



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 06:27 pm GMT

PDB ID : 3D5F
Title : Crystal Structure of PPAR-delta complex
Authors : Amano, Y.
Deposited on : 2008-05-16
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

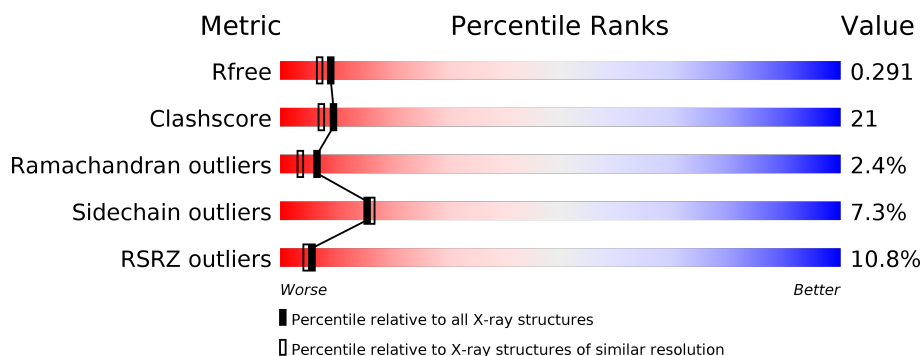
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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	267	
1	B	267	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4245 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.

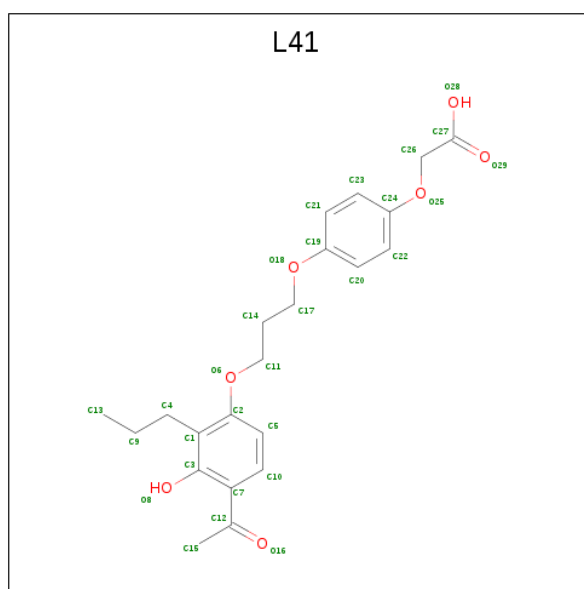
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2048	1329	345	364	10			
1	B	254	Total	C	N	O	S	0	0	0
			2052	1332	343	367	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	430	GLN	TYR	ENGINEERED	UNP Q03181
B	430	GLN	TYR	ENGINEERED	UNP Q03181

- Molecule 2 is {4-[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propoxy]phenoxy}acetic acid (three-letter code: L41) (formula: C₂₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			29	22	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			29	22	7		

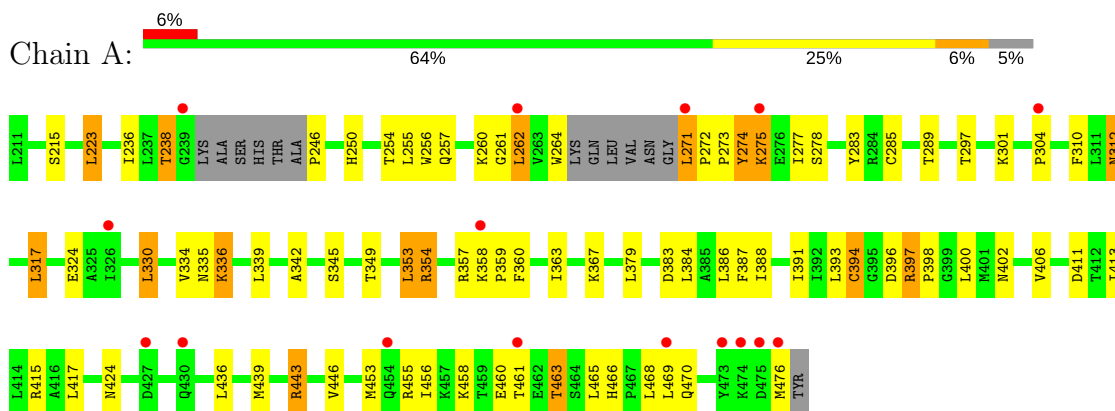
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	37	Total	O	0	0
			37	37		

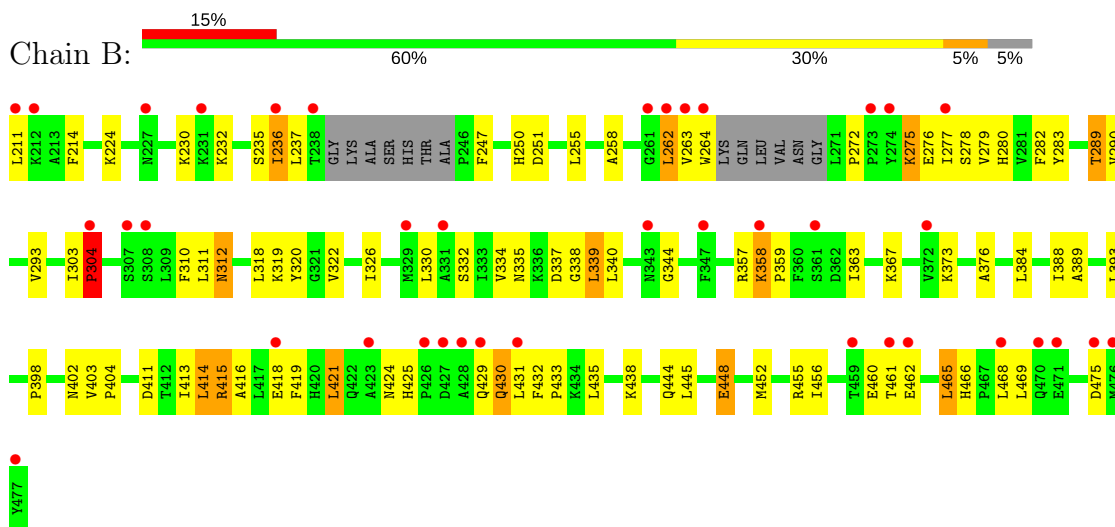
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 delta



- Molecule 1: Peroxisome proliferator-activated receptor delta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.46Å 92.83Å 96.45Å 90.00° 98.02° 90.00°	Depositor
Resolution (Å)	42.47 – 2.20 42.47 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (42.47-2.20) 97.0 (42.47-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.278 , 0.281 0.285 , 0.291	Depositor DCC
R_{free} test set	1698 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4245	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.64% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L41

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	0.40	0/2091	0.65	0/2823
1	B	0.39	0/2096	0.63	0/2832
All	All	0.40	0/4187	0.64	0/5655

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	2048	0	2094	78	0
1	B	2052	0	2079	97	0
2	A	29	0	24	2	0
2	B	29	0	24	2	0
3	A	50	0	0	3	0
3	B	37	0	0	1	0
All	All	4245	0	4221	175	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 21.

All (175) 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:293:VAL:HG22	1:B:322:VAL:HG11	1.23	1.13
1:B:247:PHE:HB3	1:B:262:LEU:HD11	1.48	0.95
1:B:275:LYS:HD3	1:B:275:LYS:H	1.32	0.93
1:B:275:LYS:HD3	1:B:275:LYS:N	1.84	0.92
1:A:465:LEU:HD23	1:A:470:GLN:HG2	1.53	0.90
1:A:312:ASN:H	1:A:312:ASN:HD22	1.18	0.90
1:B:275:LYS:H	1:B:275:LYS:CD	1.83	0.90
1:B:363:ILE:HG22	1:B:452:MET:SD	2.14	0.88
1:B:358:LYS:HE2	1:B:358:LYS:H	1.39	0.84
1:B:411:ASP:O	1:B:415:ARG:HG2	1.76	0.84
1:A:436:LEU:HA	1:A:439:MET:HE3	1.62	0.81
1:B:358:LYS:N	1:B:358:LYS:HE2	1.96	0.81
1:B:237:LEU:HD21	1:B:335:ASN:HD21	1.46	0.80
1:B:236:ILE:HD12	1:B:344:GLY:HA3	1.66	0.77
1:B:358:LYS:CE	1:B:358:LYS:H	1.98	0.76
1:A:312:ASN:N	1:A:312:ASN:HD22	1.85	0.75
1:A:285:CYS:O	1:A:289:THR:HG23	1.88	0.74
1:B:255:LEU:HD13	1:B:277:ILE:HD11	1.69	0.74
1:B:293:VAL:HG22	1:B:322:VAL:CG1	2.14	0.73
1:A:257:GLN:HG3	1:A:262:LEU:HD11	1.70	0.73
1:B:289:THR:HG21	2:B:501:L41:O28	1.88	0.72
1:B:456:ILE:O	1:B:460:GLU:HB2	1.90	0.71
1:B:335:ASN:HB3	1:B:337:ASP:H	1.55	0.71
1:A:460:GLU:HB3	1:A:463:THR:HG23	1.72	0.70
1:A:411:ASP:OD2	1:A:415:ARG:HD2	1.90	0.70
1:B:415:ARG:O	1:B:418:GLU:HB3	1.92	0.70
1:A:363:ILE:CD1	1:A:453:MET:HE2	2.23	0.69
1:B:237:LEU:HD23	1:B:237:LEU:O	1.93	0.69
1:A:466:HIS:CD2	1:A:468:LEU:H	2.11	0.69
1:B:461:THR:O	1:B:462:GLU:HB2	1.92	0.68
1:B:310:PHE:HB3	1:B:312:ASN:ND2	2.09	0.67
1:B:312:ASN:N	1:B:312:ASN:HD22	1.92	0.67
1:B:275:LYS:HG3	1:B:279:VAL:CG1	2.24	0.67
1:A:466:HIS:HD2	1:A:468:LEU:H	1.42	0.66
1:A:310:PHE:HB3	1:A:312:ASN:ND2	2.11	0.66
1:B:255:LEU:HD13	1:B:277:ILE:CD1	2.25	0.66
1:A:274:TYR:O	1:A:275:LYS:HG3	1.97	0.65
1:A:246:PRO:HA	1:A:345:SER:O	1.96	0.65
1:A:367:LYS:HD2	1:A:367:LYS:N	2.11	0.65
1:B:312:ASN:H	1:B:312:ASN:HD22	1.42	0.65
1:B:424:ASN:HD22	1:B:425:HIS:CE1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:PHE:CB	1:A:312:ASN:HD21	2.11	0.64
1:A:256:TRP:CZ2	1:A:260:LYS:HD2	2.33	0.63
1:A:272:PRO:HG2	1:A:283:TYR:CE2	2.34	0.62
1:A:310:PHE:HB3	1:A:312:ASN:HD21	1.65	0.61
1:B:358:LYS:HB2	1:B:359:PRO:HD3	1.82	0.61
1:B:373:LYS:HB2	3:B:66:HOH:O	2.00	0.61
1:B:310:PHE:HB3	1:B:312:ASN:HD21	1.65	0.60
1:A:470:GLN:HG3	3:A:42:HOH:O	2.02	0.60
1:A:386:LEU:HD13	1:A:417:LEU:HA	1.84	0.60
1:B:275:LYS:HG2	1:B:276:GLU:H	1.67	0.60
1:A:402:ASN:O	1:A:406:VAL:HG23	2.02	0.59
1:A:236:ILE:C	1:A:238:THR:H	2.05	0.59
1:B:264:TRP:HD1	1:B:264:TRP:H	1.49	0.59
1:B:432:PHE:HB3	1:B:433:PRO:HD3	1.85	0.58
1:A:363:ILE:HD13	1:A:453:MET:CE	2.34	0.58
1:B:214:PHE:CE2	1:B:304:PRO:HG2	2.39	0.57
1:A:215:SER:OG	1:A:386:LEU:HD11	2.04	0.56
1:A:363:ILE:CD1	1:A:453:MET:CE	2.84	0.55
1:A:336:LYS:HE3	3:A:29:HOH:O	2.06	0.55
1:B:275:LYS:HD2	1:B:283:TYR:HE2	1.70	0.55
1:B:255:LEU:HD23	1:B:255:LEU:C	2.28	0.54
1:B:430:GLN:O	1:B:433:PRO:HD2	2.08	0.54
1:A:393:LEU:HD13	1:A:413:ILE:HD11	1.90	0.53
1:B:465:LEU:CD1	1:B:469:LEU:HB2	2.39	0.53
1:B:236:ILE:CD1	1:B:344:GLY:HA3	2.37	0.53
1:A:317:LEU:HD13	1:A:400:LEU:HD21	1.91	0.53
1:B:275:LYS:HE3	1:B:280:HIS:HA	1.90	0.53
1:B:389:ALA:O	1:B:393:LEU:HD23	2.09	0.52
1:A:250:HIS:CD2	1:A:254:THR:HG21	2.44	0.52
1:A:357:ARG:HB3	1:A:359:PRO:HD2	1.91	0.52
1:A:310:PHE:CB	1:A:312:ASN:ND2	2.72	0.52
1:B:358:LYS:HB2	1:B:359:PRO:CD	2.40	0.52
1:B:340:LEU:HB3	1:B:344:GLY:HA2	1.91	0.52
1:A:465:LEU:HD23	1:A:470:GLN:HE21	1.75	0.52
1:A:312:ASN:N	1:A:312:ASN:ND2	2.56	0.52
1:B:237:LEU:HD21	1:B:335:ASN:ND2	2.18	0.52
1:A:324:GLU:HG3	1:A:446:VAL:HG21	1.92	0.51
1:A:411:ASP:O	1:A:415:ARG:HG3	2.10	0.51
1:A:277:ILE:HG23	1:A:278:SER:N	2.25	0.51
1:B:318:LEU:O	1:B:322:VAL:HG23	2.11	0.50
1:B:258:ALA:HB1	1:B:262:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:LEU:O	1:B:388:ILE:HG12	2.12	0.50
1:A:289:THR:HG22	2:A:501:L41:H13	1.93	0.50
1:B:340:LEU:HD22	1:B:344:GLY:HA2	1.94	0.50
1:B:319:LYS:NZ	1:B:475:ASP:HB2	2.28	0.49
1:A:394:CYS:SG	1:A:396:ASP:HB2	2.52	0.49
1:B:211:LEU:HD23	1:B:419:PHE:CD2	2.48	0.49
1:B:262:LEU:O	1:B:264:TRP:N	2.46	0.49
1:B:393:LEU:HD22	1:B:393:LEU:N	2.27	0.49
1:B:444:GLN:NE2	1:B:448:GLU:OE2	2.45	0.49
1:A:255:LEU:C	1:A:255:LEU:HD23	2.33	0.49
1:A:379:LEU:HB3	1:A:383:ASP:HB2	1.95	0.49
1:B:465:LEU:HD12	1:B:469:LEU:HB2	1.94	0.49
1:B:403:VAL:HB	1:B:404:PRO:HD3	1.95	0.48
1:B:320:TYR:CZ	1:B:398:PRO:HG2	2.48	0.48
1:B:264:TRP:N	1:B:264:TRP:CD1	2.78	0.48
1:B:275:LYS:HE3	1:B:283:TYR:HD2	1.79	0.48
1:A:310:PHE:HB2	1:A:312:ASN:HD21	1.79	0.48
1:B:461:THR:O	1:B:462:GLU:CB	2.60	0.48
1:A:312:ASN:H	1:A:312:ASN:ND2	1.97	0.47
1:B:339:LEU:HD12	1:B:340:LEU:O	2.13	0.47
1:A:255:LEU:HD13	1:A:277:ILE:HD11	1.96	0.47
1:A:465:LEU:HD23	1:A:470:GLN:CG	2.36	0.47
1:B:230:LYS:HA	1:B:332:SER:HB3	1.97	0.47
1:A:334:VAL:CG1	1:A:335:ASN:N	2.77	0.47
1:A:367:LYS:HG2	2:A:501:L41:H17	1.96	0.47
1:B:312:ASN:ND2	1:B:312:ASN:N	2.62	0.47
1:A:384:LEU:O	1:A:388:ILE:HG12	2.15	0.46
1:B:335:ASN:HB2	1:B:338:GLY:O	2.15	0.46
1:A:360:PHE:O	1:A:363:ILE:HG22	2.15	0.46
1:A:317:LEU:HD12	1:A:397:ARG:HG3	1.98	0.46
1:A:466:HIS:CD2	1:A:468:LEU:HB3	2.51	0.46
1:B:367:LYS:HD2	1:B:367:LYS:N	2.29	0.46
1:A:264:TRP:CE2	1:A:342:ALA:HB2	2.50	0.46
1:A:396:ASP:CB	1:A:443:ARG:HH22	2.28	0.46
1:B:235:SER:C	1:B:237:LEU:H	2.18	0.46
1:A:466:HIS:HD2	1:A:468:LEU:N	2.10	0.46
1:B:330:LEU:HD21	2:B:501:L41:H14A	1.97	0.46
1:A:297:THR:HG22	1:A:301:LYS:HD3	1.98	0.46
1:B:279:VAL:HG12	1:B:283:TYR:CE2	2.50	0.46
1:A:330:LEU:HD21	1:A:339:LEU:HD12	1.98	0.46
1:B:358:LYS:CA	1:B:358:LYS:HE2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ARG:HD2	3:A:59:HOH:O	2.17	0.45
1:A:397:ARG:H	1:A:397:ARG:HG2	1.38	0.45
1:B:414:LEU:O	1:B:418:GLU:N	2.41	0.45
1:B:430:GLN:C	1:B:433:PRO:HD2	2.38	0.45
1:B:303:ILE:HG23	1:B:304:PRO:HD2	1.99	0.45
1:A:317:LEU:CD1	1:A:400:LEU:HD21	2.46	0.44
1:A:393:LEU:CD1	1:A:413:ILE:HD11	2.47	0.44
1:A:274:TYR:CG	1:A:275:LYS:N	2.84	0.44
1:B:322:VAL:HG12	1:B:326:ILE:CD1	2.48	0.44
1:A:367:LYS:N	1:A:367:LYS:CD	2.80	0.44
1:B:320:TYR:CE2	1:B:398:PRO:HG2	2.52	0.44
1:B:310:PHE:CB	1:B:312:ASN:HD21	2.30	0.44
1:B:224:LYS:HB3	1:B:224:LYS:HE2	1.83	0.43
1:B:415:ARG:H	1:B:415:ARG:HG2	1.62	0.43
1:A:272:PRO:HG2	1:A:283:TYR:CD2	2.54	0.43
1:B:373:LYS:O	1:B:376:ALA:HB3	2.18	0.43
1:B:275:LYS:HG3	1:B:279:VAL:HG12	1.98	0.43
1:B:393:LEU:CD2	1:B:393:LEU:N	2.81	0.43
1:A:236:ILE:C	1:A:238:THR:N	2.71	0.43
1:A:387:PHE:CE2	1:A:391:ILE:HD11	2.52	0.43
1:B:334:VAL:CG1	1:B:335:ASN:N	2.82	0.43
1:B:430:GLN:HE21	1:B:430:GLN:HB3	1.63	0.43
1:B:277:ILE:HG23	1:B:278:SER:N	2.34	0.43
1:B:466:HIS:HB3	1:B:469:LEU:HG	2.01	0.43
1:B:444:GLN:HE21	1:B:448:GLU:CD	2.22	0.43
1:B:272:PRO:O	1:B:275:LYS:NZ	2.49	0.42
1:A:397:ARG:HA	1:A:398:PRO:HD3	1.81	0.42
1:B:421:LEU:HD21	1:B:435:LEU:HD12	2.01	0.42
1:B:272:PRO:HG2	1:B:283:TYR:CE2	2.53	0.42
1:A:396:ASP:CG	1:A:443:ARG:HH12	2.23	0.42
1:A:357:ARG:C	1:A:359:PRO:HD2	2.40	0.42
1:A:273:PRO:O	1:A:274:TYR:O	2.38	0.42
1:B:438:LYS:HA	1:B:438:LYS:HD3	1.84	0.42
1:A:349:THR:O	1:A:353:LEU:HD22	2.20	0.42
1:B:322:VAL:HG12	1:B:326:ILE:HD12	2.00	0.42
1:B:290:VAL:HG21	1:B:466:HIS:CD2	2.55	0.42
1:B:413:ILE:O	1:B:416:ALA:HB3	2.20	0.41
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.87	0.41
1:B:275:LYS:HG3	1:B:279:VAL:HG11	1.99	0.41
1:A:460:GLU:HB3	1:A:463:THR:CG2	2.47	0.41
1:A:363:ILE:HD13	1:A:453:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:HIS:CE1	1:B:251:ASP:OD2	2.74	0.41
1:A:257:GLN:CG	1:A:262:LEU:HD11	2.46	0.41
1:A:271:LEU:N	1:A:272:PRO:HD2	2.36	0.41
1:A:455:ARG:NH1	1:A:458:LYS:HG2	2.36	0.41
1:B:429:GLN:O	1:B:430:GLN:HB2	2.21	0.41
1:B:311:LEU:HD12	1:B:311:LEU:HA	1.84	0.41
1:B:357:ARG:HG2	1:B:359:PRO:HD2	2.03	0.40
1:A:367:LYS:HD2	1:A:367:LYS:H	1.85	0.40
1:A:456:ILE:O	1:A:460:GLU:HB2	2.22	0.40
1:B:275:LYS:HE3	1:B:283:TYR:CD2	2.56	0.40
1:B:279:VAL:O	1:B:282:PHE:HB3	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	248/267 (93%)	228 (92%)	14 (6%)	6 (2%)	6	3
1	B	248/267 (93%)	226 (91%)	16 (6%)	6 (2%)	6	3
All	All	496/534 (93%)	454 (92%)	30 (6%)	12 (2%)	6	3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	TYR
1	B	263	VAL
1	B	304	PRO
1	B	358	LYS
1	A	275	LYS
1	B	232	LYS
1	A	238	THR

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Mol	Chain	Res	Type
1	A	261	GLY
1	B	236	ILE
1	B	262	LEU
1	A	262	LEU
1	A	358	LYS

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	225/236 (95%)	208 (92%)	17 (8%)	14	15
1	B	224/236 (95%)	208 (93%)	16 (7%)	16	17
All	All	449/472 (95%)	416 (93%)	33 (7%)	15	16

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	LEU
1	A	271	LEU
1	A	304	PRO
1	A	312	ASN
1	A	317	LEU
1	A	330	LEU
1	A	336	LYS
1	A	353	LEU
1	A	354	ARG
1	A	394	CYS
1	A	397	ARG
1	A	424	ASN
1	A	443	ARG
1	A	461	THR
1	A	463	THR
1	A	469	LEU
1	A	476	MET
1	B	275	LYS

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Mol	Chain	Res	Type
1	B	289	THR
1	B	304	PRO
1	B	312	ASN
1	B	339	LEU
1	B	402	ASN
1	B	414	LEU
1	B	415	ARG
1	B	421	LEU
1	B	430	GLN
1	B	431	LEU
1	B	445	LEU
1	B	448	GLU
1	B	455	ARG
1	B	465	LEU
1	B	468	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	227	ASN
1	A	250	HIS
1	A	312	ASN
1	A	314	GLN
1	A	402	ASN
1	A	420	HIS
1	A	422	GLN
1	A	424	ASN
1	A	437	GLN
1	A	466	HIS
1	A	470	GLN
1	B	225	ASN
1	B	250	HIS
1	B	257	GLN
1	B	312	ASN
1	B	335	ASN
1	B	402	ASN
1	B	425	HIS
1	B	430	GLN
1	B	444	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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	L41	A	501	-	27,30,30	2.43	11 (40%)	34,39,39	1.59	8 (23%)
2	L41	B	501	-	27,30,30	2.27	10 (37%)	34,39,39	1.37	6 (17%)

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	L41	A	501	-	-	0/18/20/20	0/2/2/2
2	L41	B	501	-	-	0/18/20/20	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	L41	O8-C3	-5.88	1.23	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	L41	O8-C3	-5.24	1.24	1.37
2	B	501	L41	C3-C1	2.16	1.43	1.40
2	B	501	L41	C15-C12	2.28	1.56	1.49
2	A	501	L41	C2-C1	2.45	1.43	1.40
2	B	501	L41	O18-C19	2.51	1.43	1.37
2	A	501	L41	C23-C24	2.69	1.44	1.38
2	A	501	L41	C4-C1	2.74	1.56	1.52
2	B	501	L41	C22-C24	2.92	1.44	1.38
2	B	501	L41	C21-C23	2.95	1.43	1.38
2	A	501	L41	C21-C19	3.16	1.44	1.38
2	A	501	L41	C10-C7	3.37	1.45	1.39
2	A	501	L41	C22-C24	3.40	1.45	1.38
2	A	501	L41	C3-C1	3.41	1.45	1.40
2	B	501	L41	C23-C24	3.51	1.45	1.38
2	A	501	L41	O18-C19	3.54	1.46	1.37
2	A	501	L41	C20-C22	3.70	1.45	1.38
2	B	501	L41	C20-C22	4.07	1.45	1.38
2	B	501	L41	C21-C19	4.08	1.46	1.38
2	B	501	L41	C20-C19	4.44	1.47	1.38
2	A	501	L41	C20-C19	4.53	1.47	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	L41	C7-C3-C1	-3.46	118.18	121.36
2	A	501	L41	C7-C3-C1	-2.66	118.91	121.36
2	B	501	L41	C4-C1-C2	-2.54	118.11	121.53
2	A	501	L41	C22-C20-C19	-2.11	117.14	119.73
2	A	501	L41	C20-C22-C24	-2.09	117.17	119.73
2	A	501	L41	C10-C7-C3	2.22	120.92	118.71
2	B	501	L41	C23-C24-C22	2.28	123.73	120.18
2	B	501	L41	O16-C12-C7	2.30	123.62	120.57
2	B	501	L41	C11-O6-C2	2.32	123.36	117.69
2	A	501	L41	C21-C19-C20	2.39	123.89	120.18
2	B	501	L41	C2-C1-C3	2.51	120.58	117.38
2	A	501	L41	C23-C24-C22	2.53	124.12	120.18
2	A	501	L41	C26-O25-C24	3.10	125.41	117.64
2	A	501	L41	O16-C12-C7	3.59	125.34	120.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	L41	2	0
2	B	501	L41	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	254/267 (95%)	0.79	16 (6%) 20 19	20, 34, 54, 72	0
1	B	254/267 (95%)	1.03	39 (15%) 2 1	23, 38, 64, 78	0
All	All	508/534 (95%)	0.91	55 (10%) 6 4	20, 36, 62, 78	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	VAL	7.0
1	A	239	GLY	5.6
1	B	262	LEU	5.3
1	A	271	LEU	4.7
1	A	358	LYS	4.7
1	A	262	LEU	4.5
1	B	427	ASP	4.3
1	B	238	THR	4.0
1	B	461	THR	3.9
1	B	304	PRO	3.9
1	B	426	PRO	3.9
1	A	476	MET	3.8
1	B	264	TRP	3.7
1	B	428	ALA	3.5
1	B	429	GLN	3.5
1	B	462	GLU	3.5
1	A	461	THR	3.3
1	B	231	LYS	3.2
1	B	475	ASP	3.1
1	B	358	LYS	3.1
1	B	477	TYR	3.0
1	A	304	PRO	3.0
1	B	274	TYR	3.0
1	B	236	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	275	LYS	2.9
1	B	308	SER	2.9
1	B	331	ALA	2.8
1	B	273	PRO	2.7
1	A	430	GLN	2.7
1	B	423	ALA	2.7
1	B	470	GLN	2.7
1	A	473	TYR	2.7
1	B	431	LEU	2.6
1	A	427	ASP	2.5
1	B	307	SER	2.5
1	A	475	ASP	2.5
1	B	361	SER	2.4
1	B	347	PHE	2.4
1	B	418	GLU	2.4
1	B	261	GLY	2.3
1	B	227	ASN	2.2
1	A	474	LYS	2.2
1	B	459	THR	2.2
1	B	212	LYS	2.2
1	B	471	GLU	2.2
1	A	326	ILE	2.2
1	B	329	MET	2.2
1	B	372	VAL	2.1
1	B	476	MET	2.1
1	A	469	LEU	2.1
1	B	211	LEU	2.0
1	B	343	ASN	2.0
1	A	454	GLN	2.0
1	B	277	ILE	2.0
1	B	468	LEU	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. 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(Å ²)	Q<0.9
2	L41	B	501	29/29	0.91	0.17	23,29,34,40	0
2	L41	A	501	29/29	0.92	0.16	16,25,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.