



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:42 pm GMT

PDB ID : 4PVU
Title : Crystal structure of the complex between PPARgamma-LBD and the R enantiomer of Mbx-102 (Metaglidasen)
Authors : Pochetti, G.; Montanari, R.; Capelli, D.; Loiodice, F.; Laghezza, A.; Piemontese, L.; Lavecchia, A.
Deposited on : 2014-03-18
Resolution : 2.60 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

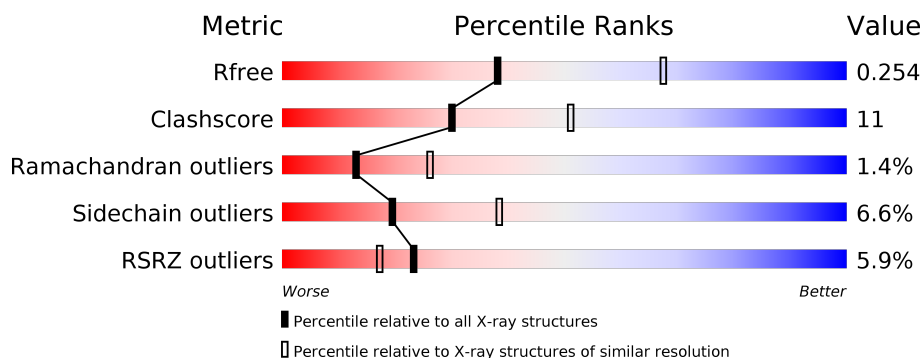
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 $\leq 5\%$. 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	<div> <div> <div></div> <div>69%</div> <div>17%</div> <div>• • 10%</div> </div> <div>9%</div> </div>
1	B	287	<div> <div> <div></div> <div>69%</div> <div>16%</div> <div>• 12%</div> </div> <div>9%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4136 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.

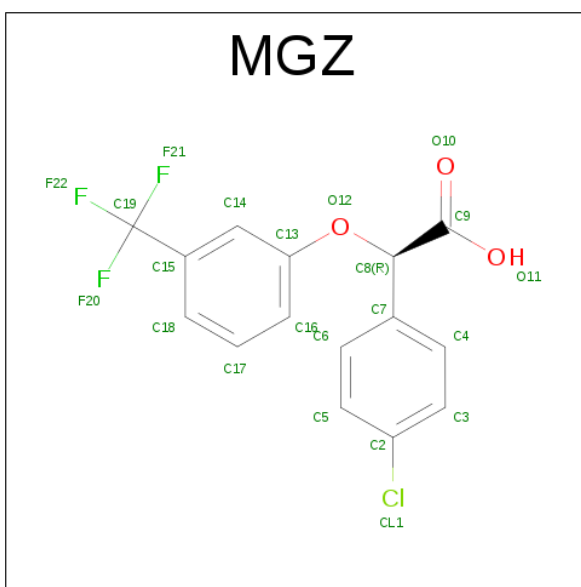
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2058	1330	335	383	10			
1	B	252	Total	C	N	O	S	0	0	0
			2010	1300	326	374	10			

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 (2R)-(4-CHLOROPHENYL)[3-(TRIFLUOROMETHYL)PHENOXY]ETHAN OIC ACID (three-letter code: MGZ) (formula: C₁₅H₁₀ClF₃O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Cl	F	O	0	0
			22	15	1	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	19	Total	O	0	0
			19	19		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.37Å 60.21Å 119.06Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	57.91 – 2.60 57.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (57.91-2.60) 97.7 (57.91-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.200 , 0.251 0.206 , 0.254	Depositor DCC
R_{free} test set	990 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	68.9	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 78.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4136	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MGZ

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	0.46	0/2092	0.66	0/2817
1	B	0.43	0/2041	0.67	1/2747 (0.0%)
All	All	0.45	0/4133	0.67	1/5564 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	SER	CA-C-N	-5.34	105.46	117.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2058	0	2120	53	0
1	B	2010	0	2073	36	0
2	B	22	0	9	2	0
3	A	27	0	0	3	0
3	B	19	0	0	2	0
All	All	4136	0	4202	88	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 (88) 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:358:LYS:HB2	1:A:359:PRO:CD	1.63	1.27
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.40	1.01
1:A:220:ASP:O	1:A:224:LYS:HG3	1.69	0.90
1:A:358:LYS:HB2	1:A:359:PRO:HD2	1.52	0.89
1:A:262:ILE:O	1:A:262:ILE:HD12	1.79	0.82
1:B:240:LYS:HA	1:B:242:THR:HG23	1.61	0.81
1:B:453:LEU:O	1:B:456:ILE:HG22	1.83	0.78
1:B:258:GLY:HA2	1:B:262:ILE:HD13	1.64	0.78
1:A:358:LYS:CB	1:A:359:PRO:CD	2.56	0.75
1:A:241:THR:HG21	1:A:244:LYS:HB2	1.70	0.74
1:A:444:GLN:HG3	3:B:618:HOH:O	1.88	0.73
1:A:290:VAL:HG23	1:A:468:LEU:HD12	1.74	0.69
1:B:253:ASN:OD1	1:B:253:ASN:N	2.26	0.68
1:A:253:ASN:OD1	1:A:253:ASN:N	2.27	0.68
1:A:471:GLU:CD	1:A:471:GLU:H	1.97	0.68
1:A:323:HIS:ND1	3:A:514:HOH:O	2.30	0.64
1:B:238:THR:C	1:B:240:LYS:H	2.00	0.64
1:A:239:GLY:O	1:A:241:THR:HG23	1.98	0.64
1:B:279:ILE:O	1:B:283:GLN:HG3	1.99	0.63
1:A:250:TYR:HA	1:A:349:THR:HG22	1.81	0.62
1:A:358:LYS:CB	1:A:359:PRO:HD3	2.23	0.62
1:B:383:ASP:OD2	1:B:425:HIS:HE1	1.83	0.61
1:B:238:THR:O	1:B:240:LYS:N	2.31	0.61
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.84	0.59
1:A:291:GLU:HA	1:A:294:GLN:NE2	2.19	0.57
1:B:461:THR:O	1:B:461:THR:HG22	2.04	0.57
1:A:291:GLU:HA	1:A:294:GLN:HE21	1.70	0.57
1:B:238:THR:C	1:B:240:LYS:N	2.58	0.56
1:A:349:THR:HG23	1:A:352:PHE:H	1.73	0.54
1:B:237:LEU:O	1:B:240:LYS:NZ	2.29	0.54
1:B:454:GLN:OE1	1:B:454:GLN:N	2.41	0.54
1:A:240:LYS:C	1:A:241:THR:HG22	2.28	0.54
1:B:466:HIS:O	1:B:470:GLN:OE1	2.26	0.53
1:B:363:PHE:CE1	1:B:364:MET:HG2	2.44	0.53
1:A:363:PHE:CE1	1:A:364:MET:HG2	2.43	0.53
1:A:440:THR:O	1:A:444:GLN:HG2	2.09	0.53
1:A:466:HIS:O	1:A:470:GLN:OE1	2.28	0.51
1:B:326:ILE:HG23	2:B:501:MGZ:H10	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.92	0.51
1:B:261:LYS:C	1:B:262:ILE:HD12	2.31	0.51
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.92	0.50
1:A:427:GLU:N	1:A:427:GLU:OE1	2.42	0.50
1:A:469:LEU:N	1:A:471:GLU:OE2	2.44	0.50
1:A:250:TYR:HA	1:A:349:THR:CG2	2.42	0.50
1:A:466:HIS:CD2	1:A:467:PRO:CD	2.96	0.49
1:A:322:VAL:HG21	1:A:472:ILE:HD13	1.95	0.49
1:B:450:VAL:O	1:B:454:GLN:OE1	2.30	0.49
1:A:287:PHE:O	1:A:290:VAL:HG12	2.13	0.48
1:A:207:GLU:HB3	3:A:504:HOH:O	2.13	0.47
1:B:358:LYS:N	3:B:608:HOH:O	2.47	0.47
1:B:404:LYS:N	1:B:405:PRO:HD2	2.29	0.47
1:A:430:GLN:HE21	1:B:415:GLN:HG2	1.79	0.47
1:B:237:LEU:HD23	1:B:335:ASN:ND2	2.30	0.47
1:A:234:ARG:NH1	1:A:332:SER:O	2.48	0.46
1:A:370:PHE:CB	1:A:445:ILE:HD11	2.45	0.46
1:A:349:THR:HG23	1:A:352:PHE:CB	2.46	0.46
1:B:234:ARG:NH1	1:B:332:SER:O	2.49	0.45
1:B:252:MET:O	1:B:255:LEU:HB3	2.17	0.45
1:B:441:ASP:O	1:B:445:ILE:HD13	2.17	0.45
1:B:466:HIS:HB2	1:B:469:LEU:HB2	1.97	0.45
2:B:501:MGZ:H4	2:B:501:MGZ:O10	2.16	0.45
1:A:466:HIS:CD2	1:A:467:PRO:HG2	2.52	0.45
1:B:252:MET:HE3	1:B:277:VAL:HG11	1.98	0.45
1:A:466:HIS:CD2	1:A:467:PRO:N	2.85	0.45
1:A:253:ASN:HA	1:A:256:MET:HG3	1.99	0.44
1:A:349:THR:HG23	1:A:352:PHE:HB3	2.00	0.44
1:A:252:MET:O	1:A:255:LEU:HB3	2.18	0.44
1:B:252:MET:CE	1:B:277:VAL:HG11	2.48	0.44
1:A:404:LYS:N	1:A:405:PRO:HD2	2.32	0.43
1:A:241:THR:OG1	1:A:244:LYS:N	2.39	0.43
1:A:290:VAL:CG2	1:A:468:LEU:HD12	2.46	0.43
1:B:237:LEU:HD12	1:B:340:LEU:HD11	2.00	0.43
1:A:452:LEU:O	1:A:456:ILE:HD12	2.18	0.43
1:A:311:LEU:HD12	1:A:312:ASN:N	2.33	0.43
1:A:465:LEU:N	1:A:465:LEU:HD12	2.33	0.43
1:B:207:GLU:HG2	1:B:208:SER:N	2.34	0.43
1:B:454:GLN:HA	1:B:457:LYS:HG3	1.99	0.42
1:A:474:LYS:CB	1:A:474:LYS:NZ	2.82	0.42
1:A:287:PHE:O	1:A:290:VAL:CG1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LYS:C	1:B:242:THR:N	2.73	0.41
1:A:207:GLU:HG2	1:A:208:SER:N	2.35	0.41
1:B:237:LEU:HD23	1:B:335:ASN:HD22	1.86	0.41
1:A:471:GLU:N	1:A:471:GLU:CD	2.72	0.41
1:B:249:ILE:O	1:B:349:THR:HG23	2.21	0.41
1:A:474:LYS:HB3	1:A:474:LYS:NZ	2.36	0.41
1:A:209:ALA:HB3	3:A:504:HOH:O	2.21	0.40
1:A:439:MET:CE	1:B:437:GLN:HG2	2.51	0.40
1:B:394:SER:O	1:B:397:ARG:HG2	2.21	0.40

There are no symmetry-related clashes.

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	253/287 (88%)	237 (94%)	12 (5%)	4 (2%)	11	23
1	B	244/287 (85%)	230 (94%)	11 (4%)	3 (1%)	15	32
All	All	497/574 (87%)	467 (94%)	23 (5%)	7 (1%)	13	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	LYS
1	B	240	LYS
1	A	208	SER
1	A	457	LYS
1	B	208	SER
1	A	239	GLY
1	B	241	THR

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	230/258 (89%)	214 (93%)	16 (7%)	18	35
1	B	225/258 (87%)	211 (94%)	14 (6%)	21	42
All	All	455/516 (88%)	425 (93%)	30 (7%)	19	38

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	SER
1	A	234	ARG
1	A	240	LYS
1	A	241	THR
1	A	245	SER
1	A	253	ASN
1	A	254	SER
1	A	255	LEU
1	A	256	MET
1	A	276	GLU
1	A	283	GLN
1	A	333	LEU
1	A	358	LYS
1	A	457	LYS
1	A	461	THR
1	A	474	LYS
1	B	208	SER
1	B	216	LYS
1	B	234	ARG
1	B	243	ASP
1	B	253	ASN
1	B	254	SER
1	B	255	LEU
1	B	276	GLU
1	B	349	THR
1	B	427	GLU
1	B	428	SER

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Mol	Chain	Res	Type
1	B	445	ILE
1	B	453	LEU
1	B	464	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	430	GLN
1	A	466	HIS
1	B	412	ASN
1	B	425	HIS
1	B	466	HIS

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 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	MGZ	B	501	-	20,23,23	1.33	1 (5%)	28,33,33	1.17	2 (7%)

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	MGZ	B	501	-	-	0/14/18/18	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	MGZ	O12-C8	-5.41	1.39	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	MGZ	O12-C8-C7	-2.72	102.62	108.07
2	B	501	MGZ	C4-C7-C8	-2.47	116.32	120.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	MGZ	2	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, 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	257/287 (89%)	0.38	3 (1%) 79 75	48, 77, 125, 145	0
1	B	252/287 (87%)	0.86	27 (10%) 7 4	50, 85, 149, 213	0
All	All	509/574 (88%)	0.62	30 (5%) 23 17	48, 81, 141, 213	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	LEU	11.4
1	B	464	SER	8.5
1	B	241	THR	6.7
1	B	361	GLY	6.5
1	B	463	MET	6.3
1	B	363	PHE	6.2
1	B	462	ASP	6.1
1	B	240	LYS	4.8
1	B	287	PHE	4.4
1	B	360	PHE	4.1
1	A	467	PRO	3.7
1	B	209	ALA	3.6
1	B	236	ILE	3.6
1	B	243	ASP	3.5
1	A	456	ILE	3.5
1	B	356	LEU	3.0
1	B	249	ILE	3.0
1	B	247	PHE	2.6
1	B	459	THR	2.6
1	B	352	PHE	2.6
1	B	238	THR	2.5
1	B	255	LEU	2.4
1	B	354	LYS	2.4
1	B	353	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	235	ALA	2.2
1	B	211	LEU	2.2
1	B	355	SER	2.2
1	B	277	VAL	2.2
1	B	461	THR	2.1
1	A	473	TYR	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, 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	LLDF	B-factors(\AA^2)	Q < 0.9
2	MGZ	B	501	22/22	0.88	0.34	0.82	87,99,112,135	0

6.5 Other polymers [i](#)

There are no such residues in this entry.