O	1:B:326:ILE:HG13	2.16	0.45
1:B:274:SER:O	1:B:276:GLU:N	2.50	0.45
1:A:273:GLN:H	1:A:273:GLN:CD	2.19	0.45
1:A:269:PRO:HD2	1:A:283:GLN:HB3	1.99	0.44
1:B:335:ASN:HD22	1:B:337:ASP:H	1.60	0.44
1:A:255:LEU:CD1	1:A:277:VAL:HG23	2.47	0.44
1:A:396:ASP:CG	1:A:396:ASP:O	2.55	0.44
1:B:453:LEU:HD22	1:B:457:LYS:NZ	2.33	0.44
1:A:288:ARG:NH1	3:A:1:OCR:H18	2.33	0.44
1:A:436:LEU:HD22	1:A:439:MET:HE1	1.99	0.44
1:B:274:SER:C	1:B:276:GLU:N	2.71	0.44
1:A:363:PHE:CZ	1:A:456:ILE:HG13	2.53	0.43
1:A:288:ARG:HH11	3:A:1:OCR:C18	2.31	0.43
1:B:357:ARG:NH1	1:B:358:LYS:HG3	2.32	0.43
1:A:235:ALA:HA	1:A:240:LYS:NZ	2.32	0.43
1:A:203:GLN:HG3	1:A:204:LEU:H	1.81	0.43
1:B:245:SER:HA	1:B:246:PRO:HD3	1.86	0.43
1:A:466:HIS:HA	1:A:467:PRO:HD3	1.83	0.43
1:A:333:LEU:HD11	3:A:1:OCR:H20	2.00	0.43
1:A:357:ARG:O	1:A:358:LYS:C	2.58	0.42
1:A:288:ARG:HH21	1:A:291:GLU:CG	2.32	0.42
1:A:288:ARG:HH21	1:A:291:GLU:HG2	1.84	0.42
1:A:379:LEU:HD11	1:A:435:LEU:HD13	2.01	0.42
1:A:275:LYS:O	1:A:276:GLU:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ALA:O	1:B:296:ILE:HG12	2.20	0.42
1:A:325:ILE:CD1	1:A:388:ILE:HG23	2.49	0.42
1:B:271:GLN:O	1:B:272:GLU:C	2.58	0.42
1:B:453:LEU:O	1:B:457:LYS:NZ	2.47	0.42
1:B:360:PHE:CZ	1:B:456:ILE:HD11	2.54	0.42
1:B:466:HIS:HB3	1:B:467:PRO:HD3	2.01	0.42
1:A:395:GLY:HA2	1:A:400:LEU:HD13	2.02	0.42
1:A:226:PHE:HA	1:A:227:PRO:HD3	1.92	0.42
1:A:454:GLN:HA	1:A:454:GLN:NE2	2.35	0.42
1:A:263:LYS:C	1:A:263:LYS:HD2	2.40	0.41
1:A:330:LEU:HD13	3:A:1:OCR:C16	2.50	0.41
1:B:453:LEU:O	1:B:457:LYS:HD2	2.20	0.41
1:B:266:HIS:HB3	1:B:267:ILE:H	1.62	0.41
1:B:384:LEU:O	1:B:388:ILE:HG12	2.20	0.41
1:A:443:ARG:HG3	1:B:440:THR:HG23	2.01	0.41
1:A:452:LEU:O	1:A:456:ILE:HG12	2.21	0.41
1:B:273:GLN:CD	1:B:280:ARG:HG2	2.40	0.41
1:B:349:THR:HG23	4:B:1072:HOH:O	2.21	0.41
1:A:356:LEU:O	1:A:357:ARG:HB2	2.21	0.41
1:B:290:VAL:CG2	1:B:473:TYR:HD1	2.33	0.41
1:B:402:ASN:OD1	1:B:405:PRO:HD3	2.21	0.41
1:A:227:PRO:HD2	4:A:1066:HOH:O	2.21	0.41
1:A:310:ASP:OD1	1:A:312:ASN:N	2.52	0.41
1:A:273:GLN:C	1:A:275:LYS:N	2.74	0.40
1:A:269:PRO:O	1:A:271:GLN:N	2.54	0.40
1:A:275:LYS:O	1:A:275:LYS:CD	2.70	0.40
1:B:349:THR:HG22	1:B:351:GLU:N	2.37	0.40
1:A:327:TYR:CE2	1:A:367:LYS:HE3	2.56	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	272/287 (95%)	250 (92%)	14 (5%)	8 (3%)	6	1
1	B	254/287 (88%)	233 (92%)	14 (6%)	7 (3%)	6	1
All	All	526/574 (92%)	483 (92%)	28 (5%)	15 (3%)	6	1

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	LEU
1	A	276	GLU
1	A	358	LYS
1	B	265	LYS
1	B	358	LYS
1	A	261	LYS
1	B	263	LYS
1	B	274	SER
1	A	239	GLY
1	A	274	SER
1	B	275	LYS
1	B	460	GLU
1	B	272	GLU
1	A	269	PRO
1	A	262	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	247/258 (96%)	237 (96%)	10 (4%)	38	30
1	B	233/258 (90%)	225 (97%)	8 (3%)	44	37
All	All	480/516 (93%)	462 (96%)	18 (4%)	40	32

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	ILE

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Mol	Chain	Res	Type
1	A	276	GLU
1	A	283	GLN
1	A	288	ARG
1	A	396	ASP
1	A	411	ASP
1	A	440	THR
1	A	441	ASP
1	A	444	GLN
1	A	469	LEU
1	B	261	LYS
1	B	270	LEU
1	B	276	GLU
1	B	318	LEU
1	B	335	ASN
1	B	340	LEU
1	B	424	ASN
1	B	452	LEU

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	205	ASN
1	A	271	GLN
1	A	283	GLN
1	A	308	ASN
1	A	410	GLN
1	A	425	HIS
1	A	430	GLN
1	A	454	GLN
1	B	217	HIS
1	B	273	GLN
1	B	283	GLN
1	B	308	ASN
1	B	335	ASN
1	B	424	ASN
1	B	437	GLN
1	B	444	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	OCR	A	1	1	19,22,22	2.15	3 (15%)	17,23,23	2.01	1 (5%)
2	MYI	A	3	-	12,16,16	3.50	4 (33%)	12,22,22	1.78	2 (16%)
3	OCR	B	2	1	19,22,22	2.25	4 (21%)	17,23,23	1.97	1 (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
3	OCR	A	1	1	-	0/19/21/21	0/0/0/0
2	MYI	A	3	-	-	0/3/6/6	0/2/2/2
3	OCR	B	2	1	-	0/19/21/21	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3	MYI	CAF-CAM	-3.58	1.31	1.38
3	A	1	OCR	C4-C5	-2.90	1.41	1.52
3	B	2	OCR	C4-C5	-2.81	1.41	1.52
3	B	2	OCR	C8-C6	2.06	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3	MYI	CAD-CAL	2.37	1.43	1.38
3	A	1	OCR	C11-C9	2.64	1.52	1.44
2	A	3	MYI	CAE-CAD	2.72	1.42	1.36
3	B	2	OCR	C11-C9	2.88	1.52	1.44
3	A	1	OCR	C9-C8	8.09	1.55	1.34
3	B	2	OCR	C9-C8	8.35	1.56	1.34
2	A	3	MYI	CAG-CAL	10.41	1.55	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	OCR	C11-C9-C8	-8.13	106.59	124.66
3	B	2	OCR	C11-C9-C8	-7.76	107.42	124.66
2	A	3	MYI	CAL-CAG-CAO	-3.29	115.02	119.99
2	A	3	MYI	CAG-CAO-CAN	4.40	122.08	120.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	OCR	5	0
2	A	3	MYI	1	0
3	B	2	OCR	6	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	A	274/287 (95%)	0.70	35 (12%) 5 5	28, 45, 101, 126	0
1	B	260/287 (90%)	0.69	37 (14%) 4 3	28, 45, 97, 115	0
All	All	534/574 (93%)	0.69	72 (13%) 4 4	28, 45, 98, 126	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	9.8
1	A	265	LYS	9.8
1	B	265	LYS	8.6
1	B	267	ILE	8.1
1	A	269	PRO	7.4
1	A	264	PHE	6.9
1	A	268	THR	5.9
1	A	267	ILE	5.9
1	B	266	HIS	5.6
1	A	261	LYS	5.4
1	B	261	LYS	5.4
1	A	266	HIS	5.2
1	A	272	GLU	5.2
1	B	269	PRO	4.9
1	B	274	SER	4.8
1	B	272	GLU	4.8
1	B	456	ILE	4.6
1	A	203	GLN	4.6
1	A	204	LEU	4.4
1	A	239	GLY	4.2
1	A	262	ILE	4.2
1	B	460	GLU	4.2
1	B	262	ILE	3.7
1	A	271	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	263	LYS	3.6
1	B	436	LEU	3.5
1	A	275	LYS	3.5
1	B	271	GLN	3.5
1	A	426	PRO	3.4
1	B	461	THR	3.3
1	B	363	PHE	3.1
1	A	206	PRO	3.1
1	B	260	ASP	3.1
1	A	285	CYS	3.1
1	A	427	GLU	3.1
1	A	260	ASP	3.0
1	B	240	LYS	2.9
1	B	470	GLN	2.9
1	B	264	PHE	2.9
1	A	358	LYS	2.9
1	B	268	THR	2.9
1	A	263	LYS	2.8
1	B	454	GLN	2.8
1	A	273	GLN	2.8
1	B	452	LEU	2.7
1	B	270	LEU	2.6
1	B	238	THR	2.6
1	A	258	GLY	2.6
1	A	401	LEU	2.5
1	B	473	TYR	2.5
1	B	256	MET	2.5
1	B	275	LYS	2.5
1	A	475	ASP	2.5
1	B	358	LYS	2.5
1	A	256	MET	2.5
1	B	244	LYS	2.5
1	B	287	PHE	2.4
1	A	241	THR	2.4
1	B	391	ILE	2.4
1	A	240	LYS	2.4
1	B	387	PHE	2.3
1	A	287	PHE	2.3
1	B	209	ALA	2.3
1	A	363	PHE	2.3
1	A	326	ILE	2.2
1	A	207	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	436	LEU	2.2
1	B	451	GLN	2.2
1	A	362	ASP	2.1
1	B	341	ILE	2.1
1	B	458	LYS	2.1
1	B	439	MET	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
2	MYI	A	3	15/15	0.61	0.51	8.51	113,114,115,115	0
3	OCR	B	2	23/23	0.38	0.56	5.30	70,74,84,85	0
3	OCR	A	1	23/23	0.56	0.43	2.55	74,80,89,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.