



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:53 PM GMT

PDB ID : 1S9P  
Title : crystal structure of the ligand-binding domain of the estrogen-related receptor gamma in complex with diethylstilbestrol  
Authors : Greschik, H.; Flaig, R.; Renaud, J.P.; Moras, D.  
Deposited on : 2004-02-05  
Resolution : 2.13 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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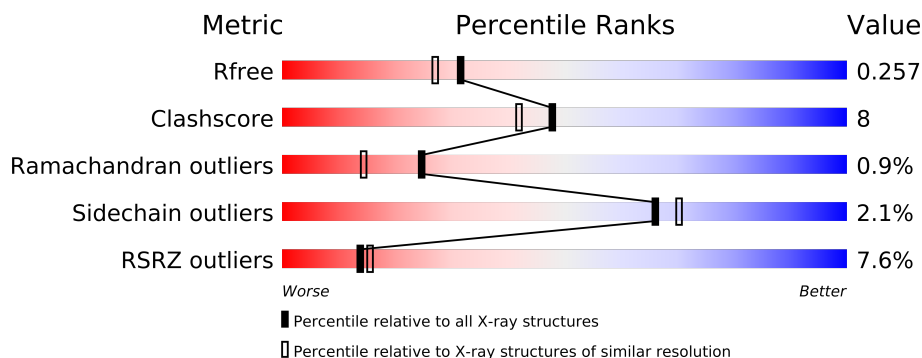
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.13 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	1116 (2.16-2.12)
Clashscore	79885	1302 (2.16-2.12)
Ramachandran outliers	78287	1281 (2.16-2.12)
Sidechain outliers	78261	1281 (2.16-2.12)
RSRZ outliers	66119	1116 (2.16-2.12)

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	227	
1	B	227	
1	C	227	
1	D	227	

## 2 Entry composition i

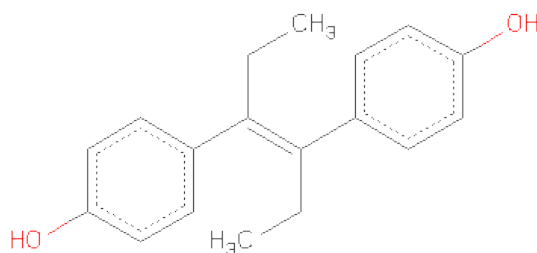
There are 3 unique types of molecules in this entry. The entry contains 7129 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Estrogen-related receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1679	1072	274	323	10			
1	B	217	Total	C	N	O	S	0	0	0
			1696	1084	277	325	10			
1	C	219	Total	C	N	O	S	0	0	0
			1696	1083	277	326	10			
1	D	225	Total	C	N	O	S	0	0	0
			1772	1137	287	336	12			

- Molecule 2 is DIETHYLSTILBESTROL (three-letter code: DES) (formula: C<sub>18</sub>H<sub>20</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	18	2		
2	B	1	Total	C	O	0	0
			20	18	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			20	18	2		
2	D	1	Total	C	O	0	0
			20	18	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total	O	0	0
			53	53		
3	B	63	Total	O	0	0
			63	63		
3	C	41	Total	O	0	0
			41	41		
3	D	49	Total	O	0	0
			49	49		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.00Å 77.46Å 95.77Å 90.00° 97.55° 90.00°	Depositor
Resolution (Å)	29.30 – 2.13 29.30 – 2.13	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.30-2.13) 99.0 (29.30-2.13)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.51 (at 2.14Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226 , 0.251 0.236 , 0.257	Depositor DCC
$R_{free}$ test set	2941 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 57918 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: DES

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	0.37	0/1707	0.61	2/2312 (0.1%)
1	B	0.35	0/1725	0.56	0/2334
1	C	0.31	0/1724	0.54	0/2336
1	D	0.34	0/1803	0.55	0/2440
All	All	0.34	0/6959	0.57	2/9422 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	PRO	N-CA-CB	5.61	110.03	103.30
1	A	233	PRO	N-CA-CB	5.03	109.34	103.30

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	1679	0	1677	27	0
1	B	1696	0	1710	26	0
1	C	1696	0	1693	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1772	0	1791	42	0
2	A	20	0	20	0	0
2	B	20	0	20	0	0
2	C	20	0	20	1	0
2	D	20	0	20	0	0
3	A	53	0	0	0	0
3	B	63	0	0	1	0
3	C	41	0	0	2	0
3	D	49	0	0	0	0
All	All	7129	0	6951	109	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 8.

All (109) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:380:MET:HG2	1:D:351:GLN:HE22	1.03	1.11
1:A:294:LEU:HD11	1:D:458:VAL:O	1.51	1.11
1:C:380:MET:HG2	1:D:351:GLN:NE2	1.83	0.93
1:A:304:ALA:HB2	1:A:377:SER:HB3	1.57	0.85
1:A:294:LEU:CD1	1:D:458:VAL:O	2.29	0.81
1:C:304:ALA:HB2	1:C:377:SER:HB3	1.65	0.76
1:D:355:LYS:HG3	1:D:359:MET:CE	2.18	0.73
1:C:333:ASP:H	1:C:336:GLN:HE21	1.35	0.73
1:C:433:GLN:HE22	1:D:433:GLN:HE22	1.37	0.73
1:D:304:ALA:HB2	1:D:377:SER:HB3	1.76	0.68
1:B:289:PHE:CE2	1:B:297:GLN:HG2	2.28	0.68
1:C:380:MET:CG	1:D:351:GLN:HE22	1.95	0.66
1:D:407:HIS:HA	1:D:409:GLU:OE2	1.95	0.66
1:B:304:ALA:HB2	1:B:377:SER:HB3	1.79	0.65
1:C:429:THR:O	1:C:433:GLN:HG3	1.97	0.65
1:C:333:ASP:H	1:C:336:GLN:NE2	1.95	0.63
1:B:438:ILE:HD12	1:B:443:LYS:HD2	1.81	0.62
1:A:339:LEU:HD23	1:A:339:LEU:O	2.00	0.61
1:C:396:HIS:CE1	1:D:412:ARG:HG2	2.36	0.61
1:C:249:ILE:HD11	1:C:278:VAL:HG21	1.81	0.60
1:D:261:ASP:O	1:D:265:LEU:HG	2.00	0.60
1:A:396:HIS:CE1	1:B:412:ARG:HG2	2.38	0.59
3:C:73:HOH:O	1:D:355:LYS:HE2	2.01	0.59
1:B:290:SER:HA	1:B:297:GLN:NE2	2.18	0.58
1:A:439:LYS:HE2	1:A:447:HIS:CB	2.33	0.58
1:B:246:PRO:HB3	1:B:278:VAL:CG1	2.34	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:386:GLU:CD	1:D:386:GLU:H	2.06	0.58
1:B:262:ILE:HD12	1:B:443:LYS:O	2.04	0.57
1:A:355:LYS:O	1:A:359:MET:HE2	2.04	0.57
1:D:438:ILE:HG23	1:D:443:LYS:HB2	1.86	0.55
1:A:294:LEU:HD11	1:D:458:VAL:C	2.25	0.55
1:A:436:TYR:O	1:A:440:LEU:CB	2.56	0.54
1:D:352:LEU:HD13	1:D:423:LEU:HG	1.89	0.54
1:D:448:LYS:O	1:D:452:GLU:HG3	2.07	0.54
1:B:262:ILE:CD1	1:B:443:LYS:HG2	2.38	0.54
1:B:249:ILE:HD13	1:B:275:GLU:HA	1.89	0.54
1:C:403:GLU:OE1	1:C:413:ARG:HD3	2.09	0.53
1:B:449:LEU:O	1:B:450:PHE:C	2.46	0.53
1:B:423:LEU:HD11	3:B:117:HOH:O	2.08	0.53
1:A:356:TYR:CD1	1:A:359:MET:HE3	2.44	0.53
1:D:276:LEU:HD22	1:D:454:LEU:HD12	1.89	0.53
1:D:338:LYS:CG	1:D:343:LEU:HD22	2.38	0.53
1:D:338:LYS:HG2	1:D:343:LEU:HD22	1.92	0.51
1:D:355:LYS:HG3	1:D:359:MET:HE1	1.92	0.51
1:B:366:PHE:CZ	1:B:370:LYS:HE2	2.46	0.51
1:C:449:LEU:O	1:C:451:LEU:N	2.44	0.50
1:A:333:ASP:OD1	1:A:336:GLN:HB2	2.11	0.50
1:A:355:LYS:CG	1:A:359:MET:HE1	2.42	0.50
1:B:282:TRP:CH2	1:B:286:ILE:HD11	2.47	0.50
1:D:437:ASN:O	1:D:441:GLU:HG3	2.12	0.50
1:C:449:LEU:C	1:C:451:LEU:H	2.15	0.50
1:C:386:GLU:O	1:C:390:LYS:HG3	2.11	0.49
1:C:235:ASN:HD21	1:C:398:ALA:HA	1.76	0.49
1:A:242:LEU:HD11	1:A:364:GLU:HG3	1.96	0.48
1:D:412:ARG:HB3	1:D:416:LYS:HE3	1.96	0.47
1:C:433:GLN:HE22	1:D:433:GLN:NE2	2.10	0.47
1:B:300:LEU:HD23	1:B:382:ILE:HD11	1.96	0.47
1:A:402:TYR:CE1	1:A:406:GLN:HG3	2.50	0.47
1:B:409:GLU:HG3	1:B:409:GLU:H	1.41	0.47
1:C:399:LEU:O	1:C:403:GLU:HG2	2.15	0.46
1:C:412:ARG:HA	3:C:179:HOH:O	2.15	0.46
1:C:304:ALA:HB2	1:C:377:SER:CB	2.41	0.46
1:C:438:ILE:HG13	2:C:500:DES:OP3	2.16	0.46
1:D:304:ALA:HB2	1:D:377:SER:CB	2.44	0.46
1:C:351:GLN:NE2	1:D:380:MET:HG2	2.31	0.46
1:B:255:PRO:C	1:B:257:VAL:N	2.68	0.45
1:A:438:ILE:HG13	1:A:439:LYS:N	2.32	0.45
1:B:407:HIS:ND1	1:B:409:GLU:OE2	2.48	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:298:MET:O	1:D:302:GLN:HG3	2.17	0.45
1:A:276:LEU:HD21	1:A:305:TRP:HB2	1.99	0.45
1:D:338:LYS:CE	1:D:343:LEU:HD22	2.48	0.44
1:B:235:ASN:OD1	1:B:238:VAL:HG23	2.18	0.44
1:A:261:ASP:OD1	1:A:262:ILE:N	2.50	0.44
1:D:276:LEU:HD22	1:D:454:LEU:CD1	2.48	0.43
1:C:415:GLY:HA3	1:D:396:HIS:CE1	2.53	0.43
1:D:253:PRO:O	1:D:255:PRO:HD3	2.17	0.43
1:B:320:PHE:N	1:B:320:PHE:CD2	2.86	0.43
1:A:355:LYS:HG3	1:A:359:MET:HE1	2.00	0.43
1:D:410:ASP:C	1:D:412:ARG:H	2.22	0.43
1:B:294:LEU:HD12	1:B:297:GLN:OE1	2.18	0.43
1:A:355:LYS:HG3	1:A:359:MET:CE	2.49	0.43
1:B:246:PRO:CB	1:B:278:VAL:CG1	2.96	0.43
1:B:368:THR:HG21	1:B:399:LEU:HB2	2.00	0.43
1:D:403:GLU:OE1	1:D:413:ARG:HD3	2.19	0.42
1:D:351:GLN:HE21	1:D:351:GLN:HB2	1.66	0.42
1:A:355:LYS:HG2	1:A:359:MET:HE1	2.01	0.42
1:D:355:LYS:HG3	1:D:359:MET:HE2	1.98	0.42
1:A:438:ILE:HG13	1:A:439:LYS:H	1.84	0.42
1:A:334:GLU:O	1:A:338:LYS:HG3	2.19	0.42
1:B:255:PRO:C	1:B:257:VAL:H	2.22	0.42
1:A:394:VAL:HG11	1:D:449:LEU:CD1	2.50	0.42
1:D:261:ASP:HA	1:D:340:ALA:HA	2.00	0.42
1:D:421:LEU:N	1:D:422:PRO:CD	2.83	0.42
1:A:440:LEU:C	1:A:442:GLY:H	2.24	0.42
1:C:282:TRP:CH2	1:C:286:ILE:HD11	2.55	0.41
1:B:249:ILE:HD11	1:B:278:VAL:HG21	2.01	0.41
1:B:294:LEU:HD12	1:B:294:LEU:HA	1.93	0.41
1:D:306:MET:O	1:D:310:ILE:HG12	2.21	0.41
1:C:235:ASN:OD1	1:C:238:VAL:HG23	2.20	0.41
1:C:249:ILE:HD13	1:C:275:GLU:HA	2.03	0.41
1:D:448:LYS:HD3	1:D:448:LYS:HA	1.84	0.41
1:A:320:PHE:CE2	1:A:325:VAL:HG21	2.56	0.41
1:D:265:LEU:HD13	1:D:438:ILE:HG21	2.03	0.40
1:C:306:MET:HG2	1:C:432:VAL:HG23	2.03	0.40
1:A:304:ALA:HB2	1:A:377:SER:CB	2.40	0.40
1:D:234:TYR:CD1	1:D:234:TYR:C	2.94	0.40
1:A:235:ASN:ND2	1:A:398:ALA:HA	2.36	0.40
1:B:286:ILE:HA	1:B:287:PRO:HD3	1.88	0.40
1:C:296:ASP:O	1:C:300:LEU:HG	2.22	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	213/227 (94%)	203 (95%)	5 (2%)	5 (2%)	10	2
1	B	215/227 (95%)	204 (95%)	10 (5%)	1 (0%)	38	30
1	C	217/227 (96%)	208 (96%)	8 (4%)	1 (0%)	38	30
1	D	223/227 (98%)	219 (98%)	3 (1%)	1 (0%)	43	39
All	All	868/908 (96%)	834 (96%)	26 (3%)	8 (1%)	25	14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	MET
1	A	443	LYS
1	C	450	PHE
1	A	445	PRO
1	D	456	ALA
1	A	235	ASN
1	A	441	GLU
1	B	445	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	182/201 (90%)	178 (98%)	4 (2%)	64	68
1	B	186/201 (92%)	182 (98%)	4 (2%)	64	68
1	C	183/201 (91%)	178 (97%)	5 (3%)	57	58
1	D	194/201 (96%)	191 (98%)	3 (2%)	76	82
All	All	745/804 (93%)	729 (98%)	16 (2%)	66	70

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	ASP
1	A	311	LEU
1	A	336	GLN
1	A	344	ASP
1	B	247	GLU
1	B	408	MET
1	B	409	GLU
1	B	433	GLN
1	C	290	SER
1	C	389	GLN
1	C	393	ASP
1	C	409	GLU
1	C	437	ASN
1	D	240	HIS
1	D	344	ASP
1	D	409	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	GLN
1	A	347	ASN
1	A	389	GLN
1	B	389	GLN
1	B	396	HIS
1	C	302	GLN
1	C	336	GLN
1	C	351	GLN
1	C	389	GLN
1	C	396	HIS
1	C	433	GLN
1	D	351	GLN
1	D	396	HIS
1	D	400	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 ⓘ

4 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	DES	A	459	-	21,21,21	1.88	9 (42%)	28,28,28	0.89	2 (7%)
2	DES	B	459	-	21,21,21	1.88	9 (42%)	28,28,28	0.89	2 (7%)
2	DES	C	500	-	21,21,21	1.84	10 (47%)	28,28,28	0.82	1 (3%)
2	DES	D	600	-	21,21,21	1.86	9 (42%)	28,28,28	1.07	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	DES	A	459	-	-	0/16/16/16	0/2/2/2
2	DES	B	459	-	-	0/16/16/16	0/2/2/2
2	DES	C	500	-	-	0/16/16/16	0/2/2/2
2	DES	D	600	-	-	0/16/16/16	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	DES	CP2-CP1	2.99	1.44	1.38
2	C	500	DES	CP2-CP1	2.79	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	DES	CP1-CP6	2.75	1.44	1.39
2	A	459	DES	C1-C2	2.69	1.43	1.38
2	B	459	DES	C1-C2	2.67	1.43	1.38
2	A	459	DES	C6-C7	2.65	1.55	1.49
2	B	459	DES	C6-C7	2.64	1.55	1.49
2	A	459	DES	CP2-CP1	2.59	1.43	1.38
2	B	459	DES	CP2-CP1	2.58	1.43	1.38
2	D	600	DES	CP5-CP6	2.56	1.43	1.39
2	C	500	DES	CP5-CP6	2.54	1.43	1.39
2	C	500	DES	C4-C5	2.54	1.43	1.38
2	D	600	DES	C1-C2	2.53	1.43	1.38
2	D	600	DES	CP1-CP6	2.53	1.43	1.39
2	B	459	DES	CP5-CP6	2.52	1.43	1.39
2	A	459	DES	CP6-CP7	2.50	1.54	1.49
2	A	459	DES	CP5-CP6	2.50	1.43	1.39
2	B	459	DES	CP6-CP7	2.49	1.54	1.49
2	A	459	DES	C5-C6	2.45	1.43	1.39
2	B	459	DES	C5-C6	2.45	1.43	1.39
2	A	459	DES	C4-C5	2.41	1.43	1.38
2	D	600	DES	CP6-CP7	2.40	1.54	1.49
2	B	459	DES	C4-C5	2.39	1.43	1.38
2	B	459	DES	CP1-CP6	2.38	1.43	1.39
2	C	500	DES	C5-C6	2.37	1.43	1.39
2	D	600	DES	C1-C6	2.36	1.43	1.39
2	D	600	DES	C6-C7	2.35	1.54	1.49
2	A	459	DES	CP1-CP6	2.35	1.43	1.39
2	C	500	DES	CP6-CP7	2.34	1.54	1.49
2	C	500	DES	C6-C7	2.33	1.54	1.49
2	B	459	DES	C1-C6	2.29	1.43	1.39
2	A	459	DES	C1-C6	2.26	1.43	1.39
2	C	500	DES	C2-C3	2.18	1.43	1.38
2	D	600	DES	C5-C6	2.12	1.43	1.39
2	C	500	DES	C1-C2	2.10	1.42	1.38
2	C	500	DES	C1-C6	2.06	1.42	1.39
2	D	600	DES	CP2-CP3	2.00	1.43	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	DES	CP9-CP8-CP7	3.04	118.11	113.03
2	B	459	DES	C8-C7-C6	-2.44	111.10	114.20
2	A	459	DES	C8-C7-C6	-2.42	111.12	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	459	DES	CP9-CP8-CP7	2.19	116.69	113.03
2	B	459	DES	CP9-CP8-CP7	2.19	116.68	113.03
2	D	600	DES	C8-C7-C6	-2.13	111.50	114.20
2	C	500	DES	C8-C7-C6	-2.03	111.61	114.20

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	215/227 (94%)	0.51	20 (9%) 9 9	25, 40, 74, 89	0
1	B	217/227 (95%)	0.41	15 (6%) 17 18	22, 41, 63, 83	0
1	C	219/227 (96%)	0.47	17 (7%) 13 14	28, 45, 64, 84	0
1	D	225/227 (99%)	0.42	15 (6%) 17 19	28, 43, 64, 85	0
All	All	876/908 (96%)	0.45	67 (7%) 14 15	22, 42, 65, 89	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	458	VAL	11.6
1	C	452	GLU	7.9
1	A	256	THR	7.4
1	C	450	PHE	7.0
1	C	451	LEU	6.7
1	A	446	MET	6.1
1	A	257	VAL	5.7
1	B	449	LEU	5.3
1	A	233	PRO	5.1
1	A	444	VAL	5.1
1	C	234	TYR	4.6
1	C	294	LEU	4.5
1	C	449	LEU	4.3
1	D	234	TYR	4.2
1	A	447	HIS	4.1
1	B	447	HIS	4.0
1	B	294	LEU	3.9
1	A	442	GLY	3.8
1	C	446	MET	3.7
1	A	258	PRO	3.7
1	D	408	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	234	TYR	3.6
1	A	436	TYR	3.6
1	D	255	PRO	3.5
1	B	450	PHE	3.4
1	B	446	MET	3.4
1	A	255	PRO	3.4
1	D	418	LEU	3.3
1	C	448	LYS	3.3
1	C	447	HIS	3.2
1	D	456	ALA	3.1
1	A	443	LYS	3.1
1	A	408	MET	3.1
1	A	440	LEU	3.0
1	B	256	THR	3.0
1	C	404	ALA	3.0
1	C	405	GLY	3.0
1	D	258	PRO	2.9
1	A	437	ASN	2.9
1	D	339	LEU	2.8
1	A	262	ILE	2.8
1	B	372	ILE	2.7
1	A	234	TYR	2.7
1	D	440	LEU	2.6
1	D	421	LEU	2.6
1	C	339	LEU	2.5
1	D	369	LEU	2.4
1	B	408	MET	2.4
1	B	373	ALA	2.4
1	B	421	LEU	2.4
1	D	446	MET	2.4
1	C	243	VAL	2.4
1	A	260	SER	2.3
1	B	310	ILE	2.3
1	B	258	PRO	2.2
1	A	445	PRO	2.2
1	C	418	LEU	2.1
1	A	438	ILE	2.1
1	C	298	MET	2.1
1	C	415	GLY	2.1
1	B	257	VAL	2.1
1	C	408	MET	2.1
1	D	373	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	369	LEU	2.0
1	A	439	LYS	2.0
1	D	457	LYS	2.0
1	D	372	ILE	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<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	DES	B	459	20/20	0.21	1.74	38,41,46,49	0
2	DES	C	500	20/20	0.15	1.45	31,37,41,43	0
2	DES	D	600	20/20	0.15	1.35	29,37,42,43	0
2	DES	A	459	20/20	0.15	0.51	38,41,46,49	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.