Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:30 AM GMT

PDB ID	:	3B3K
Title	:	Crystal structure of the complex between PPARgamma and the full agonist LT175
Authors	:	Pochetti, G.; Montanari, R.; Mazza, F.; Loiodice, F.; Fracchiolla, G.; Crestani, M.; Godio, C.
Deposited on	:	2007-10-22
Resolution	:	2.60 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:

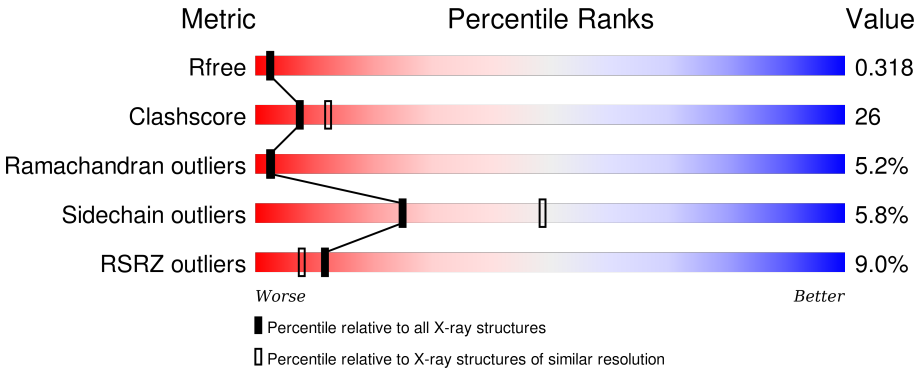
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	286	3% 49% 40% 5% 6%
1	B	286	13% 53% 36% 5% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4543 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.

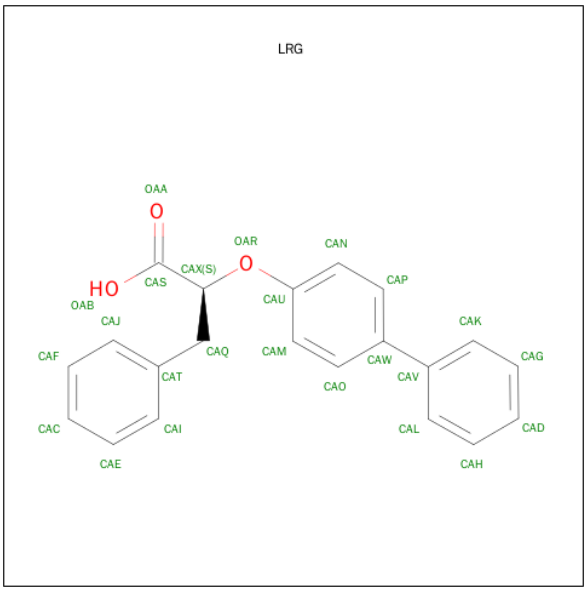
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	119	0	0
			2166	1397	354	405	10			
1	B	270	Total	C	N	O	S	127	0	0
			2166	1397	354	405	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	GLY	-	EXPRESSION TAG	UNP P37231
A	192	SER	-	EXPRESSION TAG	UNP P37231
A	193	HIS	-	EXPRESSION TAG	UNP P37231
A	194	MET	-	EXPRESSION TAG	UNP P37231
B	191	GLY	-	EXPRESSION TAG	UNP P37231
B	192	SER	-	EXPRESSION TAG	UNP P37231
B	193	HIS	-	EXPRESSION TAG	UNP P37231
B	194	MET	-	EXPRESSION TAG	UNP P37231

- Molecule 2 is (2S)-2-(BIPHENYL-4-YLOXY)-3-PHENYLPROPANOIC ACID (three-letter code: LRG) (formula: $C_{21}H_{18}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 24 21 3	0	0

- Molecule 3 is water.

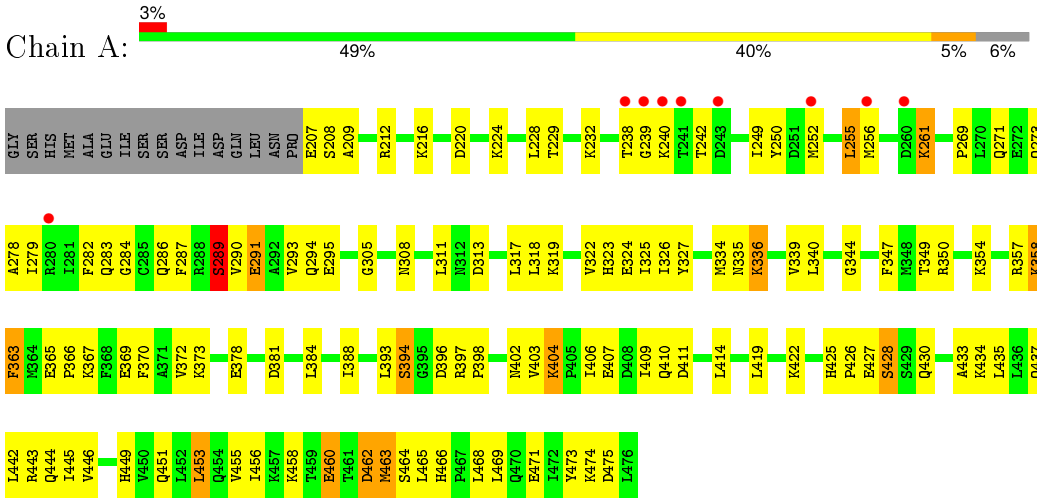
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	104	Total O 104 104	0	0
3	B	83	Total O 83 83	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

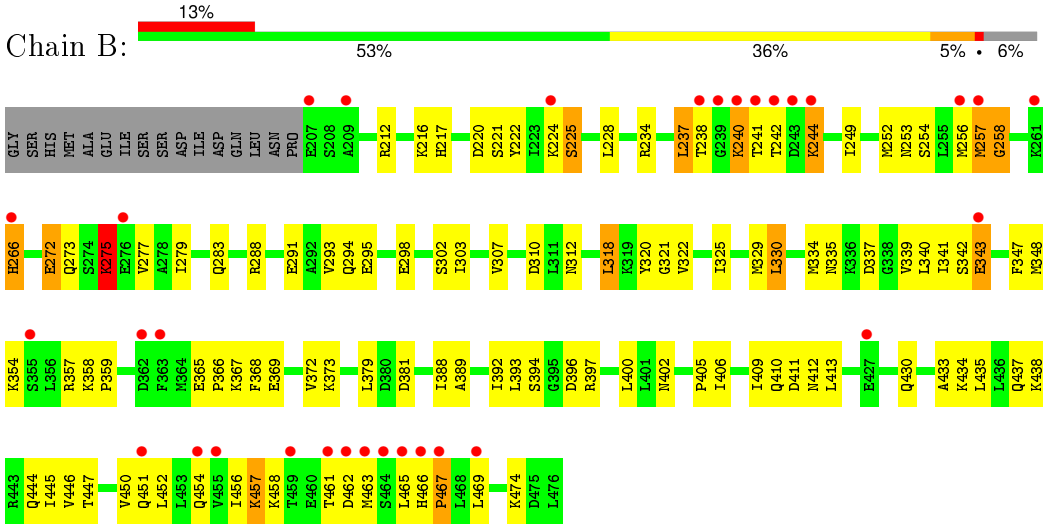
- Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain A:



- Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	93.14Å 61.57Å 118.80Å 90.00° 103.40° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60 19.73 – 2.58	Depositor EDS
% Data completeness (in resolution range)	87.9 (8.00-2.60) 99.0 (19.73-2.58)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.13 (at 2.59Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.316 0.246 , 0.318	Depositor DCC
R_{free} test set	1928 reflections (9.82%)	DCC
Wilson B-factor (Å^2)	59.2	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 72.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 20634 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4543	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% 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

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

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	0.46	2/2203 (0.1%)	0.73	4/2967 (0.1%)
1	B	0.35	0/2203	0.57	0/2967
All	All	0.41	2/4406 (0.0%)	0.65	4/5934 (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	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	SER	CA-CB	-7.58	1.41	1.52
1	A	289	SER	CB-OG	-7.46	1.32	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	462	ASP	O-C-N	-10.77	105.48	122.70
1	A	463	MET	C-N-CA	-10.71	94.92	121.70
1	A	463	MET	O-C-N	10.33	139.22	122.70
1	A	463	MET	CA-C-N	-9.82	95.59	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	462	ASP	Mainchain

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	2166	0	2232	120	0
1	B	2166	0	2232	96	0
2	A	24	0	17	5	0
3	A	104	0	0	23	0
3	B	83	0	0	17	0
All	All	4543	0	4481	213	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 26.

All (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.46	0.97
1:A:463:MET:CE	2:A:1:LRG:HAD	1.97	0.95
1:A:437:GLN:O	1:A:440:THR:HG22	1.70	0.91
1:A:473:TYR:O	1:A:474:LYS:HD2	1.72	0.90
1:A:411:ASP:HB3	3:B:536:HOH:O	1.71	0.87
1:B:393:LEU:HD23	3:B:554:HOH:O	1.74	0.87
1:B:303:ILE:HD13	3:B:554:HOH:O	1.75	0.87
1:B:465:LEU:C	1:B:467:PRO:HD2	1.95	0.87
1:A:463:MET:HG3	1:A:464:SER:H	1.38	0.86
1:B:275:LYS:HE3	1:B:275:LYS:HA	1.58	0.86
1:B:466:HIS:N	1:B:467:PRO:HD2	1.91	0.86
1:A:318:LEU:O	1:A:322:VAL:HG12	1.75	0.85
1:B:263:LYS:HE3	1:B:263:LYS:HA	1.61	0.82
1:A:463:MET:CG	1:A:464:SER:H	1.92	0.81
1:A:293:VAL:HG22	1:A:322:VAL:HG21	1.62	0.80
1:A:464:SER:HB2	3:A:518:HOH:O	1.83	0.79
1:B:451:GLN:O	1:B:454:GLN:HG2	1.83	0.78
1:B:354:LYS:HD3	1:B:365:GLU:HG3	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:PHE:HE2	1:A:456:ILE:HD11	1.47	0.77
1:A:289:SER:O	1:A:293:VAL:HG23	1.86	0.75
1:B:217:HIS:HE1	1:B:302:SER:O	1.71	0.73
1:A:286:GLN:HE22	1:A:465:LEU:HA	1.54	0.72
1:A:463:MET:CG	1:A:464:SER:N	2.52	0.72
1:A:463:MET:HE3	2:A:1:LRG:HAD	1.72	0.72
1:B:452:LEU:O	1:B:456:ILE:HG12	1.90	0.72
1:B:441:ASP:O	1:B:445:ILE:HG12	1.90	0.71
1:A:249:ILE:HD12	1:A:255:LEU:HA	1.71	0.71
1:A:340:LEU:HD23	1:A:347:PHE:HD1	1.54	0.71
1:B:329:MET:HE3	3:B:499:HOH:O	1.92	0.70
1:A:466:HIS:HB3	1:A:469:LEU:HD13	1.74	0.69
1:A:402:ASN:HB3	3:A:483:HOH:O	1.92	0.69
1:B:447:THR:O	1:B:450:VAL:HG22	1.94	0.68
1:B:354:LYS:HD3	1:B:365:GLU:CG	2.23	0.68
1:A:317:LEU:HD21	1:A:406:ILE:HD13	1.76	0.68
1:B:252:MET:O	1:B:256:MET:HG2	1.94	0.67
1:A:463:MET:HE2	2:A:1:LRG:HAD	1.73	0.67
1:A:207:GLU:HG3	1:A:209:ALA:H	1.60	0.66
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.78	0.66
1:B:264:PHE:CZ	1:B:266:HIS:HB3	2.30	0.65
1:B:307:VAL:HG13	3:B:497:HOH:O	1.96	0.65
1:A:276:GLU:CD	1:A:357:ARG:HH21	2.00	0.65
1:A:422:LYS:HD3	3:A:569:HOH:O	1.97	0.65
1:A:261:LYS:HD2	1:A:261:LYS:H	1.62	0.65
1:A:446:VAL:HG13	3:A:563:HOH:O	1.96	0.64
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.79	0.64
1:B:368:PHE:O	1:B:372:VAL:HG23	1.97	0.64
1:B:343:GLU:HB2	3:B:489:HOH:O	1.98	0.64
1:B:279:ILE:O	1:B:283:GLN:HG3	1.98	0.64
1:A:278:ALA:O	1:A:282:PHE:HD1	1.79	0.63
1:B:466:HIS:N	1:B:467:PRO:CD	2.62	0.63
1:B:291:GLU:O	1:B:295:GLU:HG3	1.98	0.62
1:A:393:LEU:HD12	1:A:409:ILE:HB	1.80	0.62
1:B:456:ILE:C	1:B:458:LYS:H	2.03	0.62
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.64	0.61
1:B:266:HIS:HD2	3:B:491:HOH:O	1.83	0.61
1:A:414:LEU:HB2	1:B:430:GLN:HG2	1.83	0.61
1:A:336:LYS:NZ	1:A:372:VAL:HG21	2.15	0.61
1:A:250:TYR:HB2	3:A:505:HOH:O	2.02	0.60
1:A:365:GLU:O	1:A:369:GLU:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:HD3	1:A:350:ARG:NH1	2.17	0.59
1:A:396:ASP:HB2	3:A:539:HOH:O	2.03	0.59
1:A:349:THR:HG22	3:A:499:HOH:O	2.02	0.58
1:A:425:HIS:N	1:A:426:PRO:HD3	2.19	0.58
1:B:220:ASP:O	1:B:224:LYS:HG2	2.03	0.58
1:B:365:GLU:N	1:B:366:PRO:HD2	2.19	0.57
1:A:238:THR:O	1:A:240:LYS:N	2.37	0.56
1:A:293:VAL:HG11	1:A:468:LEU:HD11	1.88	0.56
1:A:393:LEU:O	1:A:410:GLN:HB2	2.05	0.56
1:B:212:ARG:NH1	1:B:212:ARG:HB3	2.21	0.56
1:A:336:LYS:HD3	1:A:350:ARG:HH12	1.70	0.56
1:A:286:GLN:NE2	1:A:466:HIS:H	2.04	0.56
1:A:404:LYS:HD3	3:A:490:HOH:O	2.05	0.55
1:B:293:VAL:HG22	1:B:322:VAL:HG11	1.87	0.55
1:B:433:ALA:O	1:B:437:GLN:HG2	2.07	0.55
1:B:365:GLU:O	1:B:369:GLU:HG3	2.06	0.55
1:A:261:LYS:N	1:A:261:LYS:HD2	2.21	0.55
1:B:256:MET:O	1:B:258:GLY:N	2.37	0.54
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.90	0.54
1:A:286:GLN:NE2	1:A:465:LEU:HD12	2.22	0.54
1:B:389:ALA:HB1	3:B:554:HOH:O	2.08	0.54
1:A:284:GLY:O	1:A:287:PHE:HB3	2.08	0.54
1:B:222:TYR:CE1	1:B:381:ASP:HB3	2.43	0.54
1:B:321:GLY:O	1:B:325:ILE:HG12	2.08	0.53
1:A:208:SER:O	1:A:212:ARG:HG2	2.08	0.53
1:A:286:GLN:O	1:A:290:VAL:HG12	2.08	0.53
1:B:442:LEU:O	1:B:446:VAL:HG23	2.08	0.53
1:A:327:TYR:CE1	1:A:367:LYS:HE3	2.43	0.53
3:A:506:HOH:O	1:B:444:GLN:HG3	2.09	0.53
1:B:405:PRO:O	1:B:409:ILE:HG13	2.08	0.53
1:B:430:GLN:HG3	1:B:433:ALA:HB3	1.91	0.52
1:A:349:THR:HG21	3:A:505:HOH:O	2.08	0.52
1:B:237:LEU:HD22	3:B:494:HOH:O	2.09	0.52
1:B:340:LEU:C	1:B:341:ILE:HD12	2.29	0.52
1:B:330:LEU:O	1:B:334:MET:HG3	2.10	0.52
1:B:320:TYR:HB3	1:B:397:ARG:HD2	1.91	0.52
1:A:460:GLU:HG2	1:A:463:MET:HE1	1.92	0.52
1:A:440:THR:O	1:A:444:GLN:HG2	2.11	0.51
1:B:216:LYS:HE3	1:B:220:ASP:OD2	2.10	0.51
1:A:277:VAL:HG13	1:A:278:ALA:N	2.25	0.51
1:B:221:SER:O	1:B:225:SER:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:SER:HB2	1:A:419:LEU:HD21	1.92	0.51
1:B:340:LEU:O	1:B:341:ILE:HD12	2.11	0.51
1:A:430:GLN:HA	3:A:493:HOH:O	2.11	0.51
1:A:228:LEU:HD12	1:A:232:LYS:HB3	1.93	0.51
1:B:242:THR:HA	3:B:488:HOH:O	2.11	0.50
1:B:242:THR:O	1:B:242:THR:HG23	2.12	0.50
1:B:393:LEU:O	1:B:410:GLN:HB2	2.10	0.50
1:A:434:LYS:HE2	3:A:553:HOH:O	2.10	0.50
1:A:336:LYS:HG2	1:A:372:VAL:CG2	2.41	0.50
1:B:212:ARG:HD2	3:B:516:HOH:O	2.11	0.50
1:A:336:LYS:HZ3	1:A:372:VAL:HG11	1.77	0.50
1:A:286:GLN:HE21	1:A:465:LEU:HD12	1.77	0.50
1:A:398:PRO:HD3	3:A:491:HOH:O	2.12	0.50
1:B:462:ASP:O	1:B:463:MET:HG3	2.11	0.50
1:A:359:PRO:HG2	1:A:360:PHE:H	1.77	0.50
1:B:288:ARG:HD2	1:B:288:ARG:O	2.12	0.50
1:A:384:LEU:O	1:A:388:ILE:HG12	2.12	0.49
1:A:294:GLN:HB2	3:A:526:HOH:O	2.12	0.49
1:A:220:ASP:O	1:A:224:LYS:HG3	2.13	0.49
1:B:252:MET:SD	1:B:277:VAL:HG21	2.53	0.49
1:B:457:LYS:O	1:B:457:LYS:HG3	2.13	0.49
1:B:334:MET:HG2	1:B:339:VAL:HB	1.95	0.49
1:B:413:LEU:HD11	3:B:554:HOH:O	2.11	0.49
1:A:322:VAL:O	1:A:326:ILE:HG13	2.13	0.49
1:A:279:ILE:O	1:A:283:GLN:HG2	2.13	0.49
1:A:437:GLN:HB3	3:A:538:HOH:O	2.13	0.48
1:A:323:HIS:HB2	3:A:574:HOH:O	2.12	0.48
1:B:434:LYS:O	1:B:438:LYS:HD3	2.13	0.48
1:A:473:TYR:C	1:A:474:LYS:HD2	2.34	0.48
1:A:435:LEU:O	1:A:438:LYS:HB2	2.13	0.48
1:A:402:ASN:HB2	3:A:487:HOH:O	2.13	0.48
1:A:242:THR:HG22	1:A:242:THR:O	2.14	0.48
1:A:394:SER:HB2	1:A:397:ARG:HG2	1.95	0.48
1:B:373:LYS:HA	3:B:525:HOH:O	2.13	0.48
1:B:237:LEU:HB3	1:B:238:THR:H	1.59	0.47
1:B:212:ARG:CA	1:B:212:ARG:HH11	2.28	0.47
1:B:396:ASP:C	1:B:396:ASP:OD1	2.54	0.46
1:B:388:ILE:O	1:B:392:ILE:HG13	2.15	0.46
1:B:325:ILE:HG22	1:B:329:MET:HE2	1.97	0.46
1:A:238:THR:C	1:A:240:LYS:H	2.19	0.46
1:A:428:SER:C	3:A:529:HOH:O	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ILE:C	1:B:458:LYS:N	2.69	0.46
1:A:313:ASP:O	1:A:317:LEU:HG	2.16	0.46
1:A:212:ARG:HH21	1:A:216:LYS:NZ	2.12	0.46
1:A:336:LYS:HZ2	1:A:372:VAL:HG21	1.78	0.46
1:B:411:ASP:HB2	3:B:481:HOH:O	2.15	0.46
1:A:449:HIS:HB3	3:A:524:HOH:O	2.14	0.46
1:A:252:MET:O	1:A:256:MET:HB2	2.16	0.46
1:B:216:LYS:O	1:B:216:LYS:HD3	2.16	0.45
1:A:440:THR:HA	1:B:440:THR:HG22	1.97	0.45
1:A:336:LYS:HG2	1:A:372:VAL:HG22	1.99	0.45
1:B:240:LYS:O	1:B:241:THR:C	2.54	0.45
1:B:325:ILE:HG22	1:B:329:MET:CE	2.46	0.45
1:B:234:ARG:NH2	1:B:334:MET:O	2.45	0.45
1:A:335:ASN:C	1:A:335:ASN:OD1	2.54	0.45
1:A:469:LEU:HD12	1:A:469:LEU:N	2.31	0.45
1:A:403:VAL:O	1:A:407:GLU:HG3	2.17	0.45
1:A:229:THR:HB	1:A:381:ASP:OD2	2.17	0.45
1:A:365:GLU:N	1:A:366:PRO:HD2	2.31	0.44
1:A:440:THR:CA	1:B:440:THR:HG22	2.47	0.44
1:B:237:LEU:O	1:B:238:THR:C	2.56	0.44
1:B:348:MET:SD	1:B:353:LEU:HD21	2.58	0.44
1:A:359:PRO:HG2	1:A:360:PHE:CD1	2.53	0.43
1:B:413:LEU:CD1	3:B:554:HOH:O	2.64	0.43
1:B:320:TYR:CB	1:B:397:ARG:HD2	2.48	0.43
1:B:340:LEU:HD23	1:B:347:PHE:HD1	1.84	0.43
1:A:433:ALA:O	1:A:437:GLN:HG3	2.18	0.43
1:B:430:GLN:NE2	3:B:546:HOH:O	2.50	0.43
1:A:334:MET:HG2	1:A:339:VAL:HB	2.01	0.43
1:B:379:LEU:HD21	1:B:435:LEU:HD13	2.00	0.43
1:B:212:ARG:HA	1:B:212:ARG:HH11	1.84	0.43
1:B:258:GLY:O	1:B:262:ILE:HG22	2.18	0.43
1:A:350:ARG:NH2	1:A:365:GLU:OE2	2.48	0.43
1:B:249:ILE:HA	1:B:254:SER:HB3	2.01	0.43
1:A:282:PHE:CE1	1:A:360:PHE:HB3	2.54	0.43
1:A:407:GLU:O	1:A:411:ASP:CG	2.57	0.42
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.73	0.42
1:A:319:LYS:NZ	1:A:474:LYS:HD3	2.34	0.42
1:A:228:LEU:HA	3:A:536:HOH:O	2.19	0.42
1:A:369:GLU:O	1:A:373:LYS:HG2	2.19	0.42
1:A:358:LYS:H	1:A:358:LYS:HD3	1.84	0.42
1:A:453:LEU:HD12	1:A:453:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:HD23	1:A:311:LEU:C	2.40	0.42
1:A:463:MET:CE	2:A:1:LRG:CAD	2.84	0.42
1:A:358:LYS:N	1:A:358:LYS:HD3	2.34	0.42
1:A:463:MET:HE2	2:A:1:LRG:CAD	2.47	0.42
1:A:336:LYS:HZ3	1:A:372:VAL:HG21	1.83	0.42
1:B:462:ASP:C	1:B:463:MET:HG3	2.41	0.42
1:B:310:ASP:C	1:B:310:ASP:OD2	2.58	0.41
1:A:291:GLU:HG2	1:A:295:GLU:OE2	2.20	0.41
1:A:238:THR:C	1:A:240:LYS:N	2.73	0.41
1:A:358:LYS:CD	1:A:358:LYS:H	2.33	0.41
1:B:294:GLN:HG3	3:B:503:HOH:O	2.19	0.41
1:A:208:SER:HB2	1:A:419:LEU:CD2	2.49	0.41
1:B:367:LYS:HG2	1:B:367:LYS:H	1.68	0.41
1:A:324:GLU:HG2	1:A:442:LEU:HB3	2.03	0.41
1:B:335:ASN:CG	1:B:337:ASP:H	2.24	0.41
1:A:286:GLN:NE2	1:A:465:LEU:HA	2.30	0.41
1:B:275:LYS:CE	1:B:275:LYS:HA	2.37	0.41
1:B:253:ASN:O	1:B:257:MET:HB2	2.21	0.41
1:A:451:GLN:O	1:A:455:VAL:HG23	2.21	0.40
1:B:244:LYS:HG3	1:B:244:LYS:O	2.21	0.40
1:A:407:GLU:O	1:A:411:ASP:OD1	2.40	0.40
1:B:365:GLU:N	1:B:366:PRO:CD	2.83	0.40
1:B:456:ILE:O	1:B:458:LYS:N	2.53	0.40
1:B:402:ASN:O	1:B:405:PRO:HD2	2.20	0.40
1:A:349:THR:HG21	3:A:546:HOH:O	2.21	0.40
1:A:443:ARG:NH2	3:A:491:HOH:O	2.53	0.40
1:A:438:LYS:HA	1:A:438:LYS:HD3	1.97	0.40
1:B:400:LEU:HD13	1:B:406:ILE:CD1	2.52	0.40
1:A:419:LEU:HD12	1:A:419:LEU:HA	1.90	0.40
1:B:310:ASP:OD2	1:B:312:ASN:N	2.50	0.40
1:A:354:LYS:HB2	3:A:550:HOH:O	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	268/286 (94%)	236 (88%)	21 (8%)	11 (4%)	3 4
1	B	268/286 (94%)	229 (85%)	22 (8%)	17 (6%)	2 2
All	All	536/572 (94%)	465 (87%)	43 (8%)	28 (5%)	2 3

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	LEU
1	B	272	GLU
1	A	239	GLY
1	A	336	LYS
1	A	475	ASP
1	B	244	LYS
1	B	257	MET
1	B	263	LYS
1	B	357	ARG
1	B	474	LYS
1	A	269	PRO
1	A	276	GLU
1	A	359	PRO
1	B	240	LYS
1	B	258	GLY
1	B	394	SER
1	B	457	LYS
1	B	467	PRO
1	A	273	GLN
1	A	358	LYS
1	A	394	SER
1	B	266	HIS
1	B	342	SER
1	A	275	LYS
1	B	275	LYS
1	B	343	GLU
1	A	344	GLY
1	B	359	PRO

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	243/257 (95%)	228 (94%)	15 (6%)	23 45
1	B	243/257 (95%)	230 (95%)	13 (5%)	28 53
All	All	486/514 (95%)	458 (94%)	28 (6%)	25 49

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	LEU
1	A	261	LYS
1	A	271	GLN
1	A	289	SER
1	A	291	GLU
1	A	362	ASP
1	A	363	PHE
1	A	378	GLU
1	A	404	LYS
1	A	427	GLU
1	A	428	SER
1	A	453	LEU
1	A	458	LYS
1	A	460	GLU
1	A	471	GLU
1	B	225	SER
1	B	228	LEU
1	B	263	LYS
1	B	272	GLU
1	B	273	GLN
1	B	275	LYS
1	B	298	GLU
1	B	318	LEU
1	B	330	LEU
1	B	358	LYS
1	B	412	ASN
1	B	461	THR

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Mol	Chain	Res	Type
1	B	469	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	308	ASN
1	A	402	ASN
1	A	451	GLN
1	A	454	GLN
1	A	470	GLN
1	B	217	HIS
1	B	253	ASN
1	B	294	GLN
1	B	308	ASN
1	B	410	GLN
1	B	412	ASN
1	B	430	GLN
1	B	451	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

1 ligand is 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	LRG	A	1	-	21,26,26	0.90	1 (4%)	29,34,34	0.54	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	LRG	A	1	-	-	0/12/16/16	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	LRG	CAW-CAV	-3.56	1.39	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	LRG	5	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, 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	256/286 (89%)	0.09	9 (3%) 48 40	31, 52, 89, 99	0
1	B	256/286 (89%)	0.48	37 (14%) 3 2	28, 54, 100, 100	2 (0%)
All	All	512/572 (89%)	0.28	46 (8%) 12 8	28, 54, 99, 100	2 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	462	ASP	11.6
1	B	463	MET	8.9
1	B	263	LYS	6.9
1	B	461	THR	6.8
1	B	238	THR	5.9
1	A	240	LYS	5.1
1	B	264	PHE	4.6
1	B	459	THR	4.5
1	B	355	SER	4.4
1	B	266	HIS	4.3
1	B	467	PRO	4.2
1	B	242	THR	4.1
1	B	257	MET	4.1
1	B	464	SER	3.9
1	B	243	ASP	3.8
1	B	209	ALA	3.6
1	B	465	LEU	3.5
1	A	260	ASP	3.5
1	B	240	LYS	3.4
1	B	261	LYS	3.3
1	A	280	ARG	3.2
1	B	427	GLU	3.2
1	B	207	GLU	3.1
1	A	243	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	454	GLN	2.9
1	A	239	GLY	2.7
1	B	362	ASP	2.6
1	A	241	THR	2.6
1	B	276	GLU	2.6
1	B	469	LEU	2.5
1	A	238	THR	2.5
1	B	256	MET	2.5
1	B	224	LYS	2.5
1	B	455	VAL	2.4
1	B	466	HIS	2.4
1	A	252	MET	2.3
1	B	239	GLY	2.3
1	B	351	GLU	2.3
1	A	256	MET	2.3
1	B	265	LYS	2.3
1	B	343	GLU	2.2
1	B	262	ILE	2.2
1	B	244	LYS	2.2
1	B	363	PHE	2.1
1	B	451	GLN	2.1
1	B	241	THR	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
2	LRG	A	1	24/24	0.88	0.25	1.48	56,62,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.