Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:18 AM GMT

PDB ID	:	2Q61
Title	:	Crystal Structure of PPARgamma ligand binding domain bound to partial agonist SR145
Authors	:	Bruning, J.B.; Nettles, K.W.
Deposited on	:	2007-06-04
Resolution	:	2.20 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
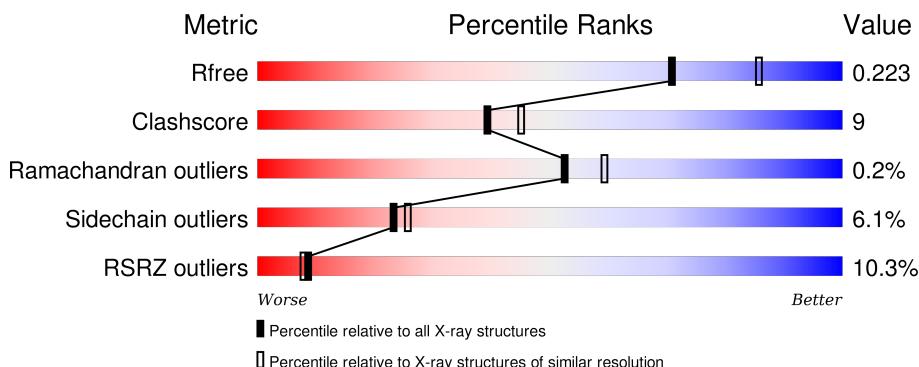
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
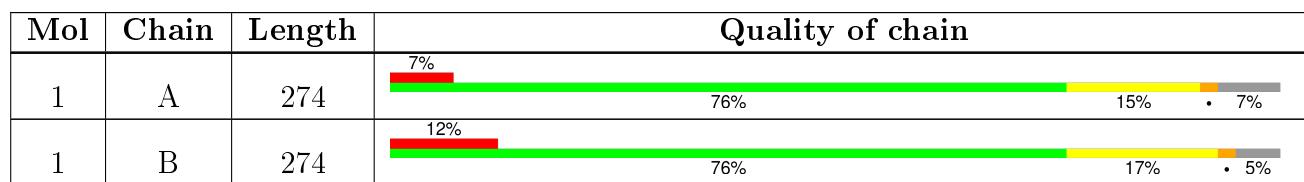
The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.223
Clashscore		9
Ramachandran outliers		0.2%
Sidechain outliers		6.1%
RSRZ outliers		10.3%

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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	274	7% 76% 15% • 7%
1	B	274	12% 76% 17% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4373 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.
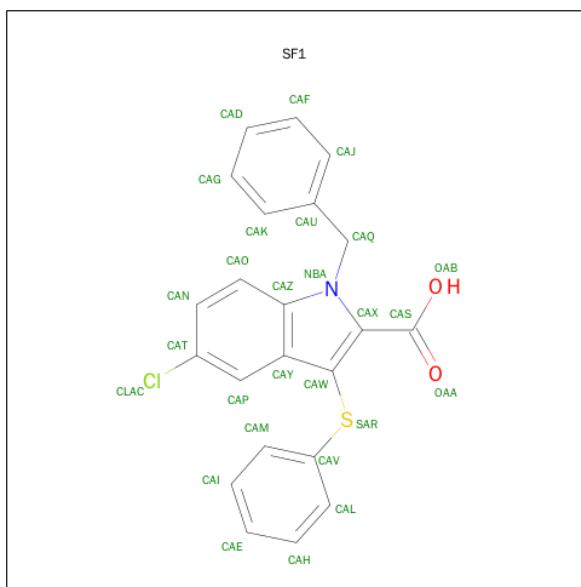
- Molecule 1 is a protein called Peroxisome Proliferator-Activated Receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total 2072	C 1343	N 335	O 383	S 11	0	8	0
1	B	259	Total 2091	C 1358	N 343	O 379	S 11	0	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	SER	-	EXPRESSION TAG	UNP P37231
B	204	SER	-	EXPRESSION TAG	UNP P37231

- Molecule 2 is 1-BENZYL-5-CHLORO-3-(PHENYLTHIO)-1H-INDOLE-2-CARBOXYLIC ACID (three-letter code: SF1) (formula: $C_{22}H_{16}ClNO_2S$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total 27	C 22	Cl 1	N 1	O 2	S 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
2	A	1	27	22	1	1	2	1	0	0
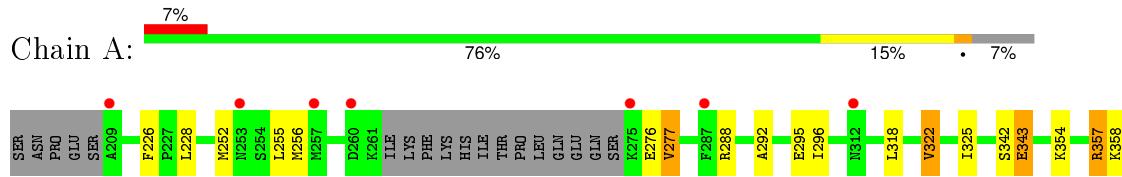
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	79	79	79	0	0
3	B	77	77	77	0	0
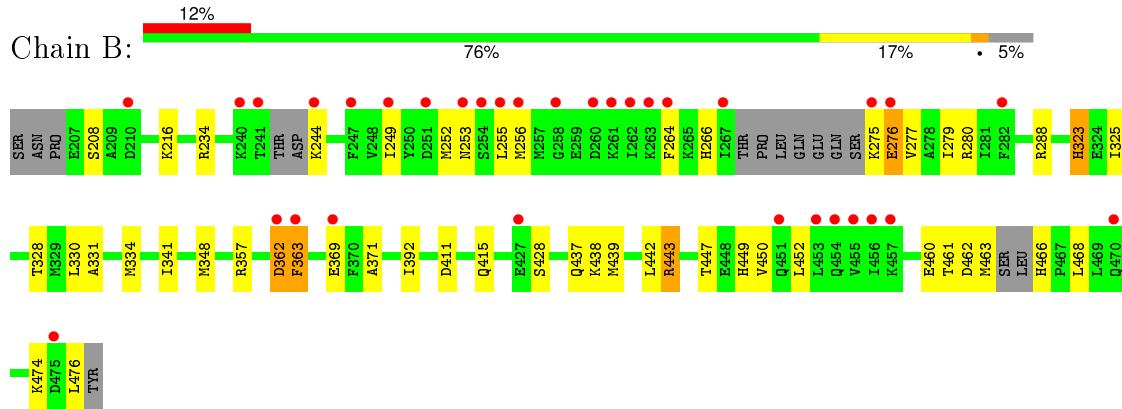
3 Residue-property plots (i)

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 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	90.13Å 62.39Å 117.93Å 90.00° 100.98° 90.00°	Depositor
Resolution (Å)	9.97 – 2.20 9.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (9.97-2.20) 99.4 (9.97-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	5.04 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.188 , 0.229 0.186 , 0.223	Depositor DCC
R_{free} test set	1650 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 60.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 32379 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4373	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF1

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	0.60	2/2130 (0.1%)	0.66	0/2872
1	B	0.65	4/2148 (0.2%)	0.63	0/2893
All	All	0.62	6/4278 (0.1%)	0.64	0/5765

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	461	THR	C-N	-10.37	1.10	1.34
1	B	460	GLU	C-N	-8.26	1.15	1.34
1	B	244	LYS	N-CA	7.80	1.61	1.46
1	A	462	ASP	CG-OD2	7.44	1.42	1.25
1	A	462	ASP	CG-OD1	6.97	1.41	1.25
1	B	244	LYS	CA-CB	6.72	1.68	1.53

There are no bond angle outliers.

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	2072	0	2135	44	0
1	B	2091	0	2149	38	0
2	A	27	0	15	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	15	6	0
3	A	79	0	0	0	0
3	B	77	0	0	6	0
All	All	4373	0	4314	76	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 9.

All (76) 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:A:357:ARG:HD2	1:A:358:LYS:O	1.60	1.01
1:A:357:ARG:HG3	1:A:357:ARG:HH11	1.24	1.00
1:B:449:HIS:HD2	3:B:5058:HOH:O	1.60	0.83
1:A:357:ARG:CD	1:A:358:LYS:O	2.26	0.83
1:B:331:ALA:HA	1:B:334:MET:HE3	1.65	0.79
1:A:444:GLN:HG3	1:B:443[A]:ARG:NH2	1.99	0.78
1:A:276:GLU:OE2	1:A:357:ARG:NH1	2.23	0.71
1:A:357:ARG:NH1	1:A:357:ARG:HG3	2.05	0.66
1:A:292:ALA:O	1:A:296[A]:ILE:HG12	1.96	0.66
1:B:362:ASP:HB2	3:B:5046:HOH:O	1.95	0.65
1:B:363:PHE:HB2	1:B:452:LEU:HD21	1.77	0.64
1:A:226:PHE:HE1	1:A:296[A]:ILE:HD13	1.62	0.64
1:B:466:HIS:N	3:B:5054:HOH:O	2.30	0.64
1:A:396:ASP:OD2	1:B:438:LYS:HE2	1.99	0.62
1:A:288[B]:ARG:HE	2:A:7001:SF1:CAS	2.14	0.59
1:A:370:PHE:CZ	1:A:442:LEU:HD13	2.36	0.59
1:A:437:GLN:HG2	1:B:439[A]:MET:CE	2.31	0.59
1:B:330:LEU:O	1:B:334:MET:HG3	2.03	0.59
1:A:454:GLN:O	1:A:458:LYS:HG2	2.04	0.56
2:A:7001:SF1:HAQ1	2:A:7001:SF1:OAA	2.06	0.56
1:B:449:HIS:CD2	3:B:5058:HOH:O	2.46	0.56
1:B:334:MET:HE1	3:B:5019:HOH:O	2.05	0.56
1:B:348:MET:HE3	2:B:5001:SF1:HAH	1.88	0.54
1:A:363:PHE:HB2	1:A:452:LEU:CD2	2.38	0.54
1:A:228:LEU:HB2	1:A:343:GLU:HG2	1.90	0.53
1:A:357:ARG:CG	1:A:357:ARG:HH11	2.07	0.53
1:A:439:MET:HE1	1:B:437:GLN:CB	2.39	0.53
1:B:334:MET:CE	1:B:371:ALA:HB2	2.38	0.53
1:A:255:LEU:HD22	1:A:277:VAL:CG2	2.38	0.53
1:B:288[B]:ARG:HE	2:B:5001:SF1:CAS	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:THR:OG1	1:B:442:LEU:HD11	2.10	0.51
1:B:334:MET:CE	3:B:5019:HOH:O	2.58	0.51
1:A:439:MET:HE1	1:B:437:GLN:HB2	1.91	0.51
1:A:255:LEU:HD22	1:A:277:VAL:HG21	1.93	0.51
1:B:462:ASP:O	1:B:463:MET:HG2	2.11	0.51
1:A:252:MET:SD	1:A:277:VAL:HG11	2.51	0.50
1:A:226:PHE:CE1	1:A:296[A]:ILE:HD13	2.45	0.50
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.93	0.50
1:B:348:MET:CE	2:B:5001:SF1:HAH	2.42	0.49
1:B:276:GLU:HG2	1:B:279:ILE:HG12	1.93	0.49
1:B:323:HIS:CE1	1:B:476:LEU:HD12	2.48	0.49
1:A:363:PHE:CB	1:A:452:LEU:HD21	2.42	0.49
1:A:437:GLN:HG2	1:B:439[A]:MET:HE3	1.94	0.49
1:B:334:MET:HE3	1:B:371:ALA:HB2	1.94	0.49
1:A:444:GLN:HG3	1:B:443[A]:ARG:CZ	2.41	0.49
1:A:437:GLN:HG2	1:B:439[A]:MET:HE1	1.94	0.48
1:A:360:PHE:O	1:A:363:PHE:HD2	1.97	0.48
2:B:5001:SF1:OAB	2:B:5001:SF1:HAQ1	2.14	0.47
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.97	0.47
1:B:266:HIS:CD2	1:B:280:ARG:HG2	2.52	0.45
1:B:411:ASP:OD2	1:B:415:GLN:NE2	2.46	0.45
1:A:370:PHE:CB	1:A:445:ILE:HD11	2.48	0.44
1:A:446:VAL:O	1:A:450:VAL:HG13	2.17	0.44
1:A:404:LYS:HE2	1:A:408:ASP:OD1	2.17	0.44
1:A:439:MET:CE	1:B:437:GLN:HB2	2.48	0.44
1:B:249:ILE:HG21	1:B:348:MET:HE2	1.99	0.44
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.48	0.44
1:A:433:ALA:O	1:A:437:GLN:HG3	2.18	0.43
2:B:5001:SF1:SAR	2:B:5001:SF1:OAA	2.76	0.43
1:A:363:PHE:CB	1:A:452:LEU:CD2	2.96	0.43
1:A:318:LEU:O	1:A:322:VAL:HB	2.18	0.43
1:A:379:LEU:HD11	1:A:435:LEU:HD13	2.01	0.43
1:A:363:PHE:HB3	1:A:452:LEU:HD21	1.99	0.43
1:B:279:ILE:HD12	1:B:463:MET:HE2	2.02	0.42
1:A:357:ARG:HD2	1:A:358:LYS:C	2.35	0.42
1:A:437:GLN:O	1:A:440:THR:HB	2.20	0.42
1:B:249:ILE:HD12	1:B:341:ILE:HD11	2.02	0.42
1:A:288[A]:ARG:HH22	1:A:295:GLU:CD	2.23	0.42
1:B:252:MET:SD	1:B:277:VAL:HG11	2.59	0.41
2:B:5001:SF1:CAZ	2:B:5001:SF1:HAJ	2.50	0.41
1:B:255:LEU:HD21	1:B:277:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:CD	1:A:357:ARG:HH12	2.24	0.41
1:A:474:LYS:HA	1:A:475:ASP:HA	1.81	0.41
1:B:447:THR:O	1:B:450:VAL:HG22	2.21	0.40
1:A:354:LYS:HA	1:A:361:GLY:O	2.21	0.40
1:A:439:MET:CE	1:B:437:GLN:CB	2.99	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	260/274 (95%)	255 (98%)	5 (2%)	0	100	100
1	B	259/274 (94%)	251 (97%)	7 (3%)	1 (0%)	39	42
All	All	519/548 (95%)	506 (98%)	12 (2%)	1 (0%)	52	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	264	PHE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/247 (94%)	218 (94%)	13 (6%)	26	29
1	B	230/247 (93%)	213 (93%)	17 (7%)	17	17
All	All	461/494 (93%)	431 (94%)	30 (6%)	23	23

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256[A]	MET
1	A	256[B]	MET
1	A	277	VAL
1	A	322	VAL
1	A	342[A]	SER
1	A	342[B]	SER
1	A	343	GLU
1	A	357	ARG
1	A	441	ASP
1	A	442	LEU
1	A	461	THR
1	A	463	MET
1	A	474	LYS
1	B	208	SER
1	B	216	LYS
1	B	234	ARG
1	B	253	ASN
1	B	256	MET
1	B	275	LYS
1	B	276	GLU
1	B	323	HIS
1	B	357	ARG
1	B	362	ASP
1	B	363	PHE
1	B	369	GLU
1	B	428	SER
1	B	443[A]	ARG
1	B	443[B]	ARG
1	B	468	LEU
1	B	474	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	449	HIS
1	A	451	GLN
1	B	253	ASN
1	B	283	GLN
1	B	449	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	SF1	A	7001	-	23,30,30	1.07	1 (4%)	25,42,42	0.76	1 (4%)
2	SF1	B	5001	-	23,30,30	1.14	2 (8%)	25,42,42	0.67	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.

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF1	A	7001	-	-	0/6/12/12	0/4/4/4
2	SF1	B	5001	-	-	0/6/12/12	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5001	SF1	CAW-SAR	-2.74	1.75	1.78
2	A	7001	SF1	CAQ-CAU	2.36	1.56	1.51
2	B	5001	SF1	CAQ-CAU	2.45	1.57	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	7001	SF1	CAV-SAR-CAW	2.08	107.51	101.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	7001	SF1	2	0
2	B	5001	SF1	6	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	256/274 (93%)	0.30	20 (7%)	16	15	12, 21, 42, 54	6 (2%)
1	B	259/274 (94%)	0.57	33 (12%)	5	4	13, 22, 44, 59	0
All	All	515/548 (93%)	0.43	53 (10%)	9	8	12, 22, 43, 59	6 (1%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	241	THR	7.7
1	B	267	ILE	5.2
1	A	287	PHE	5.0
1	A	260	ASP	4.9
1	B	451	GLN	4.8
1	B	260	ASP	4.7
1	A	209	ALA	4.5
1	B	261	LYS	4.5
1	A	474	LYS	4.2
1	B	262	ILE	4.1
1	A	464	SER	4.1
1	B	454	GLN	4.1
1	A	470	GLN	3.9
1	B	263	LYS	3.9
1	B	453	LEU	3.8
1	B	282	PHE	3.7
1	A	472	ILE	3.6
1	B	275	LYS	3.4
1	B	244	LYS	3.3
1	A	461	THR	3.3
1	A	454	GLN	3.2
1	B	456	ILE	3.2
1	A	462	ASP	3.2
1	B	240	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	463	MET	3.2
1	B	455	VAL	3.1
1	A	275	LYS	3.1
1	B	256	MET	3.1
1	B	470	GLN	3.1
1	A	477	TYR	3.0
1	B	258	GLY	3.0
1	B	249	ILE	3.0
1	B	362	ASP	2.9
1	B	363	PHE	2.9
1	A	362	ASP	2.9
1	B	475	ASP	2.8
1	B	254	SER	2.7
1	B	369	GLU	2.7
1	B	247	PHE	2.6
1	B	276	GLU	2.6
1	A	469	LEU	2.6
1	B	264	PHE	2.5
1	B	255	LEU	2.5
1	A	455	VAL	2.5
1	A	312	ASN	2.5
1	A	257	MET	2.4
1	B	427	GLU	2.4
1	A	467	PRO	2.2
1	B	210	ASP	2.2
1	B	253	ASN	2.2
1	B	251	ASP	2.1
1	A	253[A]	ASN	2.1
1	B	457	LYS	2.1

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	SF1	B	5001	27/27	0.90	0.13	-0.47	31,34,41,42	0
2	SF1	A	7001	27/27	0.91	0.12	-0.54	29,35,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.