



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:13 AM UTC

PDB ID : 3PO9 / pdb_00003po9
Title : Crystal structure of PPARgamma ligand binding domain in complex with tripropyltin
Authors : le Maire, A.; Bourguet, W.
Deposited on : 2010-11-22
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

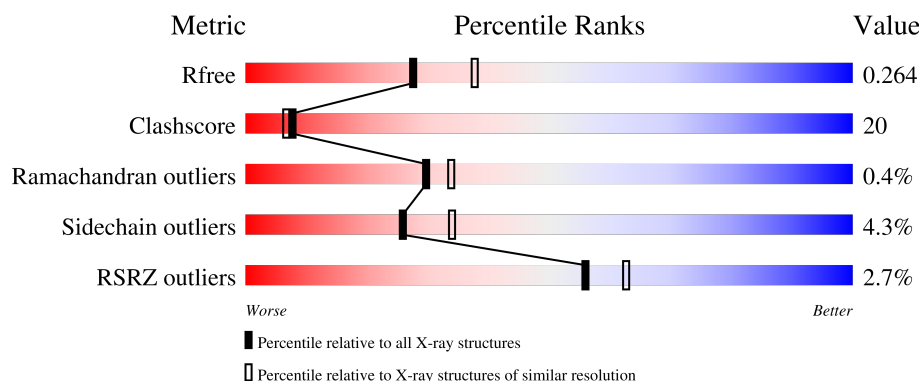
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

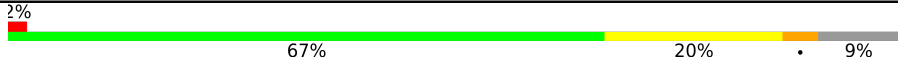
The reported resolution of this entry is 2.35 Å.

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))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	286	
1	B	286	

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	XPT	A	1[A]	-	-	X	X
2	XPT	A	1[B]	-	-	X	X
2	XPT	A	1[C]	-	-	X	X
2	XPT	B	1	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4344 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.

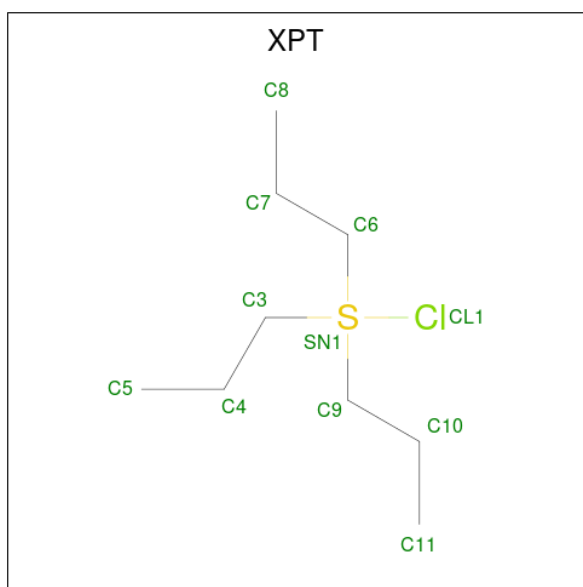
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	1	0
			2067	1332	336	389	10			
1	B	249	Total	C	N	O	S	0	2	0
			1986	1284	323	370	9			

There are 8 discrepancies between the modelled and reference sequences:

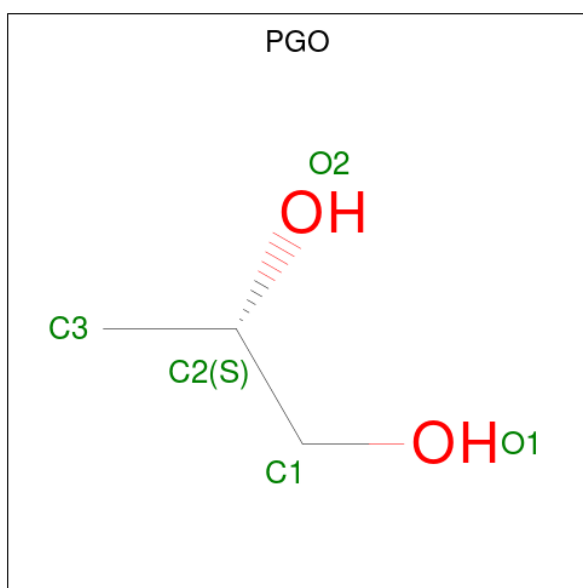
Chain	Residue	Modelled	Actual	Comment	Reference
A	192	GLY	-	expression tag	UNP P37231
A	193	SER	-	expression tag	UNP P37231
A	194	HIS	-	expression tag	UNP P37231
A	195	MET	-	expression tag	UNP P37231
B	192	GLY	-	expression tag	UNP P37231
B	193	SER	-	expression tag	UNP P37231
B	194	HIS	-	expression tag	UNP P37231
B	195	MET	-	expression tag	UNP P37231

- Molecule 2 is 1-[chloro(dipropyl)-lambda 4 -sulfanyl]propane (CCD ID: XPT) (formula: C₉H₂₁ClS).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	S	0	1
			30	27	3		
2	B	1	Total	C	S	0	0
			10	9	1		

- Molecule 3 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total	O	0	0
			118	118		
4	B	113	Total	O	0	0
			113	113		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.41Å 61.75Å 118.66Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	33.32 – 2.35 33.32 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.0 (33.32-2.35) 97.1 (33.32-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.6_289	Depositor
R, R_{free}	0.201 , 0.269 0.198 , 0.264	Depositor DCC
R_{free} test set	1351 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.6	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	0.94	EDS
Total number of atoms	4344	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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: PGO, XPT

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	0.50	0/2104	0.84	3/2841 (0.1%)
1	B	0.52	0/2024	0.79	1/2729 (0.0%)
All	All	0.51	0/4128	0.82	4/5570 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ASN	CA-C-N	7.04	128.64	119.84
1	A	205	ASN	C-N-CA	7.04	128.64	119.84
1	A	205	ASN	N-CA-C	6.75	114.30	108.22
1	B	377	LEU	N-CA-C	-5.71	106.31	113.28

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	2067	0	2100	76	0
1	B	1986	0	2012	64	0
2	A	30	0	63	37	0
2	B	10	0	21	8	0
3	B	20	0	32	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	118	0	0	5	0
4	B	113	0	0	5	0
All	All	4344	0	4228	167	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 (167) 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)
2:A:1[A]:XPT:C3	2:A:1[A]:XPT:SN1	2.13	1.36
2:A:1[A]:XPT:SN1	2:A:1[A]:XPT:C9	2.13	1.36
2:A:1[B]:XPT:SN1	2:A:1[B]:XPT:C3	2.14	1.36
2:A:1[C]:XPT:SN1	2:A:1[C]:XPT:C9	2.13	1.36
2:A:1[C]:XPT:SN1	2:A:1[C]:XPT:C3	2.13	1.36
2:B:1:XPT:C6	2:B:1:XPT:SN1	2.14	1.36
2:A:1[B]:XPT:SN1	2:A:1[B]:XPT:C6	2.14	1.36
2:A:1[C]:XPT:SN1	2:A:1[C]:XPT:C6	2.13	1.35
2:A:1[B]:XPT:SN1	2:A:1[B]:XPT:C9	2.14	1.35
2:A:1[A]:XPT:SN1	2:A:1[A]:XPT:C6	2.14	1.35
2:B:1:XPT:SN1	2:B:1:XPT:C3	2.15	1.35
2:B:1:XPT:SN1	2:B:1:XPT:C9	2.15	1.33
1:B:285:CYS:SG	2:B:1:XPT:SN1	2.49	1.10
1:A:364:MET:SD	2:A:1[B]:XPT:H9	1.96	1.05
1:B:256:MET:HE1	1:B:280:ARG:HH12	1.26	1.01
1:A:339:VAL:HG11	2:A:1[C]:XPT:H11	1.41	1.00
1:B:466:HIS:HD2	1:B:468:LEU:H	1.01	0.97
1:A:323:HIS:CE1	1:A:472:ILE:HG22	2.04	0.92
1:A:205:ASN:HD21	1:A:207:GLU:HG2	1.35	0.91
1:A:205:ASN:ND2	1:A:207:GLU:HG2	1.85	0.91
1:B:288[A]:ARG:HG3	1:B:288[A]:ARG:HH11	1.34	0.91
1:B:466:HIS:CD2	1:B:468:LEU:H	1.90	0.90
2:A:1[C]:XPT:H5A	4:A:508:HOH:O	1.76	0.84
1:B:288[B]:ARG:HD3	4:B:481:HOH:O	1.80	0.81
1:B:288[A]:ARG:HH11	1:B:288[A]:ARG:CG	1.96	0.77
1:A:330:LEU:HD11	2:A:1[C]:XPT:H10A	1.65	0.77
1:A:261:LYS:HD2	1:A:261:LYS:H	1.48	0.77
1:A:452:LEU:O	1:A:456:ILE:HG12	1.85	0.76
2:A:1[C]:XPT:H3	4:A:509:HOH:O	1.86	0.75
2:A:1[C]:XPT:H6A	2:A:1[C]:XPT:H11B	1.69	0.74
1:B:387:PHE:CE1	1:B:439:MET:HE2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:MET:SD	2:A:1[B]:XPT:C9	2.76	0.72
1:A:261:LYS:HD2	1:A:261:LYS:N	2.05	0.71
1:A:276:GLU:OE2	1:A:357:ARG:HD3	1.91	0.70
1:B:466:HIS:CD2	1:B:468:LEU:HB2	2.27	0.70
1:B:288[A]:ARG:HG3	1:B:288[A]:ARG:NH1	2.06	0.68
1:B:384:LEU:O	1:B:388:ILE:HG12	1.91	0.68
1:B:285:CYS:HB3	2:B:1:XPT:H10A	1.76	0.67
1:A:282:PHE:CE1	2:A:1[A]:XPT:H9A	2.30	0.67
1:A:219:TYR:CZ	1:A:223:ILE:HD11	2.31	0.66
1:A:261:LYS:HG2	1:A:262:ILE:H	1.59	0.66
1:A:286:GLN:HG2	4:A:528:HOH:O	1.95	0.66
1:B:247:PHE:CZ	1:B:257:MET:HG2	2.31	0.65
1:B:466:HIS:HD2	1:B:468:LEU:N	1.84	0.65
1:A:323:HIS:HE1	1:A:472:ILE:HG22	1.60	0.64
1:A:370:PHE:HA	1:A:373:LYS:HE2	1.79	0.64
1:A:474:LYS:O	1:A:475:ASP:HB2	1.96	0.64
2:A:1[A]:XPT:H10A	4:A:528:HOH:O	1.96	0.64
1:A:364:MET:HE2	2:A:1[C]:XPT:H11A	1.79	0.64
1:A:465:LEU:HD21	1:A:473:TYR:HD2	1.60	0.64
1:A:286:GLN:HE22	1:A:465:LEU:HA	1.64	0.63
2:A:1[C]:XPT:C6	2:A:1[C]:XPT:H11B	2.29	0.63
1:A:443:ARG:O	1:A:447:THR:HG23	2.01	0.61
1:A:255:LEU:O	1:A:259:GLU:HG3	2.00	0.61
1:A:456:ILE:HG21	1:A:463:MET:HE1	1.82	0.61
1:A:283:GLN:HE21	1:A:283:GLN:HA	1.65	0.61
1:A:473:TYR:HA	1:A:476:LEU:HD22	1.83	0.61
1:A:364:MET:CE	2:A:1[C]:XPT:H11A	2.31	0.61
1:A:323:HIS:CE1	1:A:472:ILE:CG2	2.80	0.60
3:B:478:PGO:H32	3:B:4:PGO:O1	2.01	0.60
1:A:323:HIS:CE1	1:A:476:LEU:HD21	2.37	0.59
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.31	0.59
1:B:364:MET:SD	2:B:1:XPT:H3	2.43	0.59
1:B:455:VAL:O	1:B:459:THR:HG22	2.03	0.58
1:B:325:ILE:HD13	1:B:388:ILE:HG23	1.85	0.58
1:A:322:VAL:HG21	1:A:472:ILE:HD13	1.86	0.58
1:A:350:ARG:HG3	1:A:368:PHE:CD2	2.39	0.58
1:B:300:ALA:HA	1:B:303:ILE:HD12	1.85	0.58
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.69	0.57
1:A:449:HIS:HE1	2:A:1[A]:XPT:H9	1.70	0.56
1:B:239:GLY:O	1:B:240:LYS:C	2.47	0.56
1:A:261:LYS:HG2	1:A:262:ILE:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:HG22	1:A:329:MET:HE2	1.87	0.56
1:A:277:VAL:HG22	1:A:280:ARG:HH21	1.72	0.55
1:B:443:ARG:O	1:B:447:THR:HG23	2.06	0.55
1:B:449:HIS:HE2	1:B:477:TYR:C	2.16	0.54
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.90	0.54
1:B:284:GLY:O	1:B:288[B]:ARG:HG2	2.08	0.54
1:B:226:PHE:CG	1:B:329:MET:HE1	2.43	0.54
1:A:205:ASN:HB2	1:A:206:PRO:HD2	1.90	0.53
1:A:434:LYS:HA	1:A:437:GLN:HG3	1.90	0.53
1:B:398:PRO:HD3	3:B:2:PGO:H11	1.91	0.53
1:B:247:PHE:HE1	1:B:257:MET:HE2	1.73	0.52
1:A:329:MET:O	1:A:332:SER:HB2	2.10	0.52
1:A:260:ASP:OD1	1:A:260:ASP:N	2.41	0.51
1:A:465:LEU:HD21	1:A:473:TYR:CD2	2.42	0.51
1:B:387:PHE:HE1	1:B:439:MET:HE2	1.72	0.51
1:A:283:GLN:HA	1:A:283:GLN:NE2	2.26	0.51
1:A:449:HIS:NE2	2:A:1[A]:XPT:H11B	2.26	0.51
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.46	0.51
1:B:256:MET:HA	1:B:256:MET:HE2	1.92	0.50
1:A:282:PHE:HE1	2:A:1[A]:XPT:H9A	1.74	0.50
1:A:402:ASN:O	1:A:405:PRO:HD2	2.11	0.50
1:A:394:SER:O	1:A:397:ARG:HG2	2.12	0.50
1:B:256:MET:HE1	1:B:280:ARG:NH1	2.09	0.49
1:B:370:PHE:HB2	1:B:445:ILE:HD11	1.94	0.49
2:B:1:XPT:H11A	2:B:1:XPT:H7	1.94	0.49
1:A:323:HIS:CD2	1:A:323:HIS:H	2.29	0.49
1:A:354:LYS:HD3	1:A:365:GLU:CG	2.42	0.49
1:A:433:ALA:O	1:A:437:GLN:HG2	2.13	0.49
1:B:255:LEU:CD2	1:B:277:VAL:HG13	2.44	0.48
1:B:387:PHE:HE1	1:B:439:MET:CE	2.26	0.48
1:B:324:GLU:OE2	1:B:443:ARG:HD3	2.12	0.48
1:A:449:HIS:CE1	2:A:1[A]:XPT:H9	2.49	0.47
1:B:370:PHE:CG	1:B:445:ILE:HD11	2.50	0.47
1:A:258:GLY:O	1:A:262:ILE:HB	2.15	0.46
1:B:370:PHE:CB	1:B:445:ILE:HD11	2.45	0.46
1:B:307:VAL:HG22	4:B:36:HOH:O	2.14	0.46
1:B:226:PHE:CD2	1:B:329:MET:HE1	2.50	0.46
1:B:288[A]:ARG:CG	1:B:288[A]:ARG:NH1	2.66	0.45
1:B:441:ASP:OD1	1:B:441:ASP:N	2.48	0.45
1:B:252:MET:SD	1:B:277:VAL:HG11	2.57	0.45
1:B:333:LEU:HB3	1:B:340:LEU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ASP:OD1	1:B:380:ASP:C	2.59	0.45
2:A:1[A]:XPT:SN1	2:A:1[A]:XPT:C4	2.99	0.45
2:A:1[B]:XPT:SN1	2:A:1[B]:XPT:C7	2.99	0.44
1:B:436:LEU:HD23	1:B:439:MET:HE3	1.99	0.44
1:A:252:MET:HE1	1:A:277:VAL:HG21	1.99	0.44
1:A:463:MET:HG2	1:A:464:SER:N	2.31	0.44
1:B:402:ASN:O	1:B:405:PRO:HD2	2.16	0.44
1:A:449:HIS:HE2	2:A:1[A]:XPT:H11B	1.82	0.44
1:A:456:ILE:CG2	1:A:463:MET:HE1	2.48	0.44
1:B:250:TYR:HB2	4:B:99:HOH:O	2.18	0.44
1:B:277:VAL:O	1:B:281:ILE:HG13	2.18	0.44
1:A:405:PRO:O	1:A:409:ILE:HG13	2.18	0.43
1:A:232:LYS:HE3	1:A:243:ASP:OD1	2.19	0.43
3:B:478:PGO:H32	3:B:4:PGO:C1	2.49	0.43
1:A:370:PHE:O	1:A:373:LYS:HG2	2.19	0.43
1:A:325:ILE:CG2	1:A:329:MET:HE2	2.48	0.42
1:A:452:LEU:HA	1:A:452:LEU:HD23	1.78	0.42
2:A:1[C]:XPT:SN1	2:A:1[C]:XPT:C10	2.99	0.42
1:B:288[A]:ARG:HD2	1:B:291:GLU:OE1	2.19	0.42
1:B:324:GLU:HG3	1:B:446:VAL:HG21	2.01	0.42
1:A:364:MET:SD	2:A:1[C]:XPT:H11A	2.60	0.42
1:A:440:THR:HG21	1:B:443:ARG:HG3	2.01	0.42
1:A:282:PHE:HE2	1:A:286:GLN:HE21	1.68	0.42
1:A:359:PRO:HG2	1:A:456:ILE:HD13	2.02	0.42
1:A:330:LEU:HD11	2:A:1[C]:XPT:C10	2.42	0.42
1:B:466:HIS:HD2	1:B:468:LEU:HB2	1.79	0.42
2:A:1[C]:XPT:SN1	2:A:1[C]:XPT:C7	3.02	0.42
1:B:325:ILE:HG23	1:B:388:ILE:HD12	2.02	0.42
1:A:303:ILE:HD11	1:A:392:ILE:HD12	2.02	0.42
1:A:327:TYR:HE2	2:A:1[B]:XPT:H11	1.85	0.42
1:B:468:LEU:O	1:B:472:ILE:HG13	2.20	0.42
1:A:257:MET:O	1:A:260:ASP:OD1	2.38	0.41
1:B:432:PHE:HB3	4:B:90:HOH:O	2.20	0.41
1:A:364:MET:SD	2:A:1[A]:XPT:H3	2.59	0.41
2:A:1[B]:XPT:SN1	2:A:1[B]:XPT:C4	3.01	0.41
2:A:1[B]:XPT:SN1	2:A:1[B]:XPT:C10	3.00	0.41
1:B:258:GLY:C	1:B:260:ASP:N	2.77	0.41
2:A:1[C]:XPT:H11B	2:A:1[C]:XPT:H8A	2.02	0.41
1:B:285:CYS:CB	2:B:1:XPT:H10A	2.48	0.41
1:B:442:LEU:O	1:B:446:VAL:HG23	2.19	0.41
1:A:261:LYS:H	1:A:261:LYS:CD	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:O	1:A:439:MET:HG2	2.20	0.41
1:B:438:LYS:HA	1:B:438:LYS:HD3	1.92	0.41
1:A:277:VAL:HG22	1:A:280:ARG:NH2	2.34	0.41
1:A:286:GLN:NE2	1:A:465:LEU:HA	2.31	0.41
1:B:318:LEU:O	1:B:322:VAL:HG13	2.21	0.41
1:B:325:ILE:HD11	1:B:392:ILE:HG12	2.03	0.41
1:A:453:LEU:HD12	1:A:453:LEU:HA	1.88	0.41
1:B:430:GLN:O	1:B:434:LYS:HG2	2.21	0.41
1:A:325:ILE:HD11	1:A:392:ILE:HG13	2.02	0.40
1:A:430:GLN:HA	4:A:67:HOH:O	2.21	0.40
1:B:288[A]:ARG:HD2	1:B:288[A]:ARG:HA	1.96	0.40
1:B:288[B]:ARG:HG3	3:B:478:PGO:H2	2.02	0.40
3:B:4:PGO:H31	4:B:169:HOH:O	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	258/286 (90%)	250 (97%)	7 (3%)	1 (0%)	30	34
1	B	243/286 (85%)	232 (96%)	10 (4%)	1 (0%)	30	34
All	All	501/572 (88%)	482 (96%)	17 (3%)	2 (0%)	30	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	GLU
1	B	239	GLY

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	229/258 (89%)	217 (95%)	12 (5%)	21	25
1	B	218/258 (84%)	210 (96%)	8 (4%)	30	40
All	All	447/516 (87%)	427 (96%)	20 (4%)	26	32

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
1	A	260	ASP
1	A	261	LYS
1	A	323	HIS
1	A	333	LEU
1	A	357	ARG
1	A	400	LEU
1	A	439	MET
1	A	452	LEU
1	A	453	LEU
1	A	456	ILE
1	A	476	LEU
1	B	276	GLU
1	B	288[A]	ARG
1	B	288[B]	ARG
1	B	311	LEU
1	B	434	LYS
1	B	441	ASP
1	B	460	GLU
1	B	468	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	283	GLN

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Mol	Chain	Res	Type
1	A	286	GLN
1	A	308	ASN
1	A	312	ASN
1	A	314	GLN
1	A	410	GLN
1	B	308	ASN
1	B	312	ASN
1	B	415	GLN
1	B	424	ASN
1	B	444	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	XPT	A	1[B]	-	6,9,10	0.34	0	3,9,12	0.29	0
3	PGO	B	478	-	4,4,4	0.79	0	4,4,4	0.59	0
2	XPT	A	1[C]	-	6,9,10	0.30	0	3,9,12	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	XPT	A	1[A]	-	6,9,10	0.32	0	3,9,12	0.43	0
3	PGO	B	2	-	4,4,4	0.85	0	4,4,4	0.71	0
3	PGO	B	4	-	4,4,4	0.80	0	4,4,4	0.69	0
3	PGO	B	3	-	4,4,4	0.86	0	4,4,4	0.74	0
2	XPT	B	1	-	6,9,10	0.34	0	3,9,12	0.33	0

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	XPT	A	1[B]	-	-	8/9/9/12	-
3	PGO	B	478	-	-	0/2/2/2	-
2	XPT	A	1[C]	-	-	4/9/9/12	-
2	XPT	A	1[A]	-	-	5/9/9/12	-
3	PGO	B	2	-	-	0/2/2/2	-
3	PGO	B	4	-	-	0/2/2/2	-
3	PGO	B	3	-	-	0/2/2/2	-
2	XPT	B	1	-	-	3/9/9/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1[A]	XPT	SN1-C3-C4-C5
2	A	1[A]	XPT	C7-C6-SN1-C3
2	A	1[B]	XPT	C4-C3-SN1-C6
2	A	1[B]	XPT	C4-C3-SN1-C9
2	A	1[B]	XPT	C7-C6-SN1-C3
2	A	1[B]	XPT	C7-C6-SN1-C9
2	A	1[B]	XPT	C11-C10-C9-SN1
2	A	1[B]	XPT	C10-C9-SN1-C3
2	A	1[B]	XPT	C10-C9-SN1-C6
2	A	1[C]	XPT	SN1-C3-C4-C5
2	A	1[C]	XPT	SN1-C6-C7-C8
2	A	1[B]	XPT	SN1-C3-C4-C5
2	A	1[A]	XPT	C7-C6-SN1-C9

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Mol	Chain	Res	Type	Atoms
2	A	1[A]	XPT	C10-C9-SN1-C3
2	A	1[A]	XPT	C10-C9-SN1-C6
2	B	1	XPT	C7-C6-SN1-C3
2	B	1	XPT	C7-C6-SN1-C9
2	A	1[C]	XPT	C7-C6-SN1-C3
2	A	1[C]	XPT	C7-C6-SN1-C9
2	B	1	XPT	C10-C9-SN1-C3

There are no ring outliers.

7 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1[B]	XPT	9	0
3	B	478	PGO	3	0
2	A	1[C]	XPT	16	0
2	A	1[A]	XPT	12	0
3	B	2	PGO	1	0
3	B	4	PGO	3	0
2	B	1	XPT	8	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	261/286 (91%)	0.25	7 (2%) 56 63	21, 39, 63, 83	1 (0%)
1	B	249/286 (87%)	0.24	7 (2%) 55 61	19, 38, 65, 80	2 (0%)
All	All	510/572 (89%)	0.24	14 (2%) 56 63	19, 39, 65, 83	3 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	ASP	3.5
1	A	444	GLN	2.8
1	A	476	LEU	2.8
1	A	204	LEU	2.7
1	B	475	ASP	2.5
1	A	275	LYS	2.5
1	A	260	ASP	2.4
1	B	275	LYS	2.3
1	B	428	SER	2.3
1	B	447	THR	2.2
1	B	451	GLN	2.2
1	A	262	ILE	2.1
1	B	209	ALA	2.1
1	B	260	ASP	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	XPT	A	1[A]	10/11	0.72	0.45	42,45,53,54	10
2	XPT	A	1[B]	10/11	0.72	0.45	38,44,46,53	10
2	XPT	A	1[C]	10/11	0.72	0.45	37,39,42,48	10
3	PGO	B	4	5/5	0.73	0.15	39,48,53,54	0
3	PGO	B	2	5/5	0.76	0.15	44,52,58,59	0
2	XPT	B	1	10/11	0.82	0.33	37,43,47,52	0
3	PGO	B	3	5/5	0.85	0.13	52,53,54,55	0
3	PGO	B	478	5/5	0.87	0.14	41,46,49,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.