



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:04 PM GMT

PDB ID : 3CDS  
Title : Crystal structure of the complex between PPAR-gamma and the agonist LT248  
(clofibric acid analogue)  
Authors : Pochetti, G.; Montanari, R.; Mazza, F.  
Deposited on : 2008-02-27  
Resolution : 2.65 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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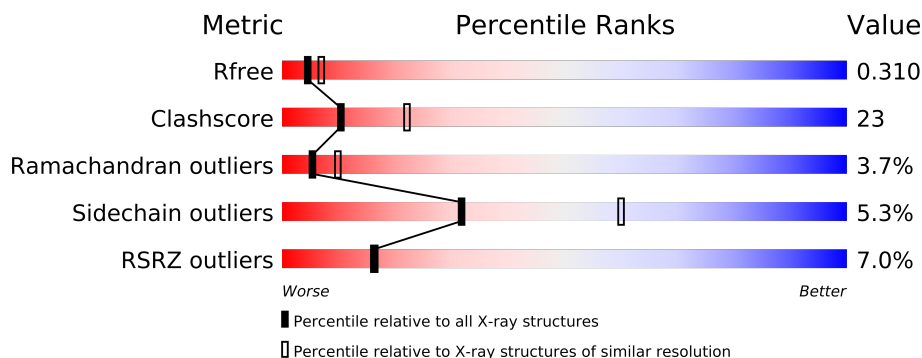
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.65 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))
$R_{free}$	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	286	
1	B	286	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GRR	A	1	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4437 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

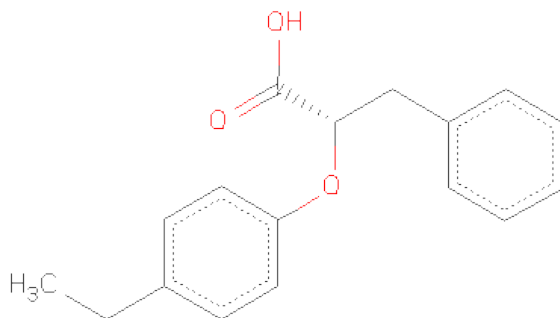
- Molecule 1 is a protein called Peroxisome proliferator-activatedreceptor gamma.

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-(4-ETHYLPHENOXY)-3-PHENYLPROPANOICACID (three-letter code: GRR) (formula: C<sub>17</sub>H<sub>18</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	17	3		

- Molecule 3 is water.

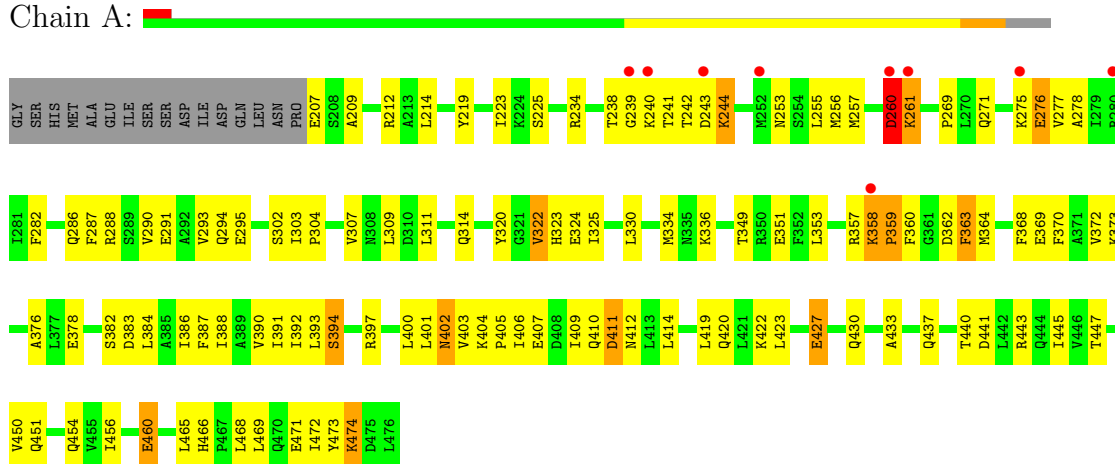
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	35	Total	O	0	0
			35	35		

### 3 Residue-property plots

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

- Molecule 1: Peroxisome proliferator-activatedreceptor gamma

Chain A:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.25Å 60.98Å 118.54Å 90.00° 102.83° 90.00°	Depositor
Resolution (Å)	10.00 – 2.65 24.61 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.65) 98.1 (24.61-2.65)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 2.64Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.241 , 0.319 0.239 , 0.310	Depositor DCC
$R_{free}$ test set	906 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 18672 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4437	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.41	0/2203	0.61	0/2967
1	B	0.37	0/2203	0.59	0/2967
All	All	0.39	0/4406	0.60	0/5934

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2166	0	2232	101	0
1	B	2166	0	2232	93	0
2	A	20	0	17	6	0
3	A	50	0	0	10	0
3	B	35	0	0	5	0
All	All	4437	0	4481	194	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (194) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.33	1.09
1:A:261:LYS:HD2	1:A:261:LYS:H	1.33	0.94
1:A:437:GLN:O	1:A:440:THR:HG22	1.67	0.93
1:A:402:ASN:HD22	1:A:402:ASN:N	1.67	0.89
1:B:466:HIS:N	1:B:467:PRO:HD2	1.91	0.85
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.60	0.83
1:A:401:LEU:C	1:A:402:ASN:HD22	1.84	0.81
1:A:419:LEU:HA	1:A:422:LYS:HE2	1.66	0.78
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.67	0.77
1:A:411:ASP:HB3	3:A:514:HOH:O	1.83	0.77
1:A:349:THR:HG22	1:A:351:GLU:H	1.50	0.76
1:B:465:LEU:C	1:B:467:PRO:HD2	2.07	0.76
1:B:238:THR:HG23	1:B:335:ASN:HD22	1.50	0.75
1:B:281:ILE:HD12	1:B:356:LEU:HD21	1.70	0.73
1:B:275:LYS:HE3	1:B:275:LYS:HA	1.69	0.72
1:A:402:ASN:ND2	1:A:402:ASN:N	2.37	0.72
1:B:212:ARG:NH1	1:B:212:ARG:HB3	2.03	0.72
1:A:212:ARG:NH1	1:A:423:LEU:HD12	2.05	0.71
1:B:324:GLU:HG3	1:B:446:VAL:HG21	1.72	0.71
1:A:419:LEU:HA	1:A:422:LYS:CE	2.23	0.68
1:B:300:ALA:HA	1:B:303:ILE:HD12	1.76	0.67
1:B:442:LEU:O	1:B:446:VAL:HG23	1.94	0.67
1:A:293:VAL:HG13	1:A:322:VAL:HG21	1.76	0.66
1:B:330:LEU:HD22	1:B:334:MET:SD	2.36	0.66
1:B:288:ARG:HD2	1:B:288:ARG:O	1.96	0.65
1:A:212:ARG:HH12	1:A:420:GLN:HA	1.62	0.64
1:A:253:ASN:HA	1:A:256:MET:CE	2.28	0.64
1:B:447:THR:O	1:B:450:VAL:HG22	1.99	0.63
1:A:384:LEU:O	1:A:388:ILE:HG12	1.98	0.63
1:B:452:LEU:O	1:B:456:ILE:HG12	1.99	0.62
1:A:336:LYS:HE2	1:A:372:VAL:HG11	1.80	0.62
1:A:369:GLU:O	1:A:373:LYS:HE2	2.00	0.62
1:B:262:ILE:HG13	1:B:263:LYS:H	1.64	0.62
2:A:1:GRR:HAK	2:A:1:GRR:CAP	2.30	0.62
1:A:403:VAL:O	1:A:407:GLU:HG3	2.00	0.61
1:A:394:SER:HA	1:A:410:GLN:NE2	2.15	0.61
1:A:474:LYS:HA	1:A:474:LYS:HE3	1.82	0.61
1:A:393:LEU:HD12	1:A:409:ILE:HB	1.82	0.61
1:B:212:ARG:HB3	1:B:212:ARG:HH11	1.64	0.61
1:A:287:PHE:HE1	1:A:288:ARG:CZ	2.14	0.60
1:A:393:LEU:O	1:A:410:GLN:HB2	2.01	0.60
1:B:403:VAL:HG12	1:B:407:GLU:HG3	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:237:LEU:O	1:B:239:GLY:N	2.35	0.60
1:A:257:MET:O	1:A:260:ASP:HB2	2.01	0.60
1:A:282:PHE:HB3	2:A:1:GRR:HAAB	1.82	0.60
1:A:253:ASN:HA	1:A:256:MET:HE3	1.83	0.59
1:A:373:LYS:O	1:A:376:ALA:HB3	2.02	0.59
1:B:466:HIS:N	1:B:467:PRO:CD	2.64	0.59
1:A:261:LYS:N	1:A:261:LYS:HD2	2.13	0.59
1:A:473:TYR:O	1:A:474:LYS:HE3	2.03	0.59
1:A:276:GLU:CD	1:A:357:ARG:HH21	2.07	0.58
1:A:450:VAL:O	1:A:454:GLN:HG2	2.03	0.58
1:A:240:LYS:O	1:A:242:THR:HG23	2.03	0.58
1:A:357:ARG:HH12	1:A:460:GLU:CD	2.06	0.57
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.85	0.57
1:B:445:ILE:HG12	3:B:37:HOH:O	2.03	0.57
1:B:434:LYS:HA	1:B:437:GLN:HE21	1.69	0.57
1:A:225:SER:O	1:A:295:GLU:HG2	2.04	0.57
1:B:275:LYS:HE2	1:B:279:ILE:HD12	1.87	0.56
1:B:220:ASP:O	1:B:224:LYS:HG2	2.05	0.56
1:A:307:VAL:HG22	3:A:493:HOH:O	2.05	0.56
1:B:462:ASP:O	1:B:463:MET:HG3	2.06	0.56
1:B:345:GLN:NE2	1:B:345:GLN:HA	2.21	0.56
1:B:300:ALA:HA	1:B:303:ILE:CD1	2.35	0.56
1:B:242:THR:O	1:B:242:THR:HG23	2.05	0.55
1:B:279:ILE:O	1:B:283:GLN:HG3	2.07	0.54
1:A:320:TYR:HB2	1:A:397:ARG:HD2	1.88	0.54
1:B:249:ILE:HA	1:B:254:SER:HB3	1.89	0.54
1:A:286:GLN:CG	2:A:1:GRR:HAAA	2.38	0.54
1:B:422:LYS:HE2	3:B:20:HOH:O	2.07	0.54
1:B:396:ASP:OD1	1:B:443:ARG:NH2	2.41	0.53
1:A:394:SER:HA	1:A:410:GLN:HE22	1.73	0.53
1:B:329:MET:O	1:B:332:SER:HB2	2.08	0.53
1:A:290:VAL:HG22	1:A:469:LEU:HD13	1.90	0.53
1:B:238:THR:CG2	1:B:335:ASN:HD22	2.18	0.53
1:B:322:VAL:O	1:B:326:ILE:HG13	2.09	0.53
1:B:212:ARG:CB	1:B:212:ARG:HH11	2.22	0.53
1:A:288:ARG:HG3	3:A:506:HOH:O	2.08	0.53
1:B:310:ASP:OD2	1:B:311:LEU:N	2.42	0.53
1:A:382:SER:C	3:A:519:HOH:O	2.48	0.53
1:A:468:LEU:O	1:A:468:LEU:HD22	2.09	0.53
1:B:262:ILE:HD11	1:B:345:GLN:HB3	1.91	0.52
1:A:324:GLU:OE2	1:A:443:ARG:HD3	2.10	0.52
1:A:212:ARG:HD3	1:A:423:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:255:LEU:HD22	1:A:277:VAL:HG23	1.92	0.52
1:B:293:VAL:HG13	1:B:322:VAL:HG21	1.92	0.52
1:A:241:THR:HG22	1:A:243:ASP:OD2	2.10	0.52
1:A:427:GLU:CD	1:A:427:GLU:H	2.13	0.51
1:A:238:THR:O	1:A:240:LYS:N	2.43	0.51
1:B:345:GLN:HE21	1:B:345:GLN:HA	1.75	0.51
1:A:363:PHE:HE2	1:A:456:ILE:HD11	1.75	0.51
1:A:311:LEU:HD23	1:A:311:LEU:C	2.32	0.51
1:A:323:HIS:CD2	1:A:473:TYR:OH	2.64	0.50
1:A:404:LYS:N	1:A:405:PRO:HD2	2.26	0.50
1:A:330:LEU:O	1:A:334:MET:HG3	2.12	0.50
1:A:294:GLN:HB2	3:A:479:HOH:O	2.11	0.50
1:B:340:LEU:O	1:B:341:ILE:HD12	2.13	0.49
1:A:363:PHE:HE2	1:A:456:ILE:CD1	2.26	0.49
1:B:307:VAL:HG13	3:B:81:HOH:O	2.12	0.49
1:A:207:GLU:HG3	1:A:209:ALA:H	1.78	0.49
1:A:242:THR:HG22	3:A:512:HOH:O	2.12	0.49
1:B:321:GLY:O	1:B:325:ILE:HG12	2.14	0.48
1:B:249:ILE:O	1:B:349:THR:HG23	2.13	0.48
1:B:311:LEU:HD23	1:B:314:GLN:NE2	2.28	0.48
1:B:234:ARG:NH2	1:B:334:MET:O	2.36	0.48
1:B:336:LYS:HG3	3:B:59:HOH:O	2.12	0.48
1:B:455:VAL:HA	1:B:458:LYS:HE2	1.93	0.48
1:A:212:ARG:HD3	1:A:423:LEU:CD1	2.44	0.48
1:B:350:ARG:O	1:B:354:LYS:HG3	2.14	0.48
1:A:255:LEU:CD2	1:A:277:VAL:HG23	2.44	0.47
1:A:276:GLU:CG	1:A:357:ARG:HH21	2.27	0.47
1:B:365:GLU:N	1:B:366:PRO:HD2	2.29	0.47
1:A:400:LEU:HD22	1:A:406:ILE:CD1	2.44	0.47
1:B:222:TYR:CE1	1:B:381:ASP:HB3	2.49	0.47
1:B:275:LYS:CE	1:B:275:LYS:HA	2.39	0.47
1:B:367:LYS:NZ	1:B:449:HIS:CD2	2.82	0.47
1:B:244:LYS:HG3	1:B:244:LYS:O	2.15	0.47
1:A:322:VAL:HG12	1:A:323:HIS:N	2.30	0.46
1:B:367:LYS:NZ	1:B:449:HIS:HD2	2.13	0.46
1:A:242:THR:C	1:A:244:LYS:N	2.69	0.46
1:B:405:PRO:O	1:B:409:ILE:HG13	2.15	0.46
1:A:212:ARG:HH11	1:A:423:LEU:HD12	1.80	0.46
1:B:216:LYS:HD3	1:B:220:ASP:OD2	2.16	0.46
1:B:380:ASP:C	1:B:380:ASP:OD1	2.54	0.46
1:B:214:LEU:HD21	1:B:413:LEU:HD23	1.97	0.46
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:440:THR:HG23	1:A:441:ASP:N	2.30	0.46
1:B:297:THR:O	1:B:301:LYS:HG3	2.15	0.46
1:B:384:LEU:O	1:B:388:ILE:HG13	2.16	0.45
1:A:309:LEU:HD13	1:A:406:ILE:HG12	1.99	0.45
1:A:419:LEU:HD12	1:A:422:LYS:HE3	1.99	0.45
1:A:303:ILE:O	1:A:304:PRO:C	2.54	0.45
1:B:256:MET:HE1	1:B:280:ARG:HH22	1.81	0.45
1:B:325:ILE:HD11	1:B:391:ILE:HB	1.98	0.45
1:B:249:ILE:HA	1:B:254:SER:CB	2.47	0.45
1:B:237:LEU:HB3	1:B:238:THR:H	1.65	0.44
1:A:359:PRO:HG2	1:A:360:PHE:H	1.82	0.44
1:A:277:VAL:HG13	1:A:278:ALA:N	2.32	0.44
2:A:1:GRR:CAK	2:A:1:GRR:CAP	2.95	0.44
1:B:348:MET:SD	1:B:353:LEU:HD21	2.58	0.44
1:A:214:LEU:HD22	1:A:412:ASN:ND2	2.33	0.44
1:A:307:VAL:HA	1:A:314:GLN:OE1	2.17	0.44
1:A:443:ARG:NH1	3:A:482:HOH:O	2.51	0.44
1:A:253:ASN:HA	1:A:256:MET:HE2	1.98	0.44
1:B:262:ILE:HD11	1:B:345:GLN:CB	2.47	0.43
1:B:367:LYS:HZ1	1:B:449:HIS:CD2	2.36	0.43
1:B:320:TYR:CZ	1:B:398:PRO:HG2	2.52	0.43
1:A:386:ILE:O	1:A:390:VAL:HG23	2.18	0.43
1:B:256:MET:CE	1:B:280:ARG:HH22	2.31	0.43
1:A:447:THR:HG22	1:A:451:GLN:HE21	1.83	0.43
1:B:454:GLN:O	1:B:458:LYS:HG3	2.17	0.43
1:B:330:LEU:HD23	1:B:330:LEU:O	2.19	0.43
1:A:288:ARG:O	1:A:291:GLU:HB3	2.17	0.43
1:B:237:LEU:O	1:B:238:THR:C	2.56	0.43
1:B:322:VAL:HG12	1:B:323:HIS:N	2.33	0.43
1:B:373:LYS:O	1:B:376:ALA:HB3	2.19	0.43
1:B:388:ILE:O	1:B:392:ILE:HG13	2.17	0.43
1:A:219:TYR:O	1:A:223:ILE:HG12	2.19	0.43
1:A:387:PHE:O	1:A:391:ILE:HG13	2.19	0.43
1:A:383:ASP:N	3:A:519:HOH:O	2.52	0.42
1:B:265:LYS:O	1:B:266:HIS:HB2	2.19	0.42
1:B:264:PHE:CE2	1:B:266:HIS:HB3	2.54	0.42
1:A:212:ARG:NH1	1:A:420:GLN:HA	2.29	0.42
1:A:261:LYS:CD	1:A:261:LYS:H	2.10	0.42
1:B:339:VAL:HG13	1:B:341:ILE:CD1	2.50	0.42
1:A:286:GLN:HG3	2:A:1:GRR:HAAA	2.01	0.42
1:B:255:LEU:HD23	1:B:277:VAL:HG13	2.02	0.42
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:241:THR:HG22	1:B:241:THR:O	2.19	0.42
1:A:353:LEU:HD12	1:A:368:PHE:HE2	1.84	0.42
1:A:433:ALA:O	1:A:437:GLN:HG3	2.19	0.41
1:A:322:VAL:HG11	1:A:472:ILE:HD13	2.02	0.41
1:A:336:LYS:HD3	1:A:372:VAL:HG21	2.01	0.41
1:B:466:HIS:O	1:B:467:PRO:C	2.59	0.41
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.44	0.41
1:B:306:PHE:HB3	3:B:81:HOH:O	2.20	0.41
1:A:212:ARG:NH2	1:A:420:GLN:OE1	2.51	0.41
1:A:207:GLU:HA	3:A:502:HOH:O	2.20	0.41
1:B:232:LYS:O	1:B:235:ALA:N	2.54	0.41
1:A:234:ARG:N	1:A:234:ARG:HD2	2.35	0.41
1:B:317:LEU:HD21	1:B:406:ILE:HD13	2.02	0.41
1:B:343:GLU:HG3	1:B:343:GLU:O	2.20	0.41
1:B:256:MET:C	1:B:258:GLY:H	2.23	0.41
1:A:414:LEU:CB	1:B:430:GLN:HG2	2.51	0.41
1:A:465:LEU:HD12	1:A:466:HIS:H	1.86	0.41
1:A:440:THR:CG2	1:A:441:ASP:N	2.84	0.41
1:B:339:VAL:HG22	1:B:340:LEU:O	2.20	0.41
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.82	0.40
1:B:330:LEU:HD21	1:B:339:VAL:HG21	2.02	0.40
1:A:364:MET:SD	2:A:1:GRR:HAF	2.61	0.40
1:A:378:GLU:HA	3:A:495:HOH:O	2.20	0.40
1:B:404:LYS:N	1:B:405:PRO:HD2	2.36	0.40
1:B:241:THR:HG22	1:B:243:ASP:OD1	2.22	0.40
1:A:414:LEU:HB2	1:B:430:GLN:HG2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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%)	240 (90%)	19 (7%)	9 (3%)	6	11
1	B	268/286 (94%)	231 (86%)	26 (10%)	11 (4%)	4	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	536/572 (94%)	471 (88%)	45 (8%)	20 (4%)	5	10

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	A	260	ASP
1	B	238	THR
1	A	358	LYS
1	A	394	SER
1	B	237	LEU
1	B	244	LYS
1	B	266	HIS
1	B	464	SER
1	A	244	LYS
1	A	269	PRO
1	A	276	GLU
1	A	359	PRO
1	B	357	ARG
1	A	275	LYS
1	B	227	PRO
1	B	233	ALA
1	B	474	LYS
1	B	461	THR
1	B	467	PRO

### 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	243/257 (95%)	229 (94%)	14 (6%)	28	55
1	B	243/257 (95%)	231 (95%)	12 (5%)	35	64
All	All	486/514 (95%)	460 (95%)	26 (5%)	32	60

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	ASP
1	A	261	LYS
1	A	271	GLN
1	A	302	SER
1	A	322	VAL
1	A	362	ASP
1	A	363	PHE
1	A	402	ASN
1	A	411	ASP
1	A	427	GLU
1	A	430	GLN
1	A	460	GLU
1	A	471	GLU
1	A	474	LYS
1	B	210	ASP
1	B	234	ARG
1	B	273	GLN
1	B	275	LYS
1	B	294	GLN
1	B	318	LEU
1	B	322	VAL
1	B	341	ILE
1	B	379	LEU
1	B	443	ARG
1	B	444	GLN
1	B	463	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	402	ASN
1	A	412	ASN
1	A	451	GLN
1	A	454	GLN
1	B	217	HIS
1	B	253	ASN
1	B	308	ASN
1	B	314	GLN
1	B	345	GLN
1	B	410	GLN
1	B	412	ASN
1	B	430	GLN

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Mol	Chain	Res	Type
1	B	437	GLN
1	B	444	GLN
1	B	449	HIS
1	B	451	GLN
1	B	470	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	GRR	A	1	-	21,21,21	0.60	0	27,27,27	2.11	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GRR	A	1	-	-	0/14/14/14	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	GRR	CAS-OAO-CAT	-10.21	113.02	118.83
2	A	1	GRR	CAN-CAT-CAP	-2.35	106.82	109.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	256/286 (89%)	-0.05	9 (3%) 42 45	16, 41, 82, 100	0
1	B	256/286 (89%)	0.25	27 (10%) 7 6	21, 47, 100, 100	2 (0%)
All	All	512/572 (89%)	0.10	36 (7%) 16 16	16, 44, 99, 100	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	463	MET	7.3
1	B	242	THR	6.9
1	B	462	ASP	6.6
1	B	465	LEU	5.6
1	B	464	SER	5.2
1	B	461	THR	4.7
1	B	263	LYS	4.5
1	B	264	PHE	4.4
1	B	238	THR	4.1
1	B	275	LYS	4.0
1	A	275	LYS	3.8
1	A	260	ASP	3.7
1	B	266	HIS	3.7
1	A	239	GLY	3.6
1	A	358	LYS	3.3
1	A	240	LYS	3.2
1	B	207	GLU	3.0
1	B	257	MET	2.9
1	B	283	GLN	2.7
1	B	451	GLN	2.7
1	B	261	LYS	2.6
1	A	280	ARG	2.4
1	A	243	ASP	2.4
1	B	256	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	243	ASP	2.4
1	B	239	GLY	2.4
1	A	252	MET	2.4
1	B	363	PHE	2.3
1	B	454	GLN	2.3
1	B	240	LYS	2.3
1	B	209	ALA	2.2
1	A	261	LYS	2.2
1	B	224	LYS	2.1
1	B	427	GLU	2.1
1	B	282	PHE	2.1
1	B	241	THR	2.1

## 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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GRR	A	1	20/20	0.36	8.56	97,98,99,100	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.