Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:59 PM GMT

PDB ID	:	1I7I
Title	:	CRYSTAL STRUCTURE OF THE LIGAND BINDING DOMAIN OF HUMAN PPAR-GAMMA IN COMPLEX WITH THE AGONIST AZ 242
Authors	:	Petersen, J.F.W.; Cronet, P.; Folmer, R.; Blomberg, N.; Sjoblom, K.; Karlsson, U.; Lindstedt, E.-L.; Bamberg, K.
Deposited on	:	2001-03-09
Resolution	:	2.35 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 (i)) were used in the production of this report:

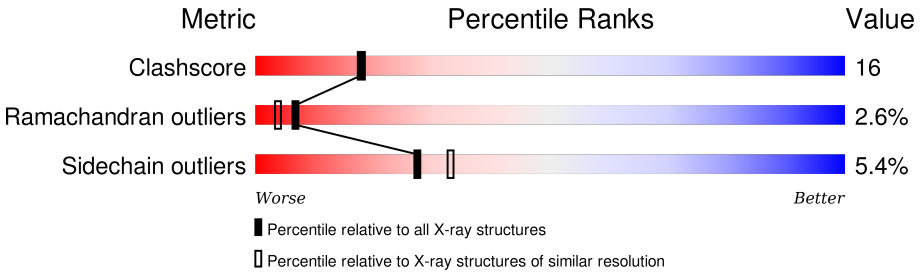
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.35 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	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	292	60% 25% • 12%
1	B	292	56% 27% 5% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4250 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.

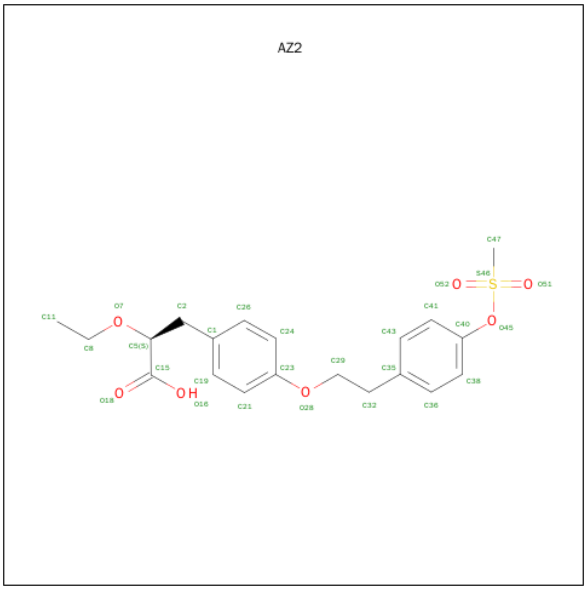
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2063	1331	336	386	10			
1	B	258	Total	C	N	O	S	0	0	0
			2069	1339	339	382	9			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	GLY	-	CLONING ARTIFACT	UNP P37231
A	187	SER	-	CLONING ARTIFACT	UNP P37231
A	188	HIS	-	CLONING ARTIFACT	UNP P37231
A	189	MET	-	CLONING ARTIFACT	UNP P37231
A	190	ALA	-	CLONING ARTIFACT	UNP P37231
A	191	GLU	-	CLONING ARTIFACT	UNP P37231
A	192	ILE	-	CLONING ARTIFACT	UNP P37231
A	193	SER	-	CLONING ARTIFACT	UNP P37231
A	194	SER	-	CLONING ARTIFACT	UNP P37231
A	195	ASP	-	CLONING ARTIFACT	UNP P37231
A	196	ILE	-	CLONING ARTIFACT	UNP P37231
B	186	GLY	-	CLONING ARTIFACT	UNP P37231
B	187	SER	-	CLONING ARTIFACT	UNP P37231
B	188	HIS	-	CLONING ARTIFACT	UNP P37231
B	189	MET	-	CLONING ARTIFACT	UNP P37231
B	190	ALA	-	CLONING ARTIFACT	UNP P37231
B	191	GLU	-	CLONING ARTIFACT	UNP P37231
B	192	ILE	-	CLONING ARTIFACT	UNP P37231
B	193	SER	-	CLONING ARTIFACT	UNP P37231
B	194	SER	-	CLONING ARTIFACT	UNP P37231
B	195	ASP	-	CLONING ARTIFACT	UNP P37231
B	196	ILE	-	CLONING ARTIFACT	UNP P37231

- Molecule 2 is (2S)-2-ETHOXY-3-[4-(2-{4-[(METHYLSULFONYL)OXY]PHENYL}ETHO

XY)PHENYL]PROPANOIC ACID (three-letter code: AZ2) (formula: $C_{20}H_{24}O_7S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 28 20 7 1	0	0
2	B	1	Total C O S 28 20 7 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	36	Total O 36 36	0	0
3	B	26	Total O 26 26	0	0

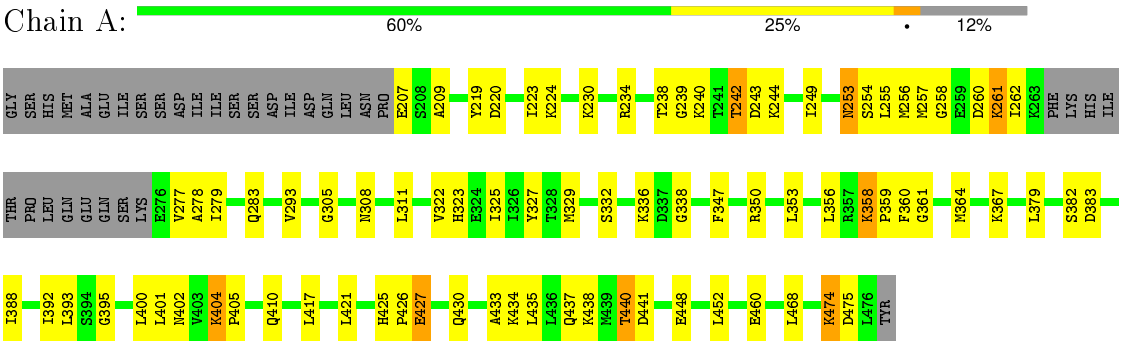
3 Residue-property plots (i)

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.

Note EDS was not executed.

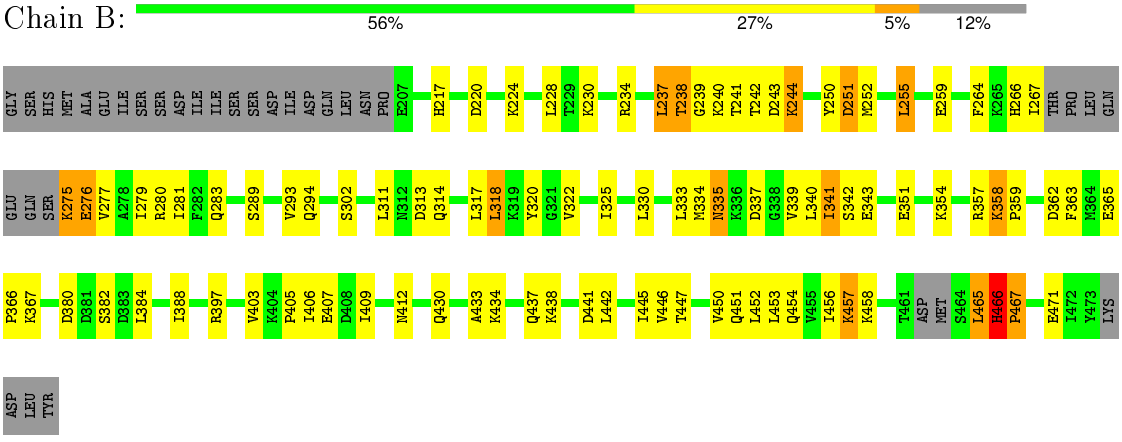
• Molecule 1: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA

Chain A:



• Molecule 1: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	92.93Å 61.78Å 118.98Å 90.00° 101.52° 90.00°	Depositor
Resolution (Å)	19.98 – 2.35	Depositor
% Data completeness (in resolution range)	91.3 (19.98-2.35)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX 2000	Depositor
R, R_{free}	0.238 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4250	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZ2

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	0.38	0/2096	0.59	0/2823
1	B	0.37	0/2103	0.59	0/2830
All	All	0.38	0/4199	0.59	0/5653

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2063	0	2126	57	0
1	B	2069	0	2137	77	0
2	A	28	0	23	0	0
2	B	28	0	23	1	0
3	A	36	0	0	1	0
3	B	26	0	0	0	0
All	All	4250	0	4309	134	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 16.

All (134) 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:325:ILE:HD12	1:B:388:ILE:HG23	1.42	0.99
1:B:451:GLN:HA	1:B:454:GLN:HE21	1.35	0.88
1:B:341:ILE:HD12	1:B:342:SER:H	1.41	0.85
1:B:275:LYS:HE3	1:B:275:LYS:HA	1.63	0.80
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.15	0.77
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.67	0.77
1:B:430:GLN:HG3	1:B:433:ALA:HB3	1.67	0.76
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.69	0.75
1:B:335:ASN:HD22	1:B:335:ASN:C	1.91	0.74
1:B:341:ILE:CD1	1:B:342:SER:H	2.02	0.73
1:B:363:PHE:O	1:B:367:LYS:HE2	1.90	0.72
1:B:441:ASP:O	1:B:445:ILE:HG12	1.91	0.71
1:B:405:PRO:O	1:B:409:ILE:HG13	1.91	0.71
1:B:380:ASP:OD1	1:B:382:SER:HB3	1.91	0.70
1:A:383:ASP:OD2	1:A:425:HIS:HE1	1.77	0.68
1:B:466:HIS:H	1:B:467:PRO:HD2	1.57	0.68
1:A:242:THR:HG22	1:A:242:THR:O	1.94	0.67
1:B:466:HIS:N	1:B:467:PRO:CD	2.58	0.66
1:A:243:ASP:O	1:A:244:LYS:HG3	1.97	0.65
1:B:466:HIS:H	1:B:467:PRO:CD	2.09	0.65
1:B:452:LEU:O	1:B:456:ILE:HG12	1.97	0.64
1:A:448:GLU:O	1:A:452:LEU:HG	1.98	0.63
1:B:359:PRO:HG2	1:B:456:ILE:CD1	2.29	0.62
1:A:359:PRO:HG2	1:A:360:PHE:CD1	2.36	0.61
1:B:255:LEU:CD1	1:B:277:VAL:HG13	2.30	0.61
1:B:433:ALA:O	1:B:437:GLN:HG3	2.01	0.61
1:A:230:LYS:O	1:A:234:ARG:HG2	2.01	0.60
1:B:341:ILE:HD12	1:B:342:SER:N	2.13	0.60
1:A:253:ASN:HA	1:A:256:MET:HG2	1.84	0.60
1:B:456:ILE:C	1:B:458:LYS:H	2.04	0.59
1:B:335:ASN:ND2	1:B:337:ASP:H	2.00	0.59
1:B:252:MET:SD	1:B:277:VAL:HG21	2.43	0.59
1:A:393:LEU:O	1:A:410:GLN:HB2	2.02	0.59
1:B:289:SER:O	1:B:293:VAL:HG23	2.03	0.58
1:A:261:LYS:HD2	1:A:261:LYS:H	1.67	0.58
1:A:437:GLN:O	1:A:440:THR:HG23	2.03	0.58
1:A:238:THR:O	1:A:240:LYS:N	2.29	0.58
1:B:279:ILE:O	1:B:283:GLN:HG3	2.05	0.57
1:A:255:LEU:CD2	1:A:277:VAL:HG23	2.35	0.57
1:A:257:MET:O	1:A:260:ASP:HB3	2.05	0.56
1:A:277:VAL:HG13	1:A:278:ALA:H	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ILE:HA	1:A:254:SER:HB3	1.87	0.56
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.89	0.55
1:B:447:THR:O	1:B:450:VAL:HG22	2.06	0.55
1:A:336:LYS:NZ	1:A:350:ARG:HH12	2.04	0.54
1:B:237:LEU:HD21	1:B:340:LEU:HG	1.89	0.54
1:B:442:LEU:O	1:B:446:VAL:HG23	2.08	0.54
1:B:311:LEU:HD23	1:B:314:GLN:NE2	2.23	0.53
1:A:277:VAL:HG13	1:A:278:ALA:N	2.24	0.53
1:B:365:GLU:N	1:B:366:PRO:HD2	2.24	0.53
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.90	0.53
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.74	0.52
1:A:474:LYS:HE3	1:A:474:LYS:HA	1.92	0.52
1:B:451:GLN:HA	1:B:454:GLN:NE2	2.17	0.52
1:B:330:LEU:O	1:B:334:MET:HG3	2.11	0.51
1:A:427:GLU:CD	1:A:427:GLU:H	2.14	0.51
1:A:327:TYR:CE1	1:A:367:LYS:HE3	2.46	0.51
1:A:356:LEU:HB2	1:A:361:GLY:HA2	1.92	0.51
1:A:401:LEU:C	1:A:402:ASN:HD22	2.14	0.51
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.92	0.51
1:A:430:GLN:O	1:A:434:LYS:HG3	2.11	0.50
1:A:353:LEU:HD13	1:A:364:MET:HG3	1.93	0.50
1:A:364:MET:HB2	3:A:26:HOH:O	2.10	0.50
1:B:217:HIS:HE1	1:B:302:SER:O	1.93	0.50
1:B:276:GLU:OE2	1:B:357:ARG:NH2	2.40	0.50
1:B:359:PRO:HG2	1:B:456:ILE:HD13	1.94	0.50
1:A:392:ILE:HG22	1:A:393:LEU:HD22	1.94	0.49
1:A:338:GLY:HA3	1:A:347:PHE:CZ	2.48	0.49
1:B:343:GLU:HG3	1:B:343:GLU:O	2.12	0.49
1:B:266:HIS:O	1:B:267:ILE:HD13	2.13	0.49
1:A:325:ILE:HG23	1:A:388:ILE:CD1	2.40	0.49
1:A:438:LYS:O	1:A:441:ASP:HB2	2.13	0.49
1:A:220:ASP:OD1	1:A:224:LYS:HE3	2.13	0.49
1:B:252:MET:SD	1:B:277:VAL:HG11	2.52	0.49
1:A:329:MET:O	1:A:332:SER:HB2	2.12	0.49
1:B:341:ILE:CG1	1:B:342:SER:H	2.26	0.48
1:B:456:ILE:O	1:B:458:LYS:N	2.41	0.48
1:B:241:THR:HG22	1:B:241:THR:O	2.13	0.47
1:B:341:ILE:CG1	1:B:342:SER:N	2.76	0.47
1:B:230:LYS:O	1:B:234:ARG:HB2	2.15	0.47
1:B:317:LEU:HD21	1:B:406:ILE:HD13	1.96	0.47
1:B:358:LYS:CD	1:B:358:LYS:H	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:VAL:HG22	1:B:280:ARG:HH21	1.78	0.47
1:A:336:LYS:HZ2	1:A:350:ARG:HH12	1.61	0.47
1:B:335:ASN:C	1:B:335:ASN:ND2	2.64	0.47
1:B:358:LYS:HD2	1:B:358:LYS:H	1.79	0.47
1:B:351:GLU:HA	1:B:354:LYS:NZ	2.30	0.47
1:B:259:GLU:HG2	1:B:264:PHE:CD1	2.50	0.46
1:A:258:GLY:O	1:A:262:ILE:HB	2.16	0.46
1:B:358:LYS:N	1:B:358:LYS:HD2	2.30	0.46
1:B:384:LEU:O	1:B:388:ILE:HG13	2.15	0.46
1:B:451:GLN:O	1:B:454:GLN:HG2	2.16	0.46
1:B:354:LYS:HB3	1:B:354:LYS:NZ	2.31	0.45
1:A:426:PRO:HG2	1:A:427:GLU:OE1	2.16	0.45
1:B:220:ASP:O	1:B:224:LYS:HD2	2.17	0.45
1:B:451:GLN:CA	1:B:454:GLN:HE21	2.19	0.44
1:A:402:ASN:HD22	1:A:402:ASN:N	2.14	0.44
1:B:403:VAL:HG12	1:B:407:GLU:HG3	2.00	0.44
1:B:457:LYS:HG3	1:B:457:LYS:O	2.17	0.44
1:A:402:ASN:ND2	1:A:402:ASN:N	2.65	0.44
1:B:293:VAL:HG22	1:B:322:VAL:HG11	1.99	0.43
1:A:219:TYR:CD1	1:A:382:SER:HA	2.53	0.43
1:B:335:ASN:ND2	1:B:337:ASP:N	2.66	0.43
1:B:357:ARG:HD2	1:B:358:LYS:O	2.19	0.43
1:A:395:GLY:HA2	1:A:400:LEU:CD1	2.48	0.43
1:B:333:LEU:HB3	1:B:340:LEU:HB2	2.00	0.43
1:A:417:LEU:O	1:A:421:LEU:HG	2.19	0.43
1:A:404:LYS:N	1:A:405:PRO:HD2	2.34	0.43
1:A:293:VAL:HG22	1:A:322:VAL:CG1	2.49	0.43
1:B:430:GLN:HG3	1:B:433:ALA:CB	2.45	0.42
1:A:322:VAL:HG12	1:A:323:HIS:N	2.33	0.42
1:B:275:LYS:CE	1:B:275:LYS:HA	2.42	0.42
1:A:393:LEU:N	1:A:393:LEU:HD22	2.34	0.42
1:B:320:TYR:HB3	1:B:397:ARG:HD2	2.01	0.42
1:A:433:ALA:O	1:A:437:GLN:HG3	2.19	0.42
1:B:237:LEU:O	1:B:238:THR:C	2.58	0.42
1:B:237:LEU:O	1:B:239:GLY:O	2.37	0.42
1:A:279:ILE:HD13	1:A:360:PHE:CZ	2.55	0.42
1:A:257:MET:O	1:A:261:LYS:HD2	2.20	0.42
1:A:207:GLU:HG3	1:A:209:ALA:H	1.84	0.42
1:B:465:LEU:O	1:B:466:HIS:HB2	2.20	0.41
1:B:250:TYR:CE1	1:B:251:ASP:OD2	2.73	0.41
1:B:456:ILE:C	1:B:458:LYS:N	2.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:LYS:O	1:B:438:LYS:HD3	2.20	0.41
1:A:279:ILE:CD1	1:A:360:PHE:CZ	3.04	0.41
1:A:388:ILE:HD13	1:A:388:ILE:HA	1.87	0.41
1:B:339:VAL:HG22	1:B:340:LEU:O	2.21	0.41
1:B:313:ASP:O	1:B:317:LEU:HG	2.21	0.41
1:B:281:ILE:HG23	2:B:478:AZ2:H381	2.03	0.41
1:B:237:LEU:O	1:B:239:GLY:N	2.53	0.40
1:B:243:ASP:O	1:B:244:LYS:HB3	2.21	0.40
1:B:318:LEU:HA	1:B:318:LEU:HD12	1.86	0.40
1:B:330:LEU:HA	1:B:330:LEU:HD23	1.96	0.40
1:A:219:TYR:CZ	1:A:223:ILE:HD11	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	254/292 (87%)	241 (95%)	9 (4%)	4 (2%)	12 10
1	B	252/292 (86%)	235 (93%)	8 (3%)	9 (4%)	4 2
All	All	506/584 (87%)	476 (94%)	17 (3%)	13 (3%)	7 4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	A	358	LYS
1	B	237	LEU
1	B	244	LYS
1	B	466	HIS
1	B	240	LYS
1	B	242	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	467	PRO
1	A	475	ASP
1	B	238	THR
1	B	276	GLU
1	B	457	LYS
1	A	242	THR

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	231/263 (88%)	221 (96%)	10 (4%)	35 45
1	B	231/263 (88%)	216 (94%)	15 (6%)	21 24
All	All	462/526 (88%)	437 (95%)	25 (5%)	27 33

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	261	LYS
1	A	283	GLN
1	A	311	LEU
1	A	404	LYS
1	A	427	GLU
1	A	440	THR
1	A	460	GLU
1	A	468	LEU
1	A	474	LYS
1	B	228	LEU
1	B	251	ASP
1	B	255	LEU
1	B	275	LYS
1	B	294	GLN
1	B	318	LEU
1	B	335	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	341	ILE
1	B	358	LYS
1	B	362	ASP
1	B	412	ASN
1	B	453	LEU
1	B	465	LEU
1	B	466	HIS
1	B	471	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	308	ASN
1	A	314	GLN
1	A	345	GLN
1	A	402	ASN
1	A	425	HIS
1	A	430	GLN
1	A	470	GLN
1	B	217	HIS
1	B	294	GLN
1	B	308	ASN
1	B	314	GLN
1	B	335	ASN
1	B	410	GLN
1	B	412	ASN
1	B	420	GLN
1	B	430	GLN
1	B	444	GLN
1	B	451	GLN
1	B	454	GLN
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 (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)

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	$\#\|Z\| > 2$
2	AZ2	A	101	-	25,29,29	1.65	7 (28%)	34,39,39	0.99	1 (2%)
2	AZ2	B	478	-	25,29,29	1.65	7 (28%)	34,39,39	1.05	3 (8%)

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	AZ2	A	101	-	-	0/18/22/22	0/2/2/2
2	AZ2	B	478	-	-	0/18/22/22	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	AZ2	O45-C40	-3.44	1.37	1.42
2	B	478	AZ2	O45-C40	-3.42	1.37	1.42
2	A	101	AZ2	C36-C35	2.07	1.43	1.38
2	B	478	AZ2	C43-C35	2.08	1.43	1.38
2	A	101	AZ2	C19-C1	2.20	1.43	1.38
2	A	101	AZ2	C26-C24	2.22	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	478	AZ2	C41-C40	2.25	1.43	1.38
2	A	101	AZ2	C38-C36	2.26	1.42	1.38
2	B	478	AZ2	C21-C23	2.27	1.43	1.38
2	B	478	AZ2	C43-C41	2.29	1.42	1.38
2	A	101	AZ2	C21-C19	2.33	1.43	1.38
2	B	478	AZ2	C19-C1	2.41	1.43	1.38
2	B	478	AZ2	C21-C19	2.64	1.43	1.38
2	A	101	AZ2	C21-C23	2.68	1.44	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	478	AZ2	O45-C40-C38	-2.21	114.37	118.74
2	B	478	AZ2	C29-O28-C23	2.40	123.83	117.91
2	A	101	AZ2	O45-C40-C41	3.14	124.94	118.74
2	B	478	AZ2	O45-C40-C41	3.49	125.62	118.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	478	AZ2	1	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.