Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:13 PM GMT

PDB ID : 4O8F

Title : Crystal Structure of the complex between PPARgamma mutant R357A and rosiglitazone

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Deposited on : 2013-12-27

Resolution : 2.60 Å(reported)

The following versions of software and data (see references (i)) 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	Percentile Ranks	Value
Rfree		0.291
Clashscore		17
Ramachandran outliers		2.3%
Sidechain outliers		3.8%
RSRZ outliers		4.6%

Worse .... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
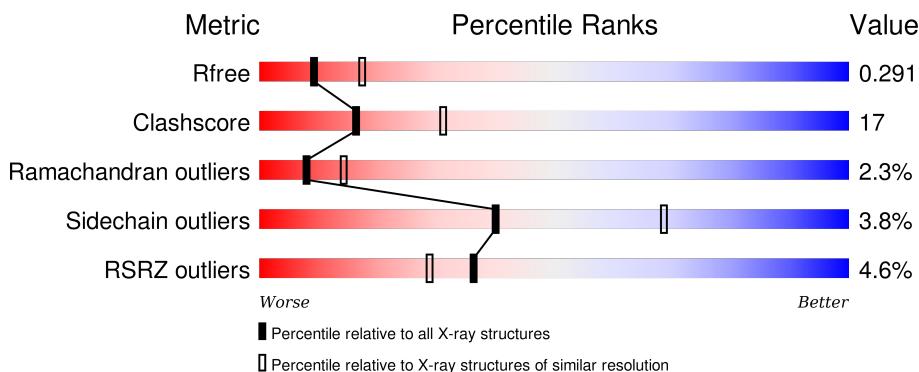
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	287	2% / 63% / 23% / · / 12%
1	B	287	6% / 56% / 26% / · · / 13%
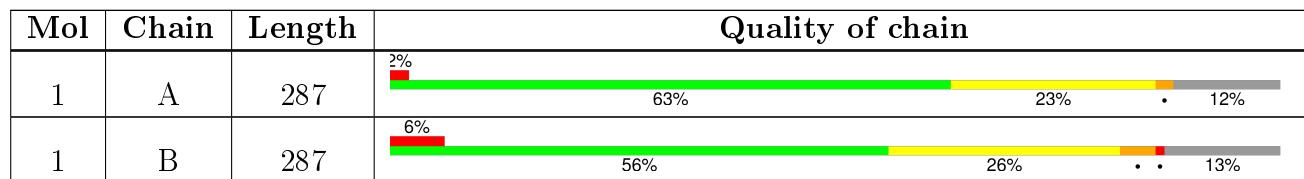
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4114 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	252	Total	C	N	O	S	0	0	0
			2013	1304	324	376	9			
1	B	249	Total	C	N	O	S	0	0	0
			1990	1288	321	372	9			

There are 10 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
A	357	ALA	ARG	ENGINEERED MUTATION	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
B	357	ALA	ARG	ENGINEERED MUTATION	UNP P37231

- Molecule 2 is 2,4-THIAZOLIDIINEDIONE, 5-[[4-[2-(METHYL-2-PYRIDINYLAMINO)ET HOXY]PHENYL]METHYL]-(9CL) (three-letter code: BRL) (formula: $C_{18}H_{19}N_3O_3S$).
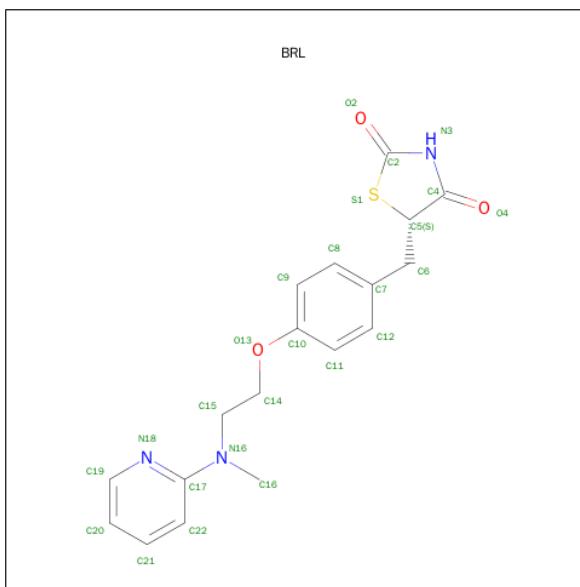
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 25	C 18	N 3	O 3	S 1	0	0
2	B	1	Total 25	C 18	N 3	O 3	S 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total 38	O 38	0	0
3	B	23	Total 23	O 23	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
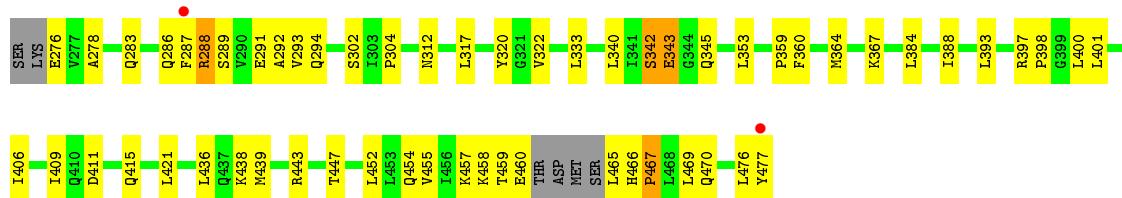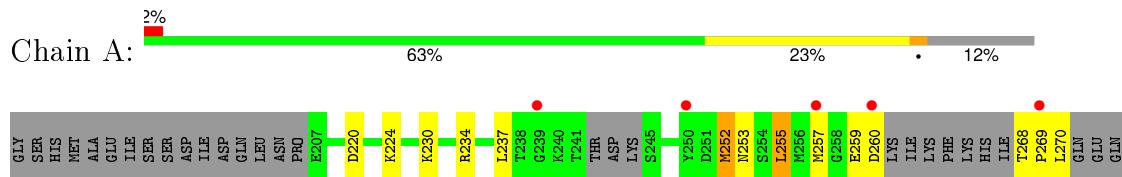
- Molecule 1: Peroxisome proliferator-activated receptor gamma
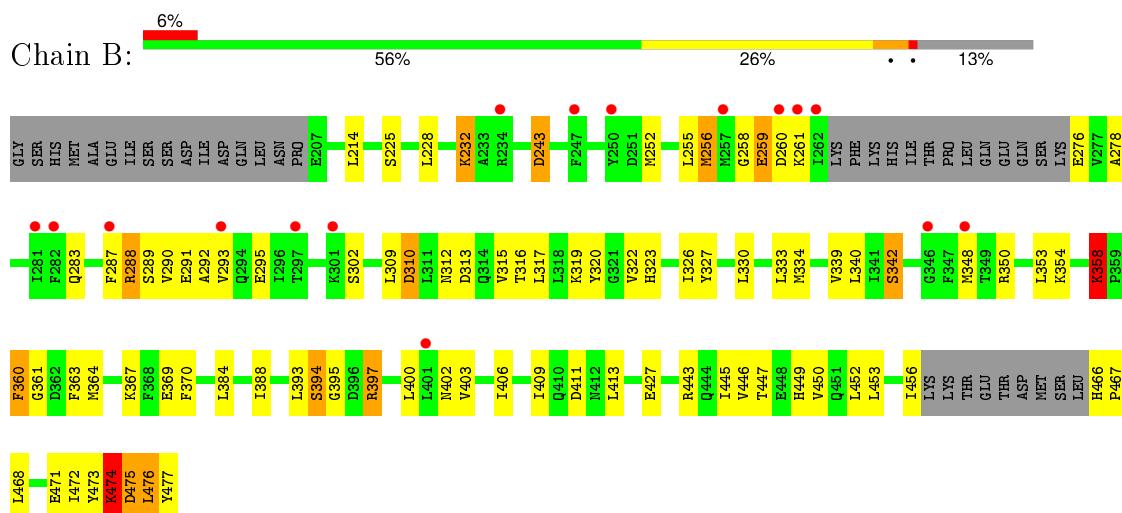
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	85.70Å 87.10Å 163.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.09 – 2.60 81.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (61.09-2.60) 90.5 (81.90-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.80 (at 2.62Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.234 , 0.297 0.240 , 0.291	Depositor DCC
R_{free} test set	1835 reflections (11.21%)	DCC
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.4	EDS
Estimated twinning fraction	0.167 for -k,-h,-l	Xtriage
L-test for twinning[2]	$<\lvert L \rvert> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	0 of 18964 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4114	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<\lvert L \rvert>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.52	0/2045	0.71	3/2754 (0.1%)
1	B	0.53	0/2023	0.71	1/2726 (0.0%)
All	All	0.52	0/4068	0.71	4/5480 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	MET	CA-CB-CG	5.97	123.45	113.30
1	A	270	LEU	CA-CB-CG	5.24	127.34	115.30
1	A	255	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	476	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2013	0	2063	53	0
1	B	1990	0	2038	88	0
2	A	25	0	19	3	0
2	B	25	0	19	7	0
3	A	38	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	23	0	0	2	0
All	All	4114	0	4139	137	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 17.

All (137) 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:319:LYS:HE2	1:B:320:TYR:HE1	1.18	1.08
1:A:401:LEU:HD22	1:B:232:LYS:HD3	1.45	0.97
1:B:289:SER:HB2	2:B:501:BRL:H8	1.45	0.96
1:B:319:LYS:HE2	1:B:320:TYR:CE1	2.04	0.90
1:B:319:LYS:HG2	1:B:320:TYR:HD1	1.37	0.89
1:A:293:VAL:HG22	1:A:322:VAL:HG21	1.61	0.83
1:B:358:LYS:HG2	1:B:360:PHE:H	1.45	0.82
1:A:288:ARG:HA	1:A:291:GLU:HG2	1.62	0.80
1:B:394:SER:OG	1:B:395:GLY:N	2.14	0.79
1:B:471:GLU:O	1:B:474:LYS:HD3	1.86	0.75
1:A:401:LEU:HD22	1:B:232:LYS:CD	2.19	0.73
1:B:258:GLY:O	1:B:261:LYS:N	2.23	0.70
1:B:474:LYS:O	1:B:476:LEU:N	2.24	0.70
1:B:453:LEU:HD11	2:B:501:BRL:O2	1.93	0.69
1:A:465:LEU:O	1:A:470:GLN:NE2	2.26	0.68
1:A:289:SER:OG	2:A:501:BRL:H5	1.94	0.67
1:B:323:HIS:HE1	1:B:473:TYR:OH	1.77	0.67
1:B:339:VAL:HG11	2:B:501:BRL:H162	1.75	0.67
1:A:447:THR:HG22	1:A:477:TYR:CE1	2.30	0.67
1:B:312:ASN:HA	1:B:315:VAL:HG22	1.75	0.66
1:A:458:LYS:O	1:A:460:GLU:N	2.27	0.66
1:A:443:ARG:O	1:A:447:THR:HG23	1.97	0.65
1:B:319:LYS:HG2	1:B:320:TYR:CD1	2.27	0.64
1:A:447:THR:HG22	1:A:477:TYR:HE1	1.63	0.63
1:A:466:HIS:CG	1:A:467:PRO:HD2	2.35	0.62
1:A:317:LEU:HD11	1:A:406:ILE:HD12	1.79	0.62
1:B:288:ARG:O	1:B:292:ALA:N	2.31	0.61
1:B:348:MET:HE2	2:B:501:BRL:H161	1.83	0.60
1:B:339:VAL:CG1	2:B:501:BRL:H162	2.31	0.60
1:B:397:ARG:HB2	1:B:400:LEU:HG	1.84	0.59
1:B:323:HIS:O	1:B:326:ILE:HG13	2.02	0.59
1:B:353:LEU:HD13	1:B:364:MET:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:LYS:N	1:B:367:LYS:HD3	2.18	0.58
1:B:319:LYS:HG3	1:B:474:LYS:HZ3	1.68	0.58
1:B:214:LEU:HD21	1:B:413:LEU:HD23	1.85	0.58
1:A:367:LYS:HD2	1:A:367:LYS:H	1.67	0.57
1:B:258:GLY:O	1:B:259:GLU:C	2.42	0.57
1:A:253:ASN:O	1:A:257:MET:HG3	2.05	0.57
1:B:354:LYS:HA	1:B:361:GLY:O	2.05	0.57
1:B:310:ASP:OD1	1:B:313:ASP:N	2.27	0.56
1:A:384:LEU:O	1:A:388:ILE:HG12	2.05	0.56
1:A:342:SER:O	1:A:345:GLN:HG3	2.06	0.56
1:B:319:LYS:HD2	1:B:474:LYS:HE2	1.88	0.56
1:B:310:ASP:OD1	1:B:312:ASN:N	2.38	0.56
1:B:393:LEU:HD22	1:B:409:ILE:HB	1.87	0.56
1:B:472:ILE:HA	1:B:474:LYS:NZ	2.22	0.55
1:A:397:ARG:HB2	1:A:400:LEU:HG	1.86	0.55
1:A:401:LEU:HD13	1:B:232:LYS:HE3	1.89	0.55
1:A:467:PRO:O	1:A:470:GLN:OE1	2.25	0.55
1:B:319:LYS:HG3	1:B:474:LYS:NZ	2.21	0.54
1:B:258:GLY:O	1:B:260:ASP:N	2.40	0.54
1:B:290:VAL:HG21	1:B:466:HIS:CE1	2.42	0.54
1:A:312:ASN:HA	1:B:243:ASP:OD2	2.08	0.54
1:B:384:LEU:O	1:B:388:ILE:HG12	2.08	0.53
1:B:252:MET:O	1:B:255:LEU:HB3	2.09	0.53
1:B:319:LYS:HE3	1:B:474:LYS:HZ3	1.74	0.53
1:B:450:VAL:HG23	1:B:453:LEU:HB2	1.90	0.52
1:B:288:ARG:HA	1:B:291:GLU:HB3	1.91	0.52
1:A:252:MET:HB2	1:A:255:LEU:HB3	1.92	0.51
1:A:353:LEU:HD13	1:A:364:MET:HG3	1.92	0.51
1:B:466:HIS:CD2	1:B:467:PRO:HD2	2.45	0.51
1:B:225:SER:OG	1:B:295:GLU:O	2.29	0.51
1:A:276:GLU:OE1	1:A:278:ALA:N	2.29	0.51
1:B:228:LEU:HG	1:B:333:LEU:HD21	1.93	0.51
1:B:358:LYS:HD3	1:B:360:PHE:CD2	2.45	0.50
1:B:358:LYS:HD3	1:B:360:PHE:CG	2.46	0.50
1:B:350:ARG:O	1:B:354:LYS:HG3	2.11	0.50
1:A:291:GLU:HG3	1:A:292:ALA:N	2.27	0.50
1:B:452:LEU:HG	1:B:452:LEU:O	2.11	0.50
1:B:312:ASN:O	1:B:316:THR:N	2.39	0.49
1:B:317:LEU:HD23	1:B:397:ARG:HG2	1.92	0.49
1:B:289:SER:O	1:B:293:VAL:HG23	2.12	0.49
1:A:289:SER:OG	2:A:501:BRL:C5	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:GLU:N	1:B:427:GLU:OE1	2.46	0.48
1:B:353:LEU:HD23	1:B:353:LEU:HA	1.74	0.48
1:A:283:GLN:HA	1:A:286:GLN:HB2	1.95	0.48
1:B:287:PHE:HA	1:B:290:VAL:HG12	1.97	0.47
1:A:237:LEU:HD21	1:A:340:LEU:HG	1.96	0.47
1:A:259:GLU:OE1	1:A:268:THR:HG21	2.15	0.47
1:A:454:GLN:OE1	1:A:457:LYS:HE3	2.14	0.47
1:A:436:LEU:O	1:A:439:MET:HB2	2.14	0.47
1:A:393:LEU:HD22	1:A:409:ILE:HB	1.95	0.47
1:A:401:LEU:CD2	1:B:232:LYS:HD3	2.32	0.47
1:B:370:PHE:HB2	1:B:445:ILE:HD11	1.96	0.47
1:A:333:LEU:HB3	1:A:340:LEU:HB2	1.96	0.46
1:B:443:ARG:NH2	1:B:477:TYR:OH	2.48	0.46
1:A:411:ASP:O	1:A:415:GLN:HG3	2.16	0.46
1:A:455:VAL:O	1:A:459:THR:HB	2.15	0.46
1:B:333:LEU:HB3	1:B:340:LEU:HB2	1.96	0.46
1:B:474:LYS:O	1:B:475:ASP:C	2.54	0.45
1:B:323:HIS:HE1	1:B:473:TYR:CZ	2.35	0.45
1:B:358:LYS:HG2	1:B:360:PHE:N	2.24	0.45
1:A:302:SER:O	1:A:304:PRO:HD3	2.16	0.45
1:B:290:VAL:HG21	1:B:466:HIS:ND1	2.31	0.45
1:A:268:THR:N	1:A:269:PRO:HD3	2.31	0.45
1:A:359:PRO:HG2	1:A:360:PHE:CE1	2.52	0.45
1:A:421:LEU:HA	1:A:421:LEU:HD23	1.78	0.45
1:B:468:LEU:O	1:B:472:ILE:HG13	2.17	0.45
1:B:443:ARG:O	1:B:446:VAL:HG22	2.16	0.45
1:B:403:VAL:O	1:B:406:ILE:HG12	2.16	0.45
1:B:322:VAL:O	1:B:326:ILE:HG23	2.17	0.44
1:A:288:ARG:O	1:A:291:GLU:HG3	2.17	0.44
1:B:283:GLN:HB3	1:B:287:PHE:CZ	2.53	0.44
1:B:475:ASP:N	1:B:475:ASP:OD1	2.50	0.44
1:B:450:VAL:HA	1:B:453:LEU:HG	1.99	0.44
1:B:334:MET:HG2	1:B:339:VAL:HB	2.00	0.43
1:A:289:SER:O	1:A:293:VAL:HG23	2.18	0.43
1:B:397:ARG:HB2	1:B:400:LEU:CG	2.46	0.43
1:A:252:MET:HA	1:A:255:LEU:H	1.84	0.43
1:A:452:LEU:HD12	1:A:452:LEU:HA	1.86	0.43
1:B:302:SER:HA	3:B:618:HOH:O	2.19	0.43
1:A:230:LYS:O	1:A:234:ARG:HG2	2.18	0.43
1:B:232:LYS:HB3	1:B:232:LYS:HZ3	1.83	0.43
1:B:278:ALA:HB1	1:B:360:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:MET:C	1:B:258:GLY:N	2.72	0.43
1:A:438:LYS:NZ	3:A:636:HOH:O	2.51	0.43
1:B:276:GLU:HG3	1:B:278:ALA:H	1.84	0.42
1:A:320:TYR:CZ	1:A:476:LEU:HD12	2.54	0.42
1:A:397:ARG:HA	1:A:398:PRO:HD3	1.83	0.42
1:B:330:LEU:HD21	2:B:501:BRL:H141	2.01	0.42
1:B:243:ASP:OD1	1:B:243:ASP:N	2.53	0.41
1:B:330:LEU:HA	1:B:330:LEU:HD12	1.79	0.41
1:A:359:PRO:HG2	1:A:360:PHE:CD1	2.54	0.41
1:B:319:LYS:CD	1:B:474:LYS:HE2	2.50	0.41
1:A:260:ASP:OD2	3:A:616:HOH:O	2.21	0.41
1:B:449:HIS:NE2	2:B:501:BRL:C2	2.83	0.41
1:B:327:TYR:CE2	1:B:446:VAL:HG12	2.56	0.41
1:A:288:ARG:CA	1:A:291:GLU:HG2	2.41	0.41
1:B:394:SER:HB3	1:B:397:ARG:NE	2.36	0.41
1:A:469:LEU:HA	1:A:469:LEU:HD23	1.88	0.41
1:B:293:VAL:HG22	1:B:322:VAL:HG21	2.03	0.41
1:B:288:ARG:NH1	3:B:619:HOH:O	2.50	0.41
1:A:220:ASP:O	1:A:224:LYS:HG3	2.21	0.41
1:B:283:GLN:HB3	1:B:287:PHE:CE2	2.56	0.40
2:A:501:BRL:H22	2:A:501:BRL:H161	1.85	0.40
1:A:291:GLU:O	1:A:294:GLN:HG2	2.21	0.40
1:B:309:LEU:HD22	1:B:406:ILE:HG22	2.03	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	242/287 (84%)	221 (91%)	18 (7%)	3 (1%)	16	33
1	B	243/287 (85%)	215 (88%)	20 (8%)	8 (3%)	5	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	485/574 (84%)	436 (90%)	38 (8%)	11 (2%)	8 14

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	310	ASP
1	B	475	ASP
1	B	358	LYS
1	A	467	PRO
1	B	394	SER
1	A	342	SER
1	A	343	GLU
1	B	474	LYS
1	B	243	ASP
1	B	259	GLU
1	B	342	SER

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	224/257 (87%)	221 (99%)	3 (1%)	76 91
1	B	221/257 (86%)	207 (94%)	14 (6%)	22 44
All	All	445/514 (87%)	428 (96%)	17 (4%)	40 68

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	PHE
1	A	288	ARG
1	A	343	GLU
1	B	232	LYS
1	B	256	MET
1	B	288	ARG
1	B	342	SER

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Mol	Chain	Res	Type
1	B	358	LYS
1	B	360	PHE
1	B	363	PHE
1	B	369	GLU
1	B	397	ARG
1	B	402	ASN
1	B	411	ASP
1	B	447	THR
1	B	456	ILE
1	B	474	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	GLN
1	B	314	GLN
1	B	323	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	BRL	A	501	-	26,27,27	1.90	4 (15%)	31,36,36	3.41	11 (35%)
2	BRL	B	501	-	26,27,27	1.57	4 (15%)	31,36,36	3.35	11 (35%)

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	BRL	A	501	-	-	0/14/26/26	0/3/3/3
2	BRL	B	501	-	-	0/14/26/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	BRL	C4-N3	-4.00	1.32	1.37
2	B	501	BRL	C4-N3	-3.85	1.32	1.37
2	A	501	BRL	C2-N3	-2.47	1.34	1.37
2	B	501	BRL	C2-N3	-2.31	1.34	1.37
2	B	501	BRL	C11-C10	2.79	1.44	1.38
2	A	501	BRL	C11-C10	3.32	1.45	1.38
2	B	501	BRL	C2-S1	3.63	1.78	1.76
2	A	501	BRL	C2-S1	6.17	1.80	1.76

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	BRL	S1-C2-N3	-9.09	103.69	110.38
2	B	501	BRL	S1-C2-N3	-8.71	103.97	110.38
2	A	501	BRL	C4-C5-S1	-7.21	99.08	105.89
2	B	501	BRL	C4-C5-S1	-7.12	99.17	105.89
2	B	501	BRL	C6-C5-S1	-2.53	110.35	113.00
2	A	501	BRL	O4-C4-N3	-2.50	121.80	124.83
2	B	501	BRL	O4-C4-N3	-2.30	122.04	124.83
2	B	501	BRL	C14-O13-C10	-2.25	112.36	117.91
2	A	501	BRL	C14-O13-C10	-2.21	112.47	117.91
2	B	501	BRL	C22-C17-N18	-2.21	119.10	123.17
2	A	501	BRL	C6-C5-S1	-2.19	110.70	113.00
2	A	501	BRL	C22-C17-N18	-2.10	119.30	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	BRL	O2-C2-S1	3.57	128.11	124.68
2	B	501	BRL	C5-C4-N3	4.05	115.77	111.96
2	A	501	BRL	C5-C4-N3	4.50	116.18	111.96
2	A	501	BRL	C19-N18-C17	4.54	122.79	116.92
2	A	501	BRL	O2-C2-S1	4.56	129.05	124.68
2	B	501	BRL	C19-N18-C17	4.72	123.03	116.92
2	B	501	BRL	C4-N3-C2	7.10	123.18	118.32
2	A	501	BRL	C4-N3-C2	7.56	123.49	118.32
2	A	501	BRL	C5-S1-C2	8.23	97.55	92.90
2	B	501	BRL	C5-S1-C2	8.89	97.92	92.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	BRL	3	0
2	B	501	BRL	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9
1	A	252/287 (87%)	0.08	7 (2%) 56	49	42, 69, 111, 163	0
1	B	249/287 (86%)	0.50	16 (6%) 23	17	45, 85, 125, 147	0
All	All	501/574 (87%)	0.29	23 (4%) 36	29	42, 76, 123, 163	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	ASP	8.8
1	B	260	ASP	8.2
1	B	297	THR	6.5
1	B	261	LYS	5.9
1	B	247	PHE	4.3
1	B	257	MET	4.2
1	B	301	LYS	3.5
1	B	262	ILE	3.4
1	A	250	TYR	3.1
1	A	239	GLY	3.0
1	B	234	ARG	3.0
1	B	293	VAL	3.0
1	B	250	TYR	2.9
1	B	346	GLY	2.8
1	B	287	PHE	2.6
1	A	477	TYR	2.5
1	B	282	PHE	2.4
1	B	401	LEU	2.4
1	B	281	ILE	2.3
1	A	257	MET	2.1
1	B	348	MET	2.0
1	A	269	PRO	2.0
1	A	287	PHE	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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	BRL	A	501	25/25	0.89	0.23	1.89	61,73,77,91	0
2	BRL	B	501	25/25	0.84	0.30	1.38	80,94,113,117	0

6.5 Other polymers (i)

There are no such residues in this entry.