



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:18 AM GMT

PDB ID : 2Q6R
Title : Crystal structure of PPAR gamma complexed with partial agonist SF147
Authors : Bruning, J.B.; Nettles, K.W.
Deposited on : 2007-06-01
Resolution : 2.41 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 (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

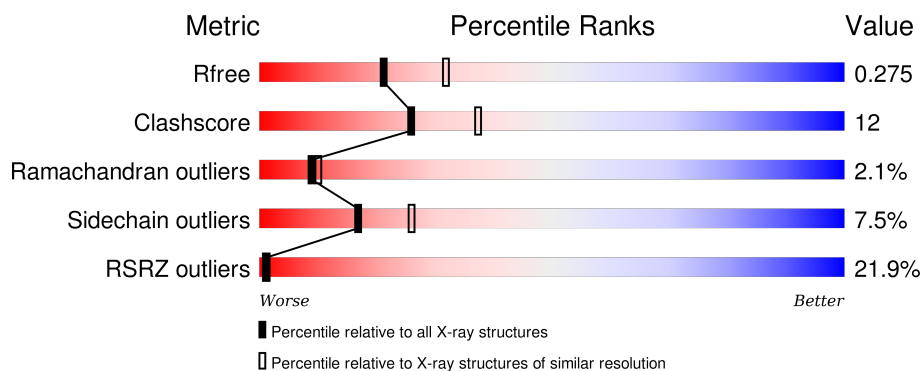
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	274	<div> <div>20%</div> <div>67%</div> <div>17%</div> <div>..</div> <div>14%</div> </div>
1	B	274	<div> <div>19%</div> <div>69%</div> <div>20%</div> <div>..</div> <div>6%</div> </div>

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	SF2	A	5001	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4069 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.

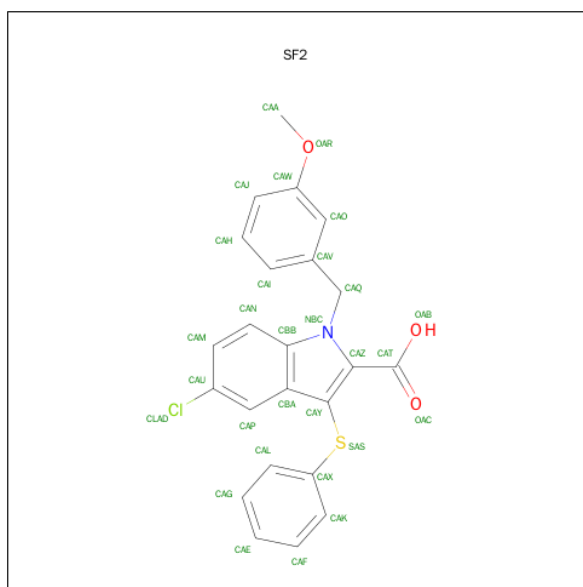
- Molecule 1 is a protein called Peroxisome Proliferator-Activated Receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1839	1182	295	353	9			
1	B	258	Total	C	N	O	S	0	0	0
			2048	1324	336	379	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	SER	-	EXPRESSION TAG	UNP P37231
B	204	SER	-	EXPRESSION TAG	UNP P37231

- Molecule 2 is 5-CHLORO-1-(3-METHOXYBENZYL)-3-(PHENYLTHIO)-1H-INDOLE-2-CARBOXYLIC ACID (three-letter code: SF2) (formula: C₂₃H₁₈ClNO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			29	23	1	1	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	S	0	0
			29	23	1	1	3	1		

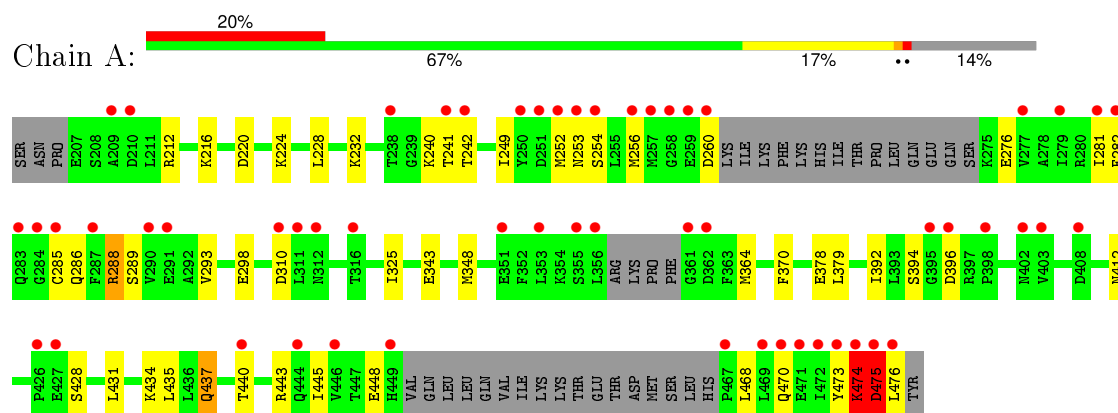
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		
3	B	68	Total	O	0	0
			68	68		

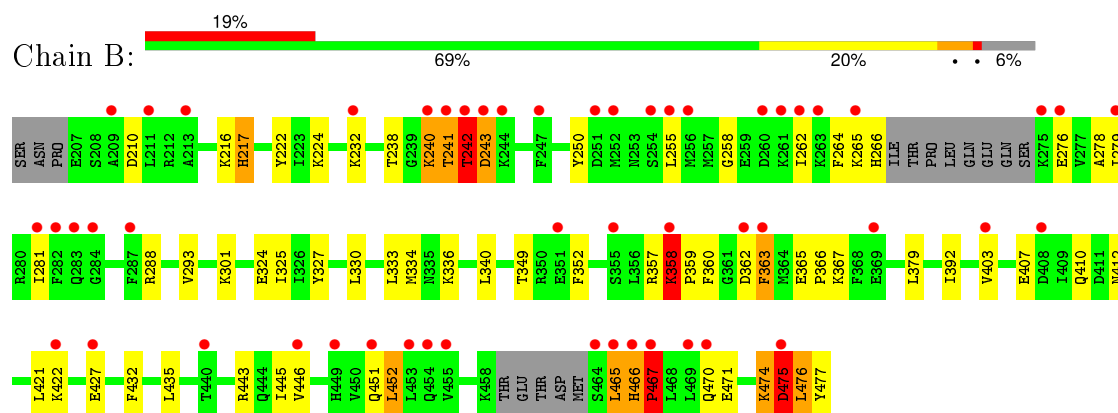
3 Residue-property plots

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, α , β , γ	90.80 Å 62.26 Å 118.07 Å 90.00° 101.12° 90.00°	Depositor
Resolution (Å)	10.00 – 2.41 10.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	90.9 (10.00-2.41) 90.9 (10.00-2.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 2.41 Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.269 , 0.284 0.264 , 0.275	Depositor DCC
R_{free} test set	1146 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 64.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 22642 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4069	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF2

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	0.42	0/1865	0.84	4/2516 (0.2%)
1	B	0.47	1/2081 (0.0%)	0.58	2/2802 (0.1%)
All	All	0.45	1/3946 (0.0%)	0.72	6/5318 (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	1	2
1	B	1	7
All	All	2	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	LYS	CE-NZ	6.91	1.66	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	ASP	N-CA-C	21.73	169.66	111.00
1	A	475	ASP	CB-CA-C	-18.43	73.55	110.40
1	A	475	ASP	C-N-CA	12.65	153.32	121.70
1	B	243	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	475	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	475	ASP	CB-CG-OD2	5.09	122.88	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	475	ASP	CA
1	B	466	HIS	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	LYS	Peptide
1	A	475	ASP	Peptide
1	B	240	LYS	Peptide
1	B	242	THR	Peptide
1	B	243	ASP	Peptide
1	B	465	LEU	Peptide
1	B	467	PRO	Peptide
1	B	475	ASP	Peptide
1	B	476	LEU	Peptide

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	1839	0	1842	41	0
1	B	2048	0	2088	57	0
2	A	29	0	17	10	0
2	B	29	0	17	2	0
3	A	56	0	0	7	0
3	B	68	0	0	2	0
All	All	4069	0	3964	98	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 12.

All (98) 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:474:LYS:HE2	1:A:474:LYS:CA	1.53	1.31
1:A:474:LYS:HA	1:A:474:LYS:CE	1.55	1.28
1:B:358:LYS:HB3	1:B:359:PRO:CD	1.72	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:LYS:HB3	1:B:359:PRO:HD3	1.09	1.04
1:B:240:LYS:O	1:B:241:THR:HG23	1.56	1.04
1:A:476:LEU:HD22	3:A:92:HOH:O	1.56	1.03
1:B:293:VAL:HG21	1:B:476:LEU:CB	1.89	1.01
1:A:394:SER:HB3	3:A:105:HOH:O	1.68	0.93
1:B:363:PHE:HB2	1:B:452:LEU:CD2	2.08	0.84
1:B:242:THR:O	1:B:242:THR:HG22	1.76	0.83
1:A:474:LYS:O	1:A:475:ASP:HB2	1.76	0.82
1:B:358:LYS:CB	1:B:359:PRO:HD3	2.03	0.82
1:B:217:HIS:O	1:B:217:HIS:CD2	2.33	0.82
1:A:474:LYS:CA	1:A:474:LYS:CE	2.30	0.82
1:B:327:TYR:HE2	1:B:367:LYS:HE2	1.44	0.79
2:A:5001:SF2:HAP	3:A:113:HOH:O	1.83	0.78
1:B:217:HIS:CD2	1:B:217:HIS:C	2.57	0.77
1:B:358:LYS:CB	1:B:359:PRO:CD	2.57	0.77
1:B:362:ASP:O	1:B:363:PHE:HB3	1.81	0.77
1:B:466:HIS:H	1:B:470:GLN:HG3	1.51	0.75
1:A:288:ARG:HG3	2:A:5001:SF2:CAT	2.15	0.75
1:B:240:LYS:O	1:B:241:THR:CG2	2.34	0.74
1:B:258:GLY:O	1:B:262:ILE:HB	1.89	0.73
1:A:474:LYS:N	1:A:474:LYS:HE2	2.03	0.72
1:A:476:LEU:CD2	3:A:92:HOH:O	2.23	0.72
1:A:474:LYS:HA	1:A:474:LYS:HE2	0.75	0.70
1:B:363:PHE:HB2	1:B:452:LEU:HD22	1.71	0.70
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.73	0.70
1:B:327:TYR:CE2	1:B:367:LYS:HE2	2.28	0.69
1:B:363:PHE:HB2	1:B:452:LEU:HD21	1.74	0.68
1:A:364:MET:HE2	2:A:5001:SF2:HAM	1.75	0.68
1:B:327:TYR:HE2	1:B:367:LYS:CE	2.09	0.65
1:B:301:LYS:O	3:B:65:HOH:O	2.13	0.65
1:B:238:THR:OG1	1:B:240:LYS:HB2	1.96	0.65
1:A:428:SER:HB3	1:A:431:LEU:HB2	1.79	0.65
1:B:242:THR:O	1:B:242:THR:CG2	2.46	0.63
1:A:281:ILE:HG23	3:A:113:HOH:O	1.97	0.63
1:B:330:LEU:HD23	1:B:367:LYS:HD3	1.81	0.63
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.81	0.61
1:B:470:GLN:O	1:B:474:LYS:HB3	2.01	0.61
1:B:474:LYS:HG2	1:B:475:ASP:N	2.16	0.60
1:A:364:MET:CE	2:A:5001:SF2:HAM	2.31	0.60
1:A:474:LYS:O	1:A:475:ASP:CB	2.47	0.59
1:A:370:PHE:CB	1:A:445:ILE:HD11	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:O	1:B:334:MET:HG3	2.04	0.58
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.33	0.58
1:B:363:PHE:CD1	1:B:363:PHE:O	2.57	0.56
1:A:440:THR:HG21	1:B:443:ARG:HD2	1.88	0.55
1:B:324:GLU:HG3	1:B:446:VAL:HG21	1.89	0.55
1:B:333:LEU:HB3	1:B:340:LEU:HB2	1.87	0.55
1:B:240:LYS:C	1:B:241:THR:HG23	2.26	0.54
1:B:362:ASP:O	1:B:363:PHE:CB	2.53	0.53
2:A:5001:SF2:HAI	2:A:5001:SF2:CBB	2.38	0.53
1:B:217:HIS:O	1:B:217:HIS:CG	2.61	0.53
1:B:293:VAL:CG2	1:B:476:LEU:CB	2.77	0.52
1:A:470:GLN:O	1:A:474:LYS:HE3	2.11	0.51
1:A:212:ARG:HD2	3:A:73:HOH:O	2.11	0.51
1:A:348:MET:HE1	2:A:5001:SF2:HAF	1.92	0.51
2:B:7001:SF2:CBB	2:B:7001:SF2:HAI	2.41	0.51
1:B:476:LEU:O	1:B:477:TYR:CB	2.59	0.50
1:A:348:MET:CE	2:A:5001:SF2:HAF	2.41	0.50
1:B:403:VAL:HG12	1:B:407:GLU:HG3	1.92	0.50
1:A:282:PHE:O	1:A:286:GLN:HB2	2.11	0.50
1:A:253:ASN:HA	1:A:256:MET:HB3	1.95	0.49
1:B:465:LEU:O	1:B:466:HIS:CB	2.60	0.49
1:B:471:GLU:O	1:B:474:LYS:NZ	2.46	0.49
1:B:240:LYS:O	1:B:241:THR:OG1	2.31	0.48
1:A:288:ARG:CG	2:A:5001:SF2:CAT	2.89	0.48
1:A:228:LEU:HD12	1:A:232:LYS:HD2	1.95	0.48
1:A:437:GLN:OE1	1:B:410:GLN:NE2	2.46	0.47
1:B:379:LEU:HD11	1:B:435:LEU:HD13	1.97	0.47
1:A:285:CYS:HB2	2:A:5001:SF2:CAP	2.45	0.47
1:B:466:HIS:HA	1:B:467:PRO:HA	1.59	0.47
1:B:365:GLU:N	1:B:366:PRO:HD2	2.30	0.47
1:A:474:LYS:N	1:A:474:LYS:CE	2.71	0.47
1:B:232:LYS:HB2	1:B:232:LYS:HE3	1.69	0.46
1:A:288:ARG:HG3	2:A:5001:SF2:OAB	2.15	0.46
1:A:289:SER:O	1:A:293:VAL:HG23	2.16	0.46
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.97	0.46
1:B:240:LYS:O	1:B:241:THR:CB	2.63	0.45
1:B:255:LEU:HD22	1:B:352:PHE:CZ	2.51	0.45
1:B:279:ILE:HD12	1:B:360:PHE:HZ	1.80	0.45
1:B:222:TYR:HD1	3:B:118:HOH:O	1.99	0.45
1:A:440:THR:CG2	1:B:443:ARG:HD2	2.45	0.45
1:B:421:LEU:HD12	1:B:432:PHE:HA	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ALA:HA	1:B:281:ILE:HD12	1.99	0.43
1:B:276:GLU:O	1:B:279:ILE:HG22	2.19	0.43
1:B:288:ARG:HG2	2:B:7001:SF2:CAT	2.49	0.42
1:A:249:ILE:HA	1:A:254:SER:HB3	2.01	0.42
1:A:288:ARG:HD2	1:A:288:ARG:HA	1.73	0.42
1:A:228:LEU:HB2	1:A:343:GLU:HG3	2.02	0.42
1:B:250:TYR:HA	1:B:349:THR:OG1	2.20	0.41
1:A:473:TYR:O	1:A:475:ASP:N	2.54	0.41
1:B:241:THR:HB	1:B:242:THR:H	1.73	0.41
1:B:325:ILE:HD11	1:B:392:ILE:HG13	2.01	0.41
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.51	0.41
1:A:298:GLU:HG3	3:A:39:HOH:O	2.22	0.40
1:A:220:ASP:O	1:A:224:LYS:HD2	2.21	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	227/274 (83%)	209 (92%)	14 (6%)	4 (2%)	11	13
1	B	252/274 (92%)	234 (93%)	12 (5%)	6 (2%)	7	7
All	All	479/548 (87%)	443 (92%)	26 (5%)	10 (2%)	9	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	241	THR
1	B	357	ARG
1	B	358	LYS
1	B	466	HIS
1	A	242	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	264	PHE
1	A	474	LYS
1	A	276	GLU
1	B	467	PRO
1	A	310	ASP

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	201/247 (81%)	187 (93%)	14 (7%)	19	29
1	B	224/247 (91%)	206 (92%)	18 (8%)	15	23
All	All	425/494 (86%)	393 (92%)	32 (8%)	17	26

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	241	THR
1	A	252	MET
1	A	260	ASP
1	A	288	ARG
1	A	378	GLU
1	A	396	ASP
1	A	412	ASN
1	A	434	LYS
1	A	437	GLN
1	A	443	ARG
1	A	448	GLU
1	A	468	LEU
1	A	474	LYS
1	B	210	ASP
1	B	216	LYS
1	B	217	HIS
1	B	224	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	242	THR
1	B	265	LYS
1	B	266	HIS
1	B	336	LYS
1	B	358	LYS
1	B	363	PHE
1	B	412	ASN
1	B	422	LYS
1	B	427	GLU
1	B	445	ILE
1	B	451	GLN
1	B	452	LEU
1	B	474	LYS
1	B	475	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	GLN
1	B	217	HIS
1	B	410	GLN

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](#)

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	SF2	A	5001	-	25,32,32	0.95	1 (4%)	28,45,45	1.37	1 (3%)
2	SF2	B	7001	-	25,32,32	0.94	0	28,45,45	1.14	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	SF2	A	5001	-	-	0/8/14/14	0/4/4/4
2	SF2	B	7001	-	-	0/8/14/14	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5001	SF2	CAQ-CAV	2.34	1.56	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7001	SF2	CAA-OAR-CAW	-2.11	112.57	117.51
2	B	7001	SF2	CAX-SAS-CAY	4.19	113.13	101.96
2	A	5001	SF2	CAX-SAS-CAY	5.94	117.81	101.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	SF2	10	0
2	B	7001	SF2	2	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, 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	235/274 (85%)	1.16	56 (23%) ⓘ ⓘ	47, 90, 173, 225	5 (2%)
1	B	258/274 (94%)	0.89	52 (20%) ⓘ ⓘ	39, 71, 137, 156	0
All	All	493/548 (89%)	1.02	108 (21%) ⓘ ⓘ	39, 82, 155, 225	5 (1%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	242	THR	13.5
1	B	243	ASP	10.4
1	A	470	GLN	8.0
1	A	260	ASP	7.0
1	B	454	GLN	6.7
1	A	475	ASP	6.3
1	A	471	GLU	5.8
1	B	470	GLN	5.8
1	B	256	MET	5.7
1	B	241	THR	5.7
1	A	259	GLU	5.0
1	A	282	PHE	4.7
1	A	256	MET	4.7
1	A	440	THR	4.6
1	B	469	LEU	4.6
1	A	398	PRO	4.4
1	A	469	LEU	4.4
1	B	287	PHE	4.4
1	B	451	GLN	4.3
1	B	260	ASP	4.2
1	A	257	MET	4.1
1	B	358	LYS	4.1
1	A	283	GLN	4.1
1	B	251	ASP	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	472	ILE	4.1
1	A	403	VAL	3.9
1	B	240	LYS	3.9
1	A	287	PHE	3.8
1	A	467	PRO	3.7
1	A	312	ASN	3.6
1	A	250	TYR	3.6
1	A	284	GLY	3.6
1	B	209	ALA	3.5
1	B	363	PHE	3.5
1	A	396	ASP	3.5
1	B	283	GLN	3.5
1	B	351	GLU	3.4
1	A	258	GLY	3.4
1	A	290	VAL	3.4
1	A	356	LEU	3.3
1	B	465	LEU	3.3
1	A	242	THR	3.3
1	B	453	LEU	3.3
1	A	395	GLY	3.2
1	B	467	PRO	3.1
1	B	466	HIS	3.1
1	A	444	GLN	3.1
1	A	473	TYR	3.1
1	A	311	LEU	3.1
1	A	210	ASP	3.0
1	A	474	LYS	3.0
1	B	261	LYS	2.9
1	B	282	PHE	2.9
1	B	440	THR	2.9
1	B	276	GLU	2.9
1	B	262	ILE	2.9
1	A	277	VAL	2.9
1	A	253	ASN	2.9
1	A	351	GLU	2.9
1	B	475	ASP	2.8
1	A	279	ILE	2.8
1	A	254	SER	2.8
1	B	449	HIS	2.8
1	A	310	ASP	2.8
1	B	255	LEU	2.8
1	A	316	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	209	ALA	2.8
1	A	355	SER	2.8
1	B	275	LYS	2.7
1	A	241	THR	2.7
1	B	355	SER	2.7
1	B	213	ALA	2.7
1	B	244	LYS	2.7
1	B	211	LEU	2.6
1	B	265	LYS	2.6
1	A	238	THR	2.6
1	A	362	ASP	2.6
1	A	476	LEU	2.6
1	B	281	ILE	2.6
1	A	252	MET	2.5
1	A	446	VAL	2.5
1	B	464	SER	2.5
1	A	361	GLY	2.4
1	B	455	VAL	2.4
1	A	291	GLU	2.3
1	A	402	ASN	2.3
1	B	369	GLU	2.2
1	B	446	VAL	2.2
1	B	279	ILE	2.2
1	A	251	ASP	2.2
1	B	362	ASP	2.2
1	B	263	LYS	2.2
1	B	422	LYS	2.2
1	A	281	ILE	2.2
1	A	353	LEU	2.1
1	A	449	HIS	2.1
1	B	254	SER	2.1
1	B	403	VAL	2.1
1	B	252	MET	2.1
1	B	427	GLU	2.1
1	B	408	ASP	2.1
1	A	408	ASP	2.1
1	B	247	PHE	2.1
1	A	426	PRO	2.0
1	A	285	CYS	2.0
1	A	427	GLU	2.0
1	B	232	LYS	2.0
1	B	284	GLY	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	SF2	A	5001	29/29	0.81	0.22	0.05	60,77,85,87	0
2	SF2	B	7001	29/29	0.90	0.15	-0.71	55,60,68,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.