Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:23 AM GMT

PDB ID	:	2GWX
Title	:	MOLECULAR RECOGNITION OF FATTY ACIDS BY PEROXISOME PR OLIFERATOR-ACTIVATED RECEPTORS
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Deposited on	:	1999-03-11
Resolution	:	2.30 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 (1)) were used in the production of this report:

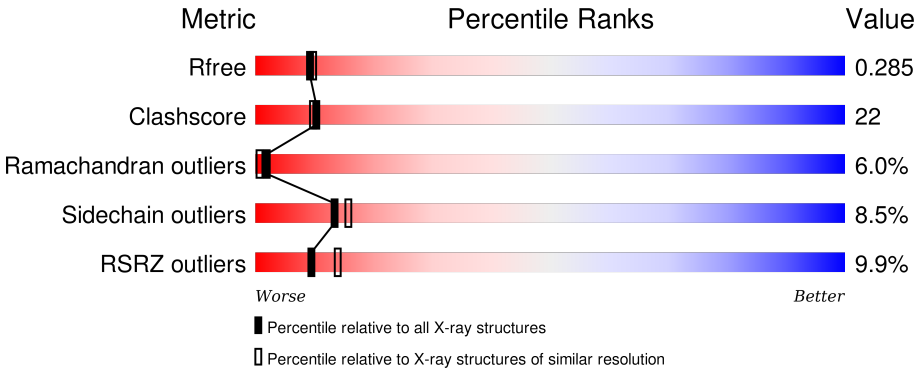
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	267	9% 64% 26% 7%
1	B	267	11% 56% 38% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4384 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 PROTEIN (PPAR-DELTA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	1
			2087	1347	356	375	9			
1	B	267	Total	C	N	O	S	0	0	0
			2112	1365	357	380	10			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is water.

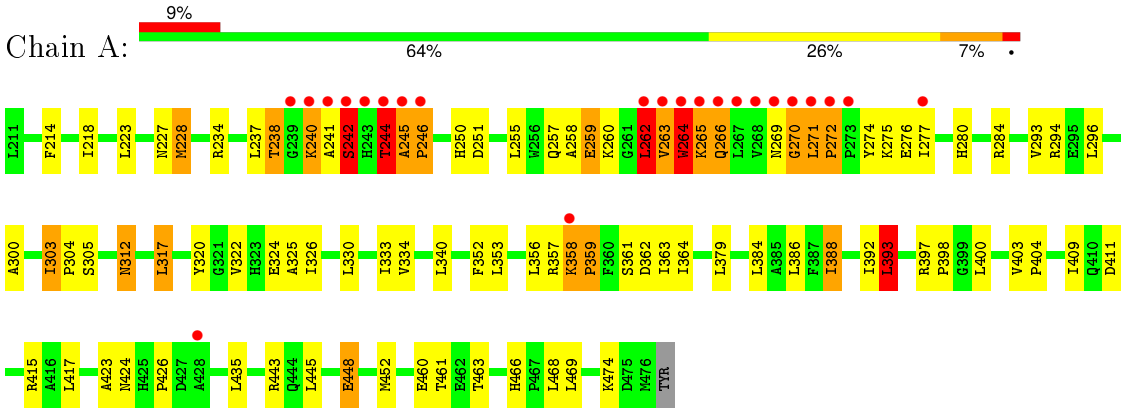
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	96	Total	O	0	0
			96	96		
2	B	89	Total	O	0	0
			89	89		

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.

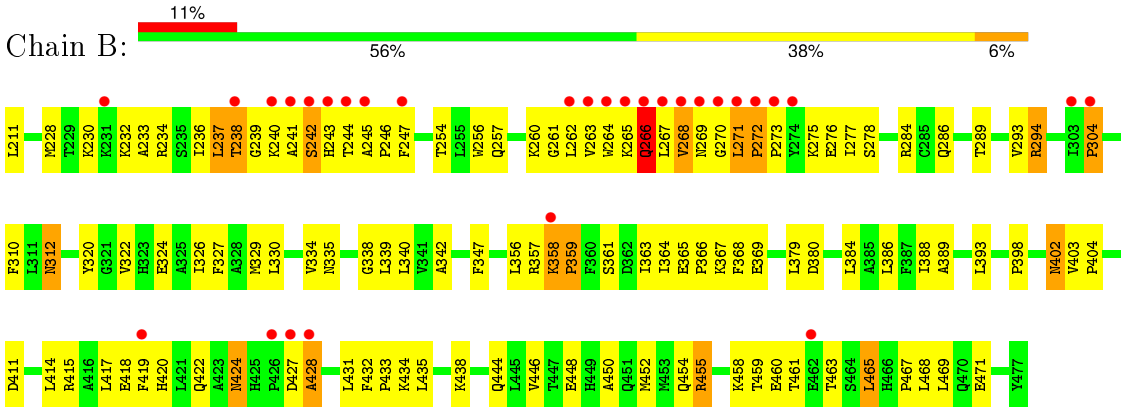
- Molecule 1: PROTEIN (PPAR-DELTA)

Chain A:



- Molecule 1: PROTEIN (PPAR-DELTA)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	39.77Å 94.22Å 96.70Å 90.00° 97.77° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.5 (8.00-2.30) 58.7 (8.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 2.00Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.246 , 0.288 0.244 , 0.285	Depositor DCC
R_{free} test set	2665 reflections (11.00%)	DCC
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 33836 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4384	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.45	0/2130	0.72	5/2883 (0.2%)
1	B	0.41	0/2157	0.66	0/2919
All	All	0.43	0/4287	0.69	5/5802 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	245	ALA	N-CA-C	12.12	143.73	111.00
1	A	244	THR	C-N-CA	6.20	137.19	121.70
1	A	262	LEU	CA-CB-CG	5.66	128.32	115.30
1	A	272	PRO	N-CA-CB	5.66	110.10	103.30
1	A	393	LEU	CA-CB-CG	-5.29	103.12	115.30

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	2087	0	2097	81	0
1	B	2112	0	2119	101	0
2	A	96	0	0	2	0
2	B	89	0	0	1	0
All	All	4384	0	4216	182	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 22.

All (182) 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:266:GLN:NE2	1:B:284:ARG:HH21	1.58	1.00
1:B:312:ASN:H	1:B:312:ASN:HD22	1.14	0.89
1:B:272:PRO:HD2	1:B:275:LYS:CB	2.04	0.87
1:A:384:LEU:O	1:A:388:ILE:HG22	1.73	0.87
1:A:445:LEU:O	1:A:448:GLU:HG3	1.76	0.85
1:B:266:GLN:HE22	1:B:284:ARG:NH2	1.73	0.84
1:A:228:MET:HG2	1:A:333:ILE:HD11	1.60	0.83
1:A:244:THR:O	1:A:246:PRO:HD2	1.79	0.83
1:A:312:ASN:H	1:A:312:ASN:HD22	1.28	0.81
1:B:432:PHE:HB3	1:B:433:PRO:CD	2.10	0.81
1:A:325:ALA:HB1	1:A:388:ILE:HD13	1.61	0.80
1:A:271:LEU:HB3	1:A:276:GLU:HA	1.64	0.78
1:B:269:ASN:HD21	1:B:271:LEU:HG	1.48	0.77
1:B:266:GLN:HE22	1:B:284:ARG:HH21	1.22	0.76
1:B:312:ASN:N	1:B:312:ASN:HD22	1.85	0.75
1:A:325:ALA:CB	1:A:388:ILE:HD13	2.17	0.75
1:B:432:PHE:HB3	1:B:433:PRO:HD3	1.67	0.74
1:B:266:GLN:NE2	1:B:284:ARG:NH2	2.30	0.74
1:B:240:LYS:HG3	1:B:241:ALA:H	1.51	0.74
1:A:270:GLY:O	1:A:271:LEU:HD23	1.88	0.73
1:B:465:LEU:H	1:B:465:LEU:HD22	1.54	0.72
1:B:460:GLU:O	1:B:463:THR:HG22	1.92	0.69
1:A:305:SER:HB2	1:A:409:ILE:HD13	1.75	0.69
1:B:339:LEU:HD23	1:B:340:LEU:O	1.93	0.69
1:B:455:ARG:HH21	1:B:455:ARG:HG2	1.57	0.69
1:A:270:GLY:O	1:A:275:LYS:CB	2.41	0.68
1:A:333:ILE:HG22	1:A:333:ILE:O	1.93	0.68
1:A:333:ILE:CG2	1:A:340:LEU:HB2	2.23	0.67
1:B:432:PHE:CB	1:B:433:PRO:HD3	2.24	0.67
1:A:300:ALA:O	1:A:303:ILE:HG23	1.94	0.67
1:B:357:ARG:HG2	1:B:359:PRO:HD2	1.75	0.67
1:B:358:LYS:CA	1:B:358:LYS:HE2	2.26	0.66
1:A:322:VAL:O	1:A:326:ILE:HG13	1.96	0.66
1:B:358:LYS:N	1:B:358:LYS:HE2	2.10	0.65
1:B:327:PHE:CZ	1:B:367:LYS:HE3	2.31	0.65
1:B:358:LYS:HA	1:B:358:LYS:HE2	1.80	0.64
1:A:262:LEU:HD12	1:A:263:VAL:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HD13	1:A:400:LEU:HD21	1.78	0.64
1:B:271:LEU:CD2	1:B:277:ILE:HA	2.28	0.63
1:B:228:MET:HE1	1:B:233:ALA:HA	1.79	0.63
1:A:264:TRP:HB3	1:A:284:ARG:HH22	1.62	0.63
1:A:312:ASN:N	1:A:312:ASN:HD22	1.97	0.63
1:B:271:LEU:HD21	1:B:277:ILE:HA	1.80	0.63
1:A:228:MET:HG2	1:A:333:ILE:CD1	2.30	0.62
1:B:236:ILE:O	1:B:237:LEU:HB2	1.98	0.62
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.34	0.62
1:B:432:PHE:CB	1:B:433:PRO:CD	2.73	0.62
1:A:250:HIS:CE1	1:A:251:ASP:OD2	2.53	0.62
1:A:324:GLU:OE2	1:A:443:ARG:HD3	2.00	0.62
1:B:432:PHE:HB3	1:B:433:PRO:HD2	1.81	0.62
1:A:330:LEU:HD13	1:A:334:VAL:HG21	1.83	0.61
1:A:293:VAL:HG22	1:A:322:VAL:HG21	1.83	0.61
1:A:393:LEU:HD22	1:A:409:ILE:HG21	1.83	0.60
1:A:388:ILE:O	1:A:388:ILE:HD12	2.00	0.60
1:A:379:LEU:HD11	1:A:435:LEU:HD21	1.84	0.60
1:A:333:ILE:HG23	1:A:340:LEU:HD12	1.85	0.59
1:A:271:LEU:HB3	1:A:276:GLU:CA	2.32	0.59
1:A:333:ILE:HG22	1:A:340:LEU:H	1.68	0.59
1:B:330:LEU:O	1:B:334:VAL:HG23	2.03	0.58
1:B:270:GLY:O	1:B:271:LEU:HB2	2.04	0.58
1:A:423:ALA:O	1:A:426:PRO:HD3	2.04	0.57
1:A:264:TRP:HB3	1:A:284:ARG:NH2	2.20	0.57
1:A:333:ILE:HG21	1:A:340:LEU:HB2	1.86	0.57
1:A:262:LEU:HD12	1:A:262:LEU:O	2.05	0.57
1:B:271:LEU:HD11	1:B:277:ILE:HB	1.87	0.56
1:A:305:SER:HB2	1:A:409:ILE:CD1	2.35	0.56
1:B:264:TRP:C	1:B:265:LYS:HG3	2.25	0.56
1:A:330:LEU:CD1	1:A:334:VAL:HG21	2.37	0.55
1:B:320:TYR:CZ	1:B:398:PRO:HG2	2.42	0.54
1:A:296:LEU:HD13	1:A:322:VAL:HG23	1.88	0.54
1:B:271:LEU:HD22	1:B:276:GLU:C	2.28	0.54
1:B:294:ARG:CG	1:B:294:ARG:HH11	2.20	0.54
1:B:268:VAL:CB	2:B:487:HOH:O	2.55	0.54
1:B:330:LEU:HD11	1:B:339:LEU:HD11	1.89	0.54
1:B:356:LEU:O	1:B:361:SER:HB3	2.08	0.53
1:B:264:TRP:HB3	1:B:266:GLN:NE2	2.23	0.53
1:B:272:PRO:HB2	1:B:273:PRO:CD	2.38	0.53
1:B:271:LEU:HD22	1:B:276:GLU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:ARG:O	1:B:459:THR:HG22	2.08	0.53
1:A:363:ILE:HG22	1:A:452:MET:SD	2.49	0.53
1:A:388:ILE:HD11	1:A:392:ILE:HD11	1.91	0.53
1:B:310:PHE:HB3	1:B:312:ASN:ND2	2.24	0.52
1:B:312:ASN:H	1:B:312:ASN:ND2	1.93	0.52
1:B:247:PHE:CZ	1:B:257:GLN:HG3	2.46	0.51
1:B:236:ILE:HG13	1:B:236:ILE:O	2.11	0.51
1:A:270:GLY:C	1:A:271:LEU:HD23	2.31	0.51
1:A:358:LYS:O	1:A:362:ASP:OD2	2.30	0.50
1:A:258:ALA:C	1:A:260:LYS:H	2.14	0.50
1:B:366:PRO:HA	1:B:369:GLU:OE2	2.10	0.50
1:A:241:ALA:O	1:A:242:SER:C	2.49	0.50
1:A:255:LEU:HD23	1:A:277:ILE:CD1	2.42	0.50
1:A:386:LEU:HD13	1:A:417:LEU:HA	1.92	0.50
1:A:294:ARG:HH11	1:A:294:ARG:HG2	1.76	0.50
1:A:411:ASP:O	1:A:415:ARG:HG3	2.11	0.50
1:B:246:PRO:HB2	1:B:347:PHE:HB2	1.94	0.50
1:A:264:TRP:O	1:A:265:LYS:O	2.30	0.50
1:A:241:ALA:O	1:A:242:SER:O	2.30	0.49
1:B:411:ASP:O	1:B:415:ARG:HG3	2.11	0.49
1:B:386:LEU:HD13	1:B:417:LEU:HA	1.93	0.49
1:B:340:LEU:HD23	1:B:347:PHE:HD2	1.78	0.49
1:B:432:PHE:CD2	1:B:433:PRO:HD3	2.48	0.48
1:B:261:GLY:O	1:B:262:LEU:HD23	2.12	0.48
1:A:277:ILE:HD11	1:A:352:PHE:HZ	1.79	0.48
1:B:312:ASN:ND2	1:B:312:ASN:N	2.56	0.48
1:B:329:MET:HG2	1:B:388:ILE:HD11	1.95	0.47
1:A:238:THR:O	1:A:238:THR:HG22	2.15	0.47
1:A:460:GLU:HB3	1:A:463:THR:HG23	1.97	0.47
1:A:255:LEU:HD23	1:A:277:ILE:HD13	1.96	0.47
1:A:262:LEU:HD12	1:A:262:LEU:C	2.35	0.47
1:B:256:TRP:O	1:B:260:LYS:HG3	2.15	0.47
1:B:363:ILE:HG22	1:B:452:MET:SD	2.55	0.47
1:A:364:ILE:HG23	2:A:512:HOH:O	2.14	0.47
1:A:466:HIS:CD2	1:A:468:LEU:H	2.33	0.47
1:A:403:VAL:HB	1:A:404:PRO:HD3	1.97	0.47
1:A:269:ASN:O	1:A:270:GLY:O	2.33	0.46
1:B:277:ILE:HG23	1:B:278:SER:N	2.31	0.46
1:B:455:ARG:HG2	1:B:455:ARG:NH2	2.29	0.46
1:B:254:THR:HA	1:B:257:GLN:HG2	1.97	0.46
1:B:434:LYS:O	1:B:438:LYS:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ASN:C	1:B:270:GLY:O	2.54	0.46
1:B:271:LEU:CD1	1:B:277:ILE:HB	2.46	0.46
1:A:294:ARG:NH1	1:A:294:ARG:HG2	2.31	0.46
1:B:324:GLU:HG3	1:B:446:VAL:HG21	1.97	0.46
1:B:310:PHE:HB3	1:B:312:ASN:HD21	1.79	0.46
1:A:356:LEU:HB2	1:A:361:SER:HB3	1.98	0.46
1:B:289:THR:O	1:B:293:VAL:HG23	2.16	0.45
1:B:247:PHE:HZ	1:B:257:GLN:HG3	1.82	0.45
1:B:266:GLN:O	1:B:267:LEU:C	2.53	0.45
1:B:271:LEU:N	1:B:272:PRO:CD	2.80	0.45
1:B:379:LEU:HD11	1:B:435:LEU:HD21	1.99	0.45
1:A:259:GLU:HA	1:A:259:GLU:OE1	2.16	0.45
1:B:242:SER:C	1:B:244:THR:H	2.18	0.45
1:B:241:ALA:C	1:B:243:HIS:H	2.20	0.45
1:A:303:ILE:HA	1:A:304:PRO:HD3	1.88	0.45
1:B:230:LYS:O	1:B:234:ARG:HG2	2.16	0.44
1:B:450:ALA:O	1:B:454:GLN:HG3	2.17	0.44
1:B:380:ASP:OD2	1:B:424:ASN:ND2	2.51	0.44
1:B:237:LEU:O	1:B:238:THR:CB	2.65	0.44
1:B:264:TRP:HB3	1:B:266:GLN:HE22	1.82	0.44
1:A:259:GLU:OE2	1:A:280:HIS:CE1	2.71	0.44
1:A:320:TYR:CB	1:A:397:ARG:HD2	2.48	0.44
1:A:312:ASN:H	1:A:312:ASN:ND2	2.06	0.43
1:B:365:GLU:N	1:B:366:PRO:CD	2.81	0.43
1:B:322:VAL:O	1:B:326:ILE:HG13	2.17	0.43
1:B:264:TRP:CB	1:B:266:GLN:HE22	2.31	0.43
1:B:294:ARG:NH1	1:B:294:ARG:CG	2.81	0.43
1:A:271:LEU:HA	1:A:275:LYS:C	2.39	0.43
1:A:262:LEU:CD1	1:A:262:LEU:O	2.67	0.43
1:A:325:ALA:HB2	1:A:388:ILE:HD13	1.97	0.43
1:A:466:HIS:HD2	1:A:468:LEU:HB3	1.83	0.43
1:B:389:ALA:O	1:B:393:LEU:HD23	2.18	0.43
1:B:427:ASP:O	1:B:428:ALA:O	2.37	0.43
1:A:214:PHE:CZ	1:A:218:ILE:HD11	2.54	0.43
1:B:467:PRO:O	1:B:471:GLU:HG2	2.18	0.43
1:B:402:ASN:HD22	1:B:402:ASN:C	2.22	0.43
1:B:271:LEU:N	1:B:271:LEU:HD23	2.33	0.43
1:B:419:PHE:O	1:B:422:GLN:N	2.52	0.42
1:A:466:HIS:CD2	1:A:468:LEU:HB3	2.54	0.42
1:B:211:LEU:HA	1:B:211:LEU:HD12	1.87	0.42
1:B:419:PHE:O	1:B:420:HIS:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:GLN:NE2	1:B:448:GLU:OE2	2.52	0.42
1:B:284:ARG:HA	1:B:284:ARG:HD3	1.77	0.42
1:A:244:THR:C	1:A:246:PRO:HD2	2.39	0.42
1:B:459:THR:HG23	1:B:460:GLU:N	2.35	0.42
1:A:255:LEU:CD2	1:A:277:ILE:CD1	2.98	0.42
1:A:397:ARG:HA	1:A:398:PRO:HD3	1.82	0.42
1:A:325:ALA:CB	1:A:388:ILE:CD1	2.94	0.42
1:B:403:VAL:HB	1:B:404:PRO:HD3	2.01	0.41
1:B:334:VAL:CG1	1:B:335:ASN:N	2.82	0.41
1:B:237:LEU:HD21	1:B:335:ASN:ND2	2.34	0.41
1:A:357:ARG:HB3	1:A:359:PRO:HD3	2.00	0.41
1:A:448:GLU:HB3	2:A:567:HOH:O	2.20	0.41
1:B:294:ARG:HG3	1:B:294:ARG:HH11	1.85	0.41
1:B:339:LEU:CD2	1:B:340:LEU:O	2.67	0.41
1:A:393:LEU:HD22	1:A:409:ILE:CG2	2.48	0.41
1:B:264:TRP:O	1:B:265:LYS:HG3	2.21	0.41
1:B:286:GLN:HB2	1:B:469:LEU:HD11	2.02	0.41
1:A:240:LYS:HE2	1:A:240:LYS:HB3	1.89	0.41
1:B:228:MET:HE1	1:B:236:ILE:HD11	2.04	0.40
1:A:466:HIS:HD2	1:A:468:LEU:H	1.68	0.40
1:A:265:LYS:O	1:A:266:GLN:CB	2.67	0.40
1:B:465:LEU:N	1:B:465:LEU:HD13	2.36	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	264/267 (99%)	233 (88%)	15 (6%)	16 (6%)	2	1
1	B	265/267 (99%)	227 (86%)	22 (8%)	16 (6%)	2	1
All	All	529/534 (99%)	460 (87%)	37 (7%)	32 (6%)	2	1

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	SER
1	A	245	ALA
1	A	246	PRO
1	A	263	VAL
1	A	264	TRP
1	A	265	LYS
1	A	266	GLN
1	A	272	PRO
1	B	237	LEU
1	B	238	THR
1	B	268	VAL
1	B	304	PRO
1	B	428	ALA
1	A	270	GLY
1	A	474	LYS
1	B	232	LYS
1	B	266	GLN
1	A	240	LYS
1	A	259	GLU
1	B	242	SER
1	B	272	PRO
1	B	342	ALA
1	A	359	PRO
1	B	239	GLY
1	A	238	THR
1	B	245	ALA
1	B	263	VAL
1	B	359	PRO
1	B	461	THR
1	A	271	LEU
1	A	274	TYR
1	B	358	LYS

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	222/236 (94%)	201 (90%)	21 (10%)	11 12
1	B	225/236 (95%)	208 (92%)	17 (8%)	16 20
All	All	447/472 (95%)	409 (92%)	38 (8%)	13 16

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	LEU
1	A	227	ASN
1	A	228	MET
1	A	234	ARG
1	A	237	LEU
1	A	242	SER
1	A	244	THR
1	A	257	GLN
1	A	262	LEU
1	A	264	TRP
1	A	303	ILE
1	A	312	ASN
1	A	317	LEU
1	A	353	LEU
1	A	358	LYS
1	A	388	ILE
1	A	393	LEU
1	A	424	ASN
1	A	448	GLU
1	A	461	THR
1	A	469	LEU
1	B	266	GLN
1	B	271	LEU
1	B	294	ARG
1	B	304	PRO
1	B	312	ASN
1	B	364	ILE
1	B	368	PHE
1	B	384	LEU
1	B	402	ASN
1	B	414	LEU
1	B	418	GLU
1	B	424	ASN
1	B	431	LEU
1	B	455	ARG

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Mol	Chain	Res	Type
1	B	458	LYS
1	B	465	LEU
1	B	468	LEU

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	220	ASN
1	A	250	HIS
1	A	257	GLN
1	A	280	HIS
1	A	312	ASN
1	A	314	GLN
1	A	420	HIS
1	A	424	ASN
1	A	437	GLN
1	A	454	GLN
1	A	466	HIS
1	B	217	HIS
1	B	220	ASN
1	B	225	ASN
1	B	266	GLN
1	B	269	ASN
1	B	312	ASN
1	B	375	ASN
1	B	402	ASN
1	B	424	ASN
1	B	437	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

There are no ligands in this entry.

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, 95^{th} 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	266/267 (99%)	0.56	23 (8%) 13 18	15, 34, 94, 102	0
1	B	267/267 (100%)	0.66	30 (11%) 7 10	20, 42, 88, 102	0
All	All	533/534 (99%)	0.61	53 (9%) 9 14	15, 38, 93, 102	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	272	PRO	12.0
1	B	270	GLY	11.7
1	A	239	GLY	10.8
1	B	263	VAL	10.6
1	A	273	PRO	9.6
1	A	241	ALA	9.5
1	A	264	TRP	8.4
1	A	271	LEU	8.4
1	A	270	GLY	8.3
1	A	268	VAL	8.3
1	B	264	TRP	8.1
1	A	263	VAL	7.8
1	A	265	LYS	7.1
1	B	242	SER	6.9
1	B	240	LYS	6.9
1	A	267	LEU	6.6
1	A	242	SER	6.1
1	B	241	ALA	5.8
1	B	267	LEU	5.8
1	B	273	PRO	5.6
1	B	428	ALA	5.5
1	B	272	PRO	5.1
1	A	240	LYS	5.1
1	A	262	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	269	ASN	4.6
1	B	269	ASN	4.6
1	B	266	GLN	4.5
1	B	243	HIS	4.5
1	B	274	TYR	4.5
1	B	262	LEU	4.3
1	B	244	THR	4.3
1	A	266	GLN	4.1
1	B	265	LYS	4.0
1	A	244	THR	3.9
1	B	419	PHE	3.6
1	B	238	THR	3.5
1	B	271	LEU	3.3
1	B	247	PHE	3.2
1	B	303	ILE	3.0
1	A	358	LYS	2.8
1	A	277	ILE	2.8
1	A	428	ALA	2.8
1	B	268	VAL	2.6
1	B	245	ALA	2.4
1	A	245	ALA	2.3
1	A	246	PRO	2.3
1	B	304	PRO	2.2
1	B	231	LYS	2.2
1	B	462	GLU	2.2
1	B	427	ASP	2.1
1	B	426	PRO	2.1
1	A	243	HIS	2.1
1	B	358	LYS	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.