



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:00 PM GMT

PDB ID : 1DKF  
Title : CRYSTAL STRUCTURE OF A HETERODIMERIC COMPLEX OF RAR  
AND RXR LIGAND-BINDING DOMAINS  
Authors : Bourguet, W.; Vivat, V.; Wurtz, J.M.; Chambon, P.; Gronemeyer, H.; Moras,  
D.; Structural Proteomics in Europe (SPINE)  
Deposited on : 1999-12-07  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (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

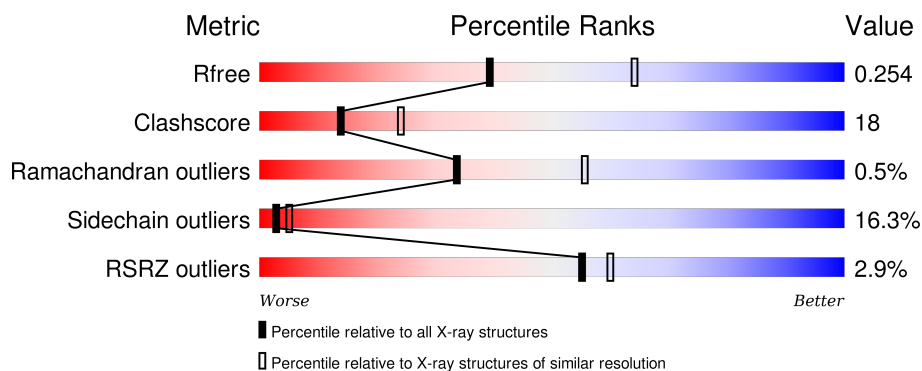
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

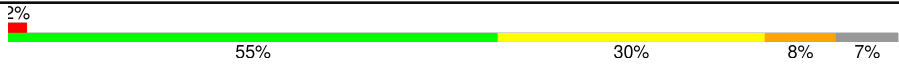

The reported resolution of this entry is 2.50 Å.

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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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  $\leq 5\%$ . 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	233	
2	B	235	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BMS	B	600	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3743 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 PROTEIN (RETINOID X RECEPTOR-ALPHA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1701	1088	291	312	10			

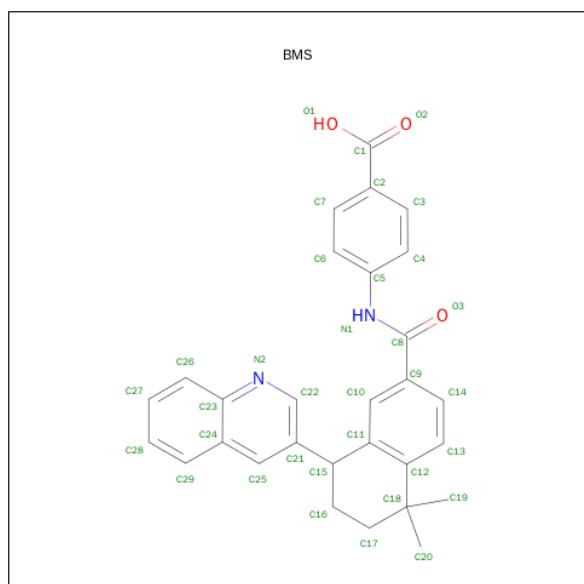
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	ALA	PHE	ENGINEERED	UNP P28700

- Molecule 2 is a protein called PROTEIN (RETINOIC ACID RECEPTOR-ALPHA).

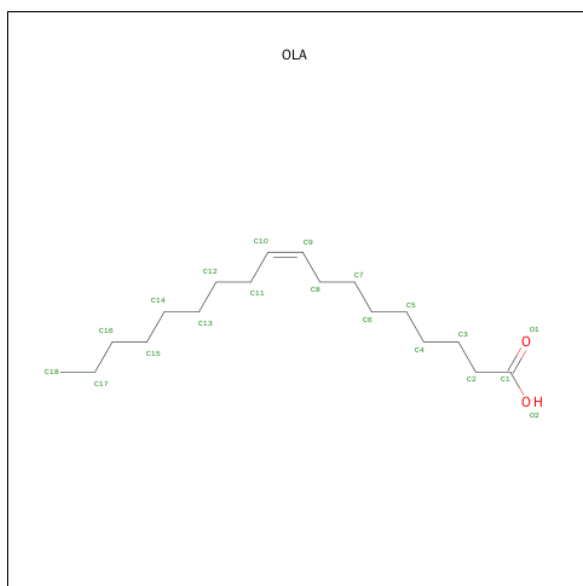
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	232	Total	C	N	O	S	0	0	0
			1831	1164	307	344	16			

- Molecule 3 is 4-[(4,4-DIMETHYL-1,2,3,4-TETRAHYDRO-[1,2']BINAPHTHALENYL-7-CARBONYL)-AMINO]-BENZOIC ACID (three-letter code: BMS) (formula:  $C_{29}H_{26}N_2O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			34	29	2	3		

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula:  $C_{18}H_{34}O_2$ ).



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

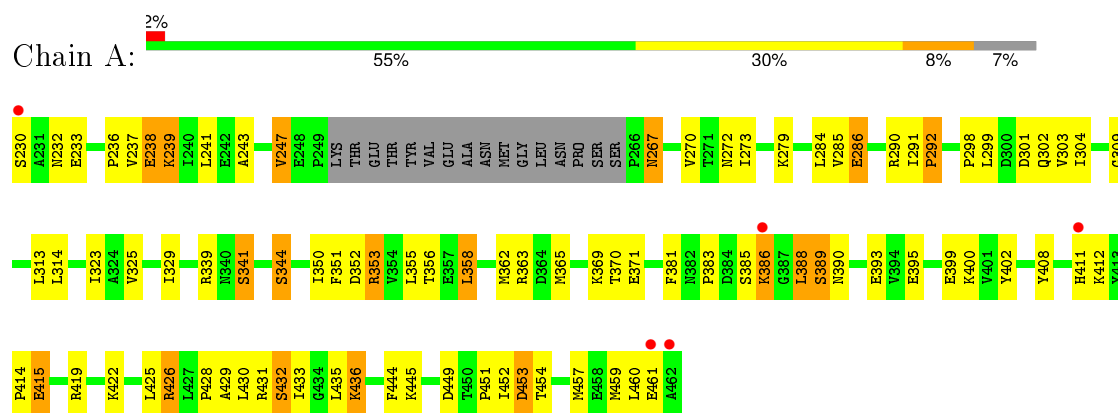
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O	0	0
			79	79		
5	B	78	Total	O	0	0
			78	78		

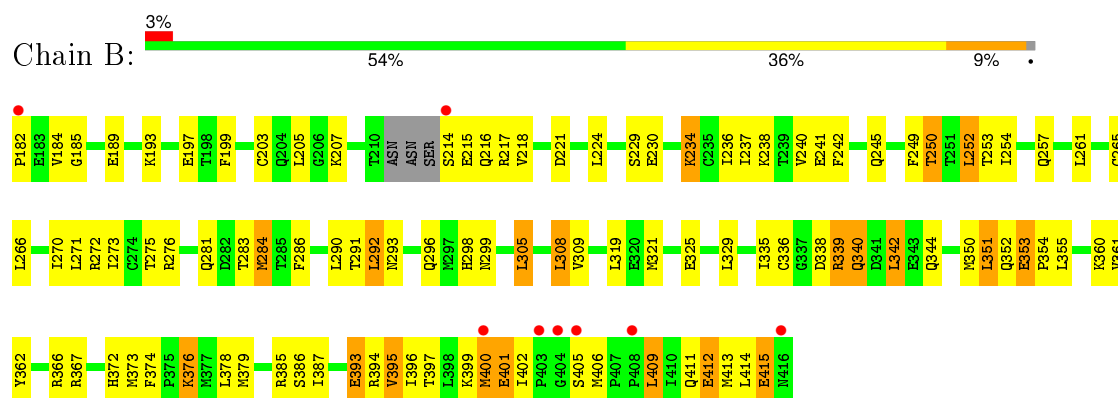
### 3 Residue-property plots

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: PROTEIN (RETINOID X RECEPTOR-ALPHA)



#### • Molecule 2: PROTEIN (RETINOIC ACID RECEPTOR-ALPHA)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.60 Å 116.60 Å 207.80 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.82 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 88.3 (19.82-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 2.50 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.203 , 0.262 0.203 , 0.254	Depositor DCC
$R_{free}$ test set	1286 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.9	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29122 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3743	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: OLA, BMS

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	0/1734	0.58	0/2344
2	B	0.42	0/1860	0.61	0/2511
All	All	0.41	0/3594	0.60	0/4855

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	1701	0	1734	62	0
2	B	1831	0	1888	74	0
3	B	34	0	24	1	0
4	A	20	0	33	1	0
5	A	79	0	0	2	0
5	B	78	0	0	3	0
All	All	3743	0	3679	134	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 18.

All (134) 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:353:ARG:HH22	1:A:432:SER:HB3	1.12	1.05
1:A:353:ARG:NH2	1:A:432:SER:HB3	1.81	0.96
2:B:411:GLN:O	2:B:415:GLU:HG2	1.83	0.79
2:B:393:GLU:O	2:B:396:ILE:HG13	1.82	0.79
2:B:261:LEU:HD12	2:B:414:LEU:HD22	1.68	0.75
2:B:399:LYS:HA	2:B:405:SER:OG	1.88	0.73
2:B:293:ASN:CG	2:B:296:GLN:HE21	1.91	0.73
1:A:353:ARG:HH22	1:A:432:SER:CB	1.98	0.72
1:A:323:ILE:HG23	1:A:363:ARG:HB2	1.72	0.71
1:A:230:SER:HA	1:A:233:GLU:HG3	1.73	0.70
1:A:350:ILE:H	1:A:350:ILE:HD12	1.56	0.70
2:B:240:VAL:HG22	2:B:261:LEU:HD13	1.74	0.69
2:B:271:LEU:O	2:B:275:THR:HG23	1.94	0.68
2:B:273:ILE:HG13	2:B:284:MET:HG2	1.76	0.67
2:B:400:MET:HG2	2:B:401:GLU:N	2.09	0.66
2:B:308:LEU:HD23	2:B:387:ILE:HG12	1.77	0.66
2:B:207:LYS:HG2	2:B:291:THR:OG1	1.96	0.65
1:A:267:ASN:C	1:A:267:ASN:HD22	2.01	0.65
1:A:431:ARG:HH11	1:A:431:ARG:HG2	1.62	0.64
2:B:237:ILE:O	2:B:241:GLU:HG3	1.96	0.64
2:B:352:GLN:HA	2:B:355:LEU:HD12	1.79	0.64
1:A:303:VAL:HG23	1:A:460:LEU:HD12	1.81	0.63
2:B:276:ARG:HG3	2:B:276:ARG:HH11	1.64	0.62
2:B:409:LEU:HD11	2:B:413:MET:HE1	1.82	0.62
1:A:358:LEU:HD22	1:A:433:ILE:HD13	1.81	0.62
1:A:232:ASN:ND2	1:A:236:PRO:HA	2.15	0.61
2:B:395:VAL:HG22	2:B:406:MET:HE3	1.84	0.60
2:B:412:GLU:HA	2:B:415:GLU:HG3	1.83	0.60
1:A:431:ARG:NH1	1:A:431:ARG:HG2	2.16	0.59
2:B:281:GLN:HB3	2:B:283:THR:HG23	1.85	0.59
1:A:385:SER:HB2	1:A:388:LEU:HD22	1.85	0.59
2:B:395:VAL:HG13	2:B:406:MET:HE1	1.86	0.58
1:A:371:GLU:OE2	1:A:419:ARG:HD3	2.03	0.58
2:B:250:THR:HA	2:B:257:GLN:NE2	2.19	0.57
2:B:319:LEU:HD11	2:B:376:LYS:HD3	1.86	0.57
2:B:339:ARG:HG2	2:B:339:ARG:HH11	1.68	0.57
1:A:353:ARG:HE	1:A:436:LYS:HE3	1.69	0.57
2:B:266:LEU:O	2:B:270:ILE:HG13	2.05	0.57
1:A:329:ILE:HD12	1:A:351:PHE:CZ	2.40	0.56
2:B:319:LEU:HA	2:B:373:MET:HE1	1.87	0.56
2:B:276:ARG:HG3	2:B:276:ARG:NH1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:ND2	1:A:272:ASN:HD21	2.04	0.55
1:A:298:PRO:HG2	1:A:301:ASP:HB2	1.89	0.55
1:A:390:ASN:ND2	1:A:393:GLU:HB2	2.22	0.55
2:B:218:VAL:H	2:B:299:ASN:HD21	1.55	0.55
2:B:249:PHE:O	2:B:252:LEU:HB2	2.08	0.54
2:B:361:VAL:HG23	2:B:362:TYR:N	2.24	0.53
1:A:371:GLU:CD	1:A:419:ARG:HH11	2.11	0.52
2:B:261:LEU:HD12	2:B:414:LEU:CD2	2.40	0.52
2:B:395:VAL:HG22	2:B:406:MET:CE	2.40	0.51
2:B:308:LEU:CD2	2:B:387:ILE:HG12	2.41	0.51
2:B:393:GLU:HB3	5:B:144:HOH:O	2.09	0.50
1:A:358:LEU:O	1:A:362:MET:HG3	2.11	0.50
2:B:182:PRO:HD2	2:B:184:VAL:HG12	1.92	0.50
1:A:323:ILE:O	1:A:363:ARG:NH1	2.42	0.50
1:A:304:ILE:HG21	1:A:388:LEU:HD13	1.94	0.49
1:A:429:ALA:O	1:A:433:ILE:HD12	2.12	0.49
2:B:215:GLU:HG3	2:B:216:GLN:N	2.26	0.49
2:B:286:PHE:HD1	2:B:290:LEU:O	1.95	0.49
2:B:399:LYS:HA	2:B:405:SER:HG	1.77	0.49
1:A:309:GLY:O	1:A:313:LEU:HG	2.13	0.49
1:A:365:MET:O	1:A:419:ARG:NH2	2.45	0.48
2:B:292:LEU:HG	2:B:296:GLN:HB3	1.95	0.48
1:A:459:MET:HE2	5:A:92:HOH:O	2.12	0.48
2:B:362:TYR:CE1	2:B:366:ARG:HD2	2.49	0.48
1:A:399:GLU:HG2	2:B:372:HIS:HB2	1.96	0.48
1:A:371:GLU:OE1	1:A:419:ARG:NH1	2.47	0.47
2:B:336:CYS:SG	2:B:338:ASP:HB2	2.54	0.47
1:A:451:PRO:HG2	1:A:454:THR:OG1	2.13	0.47
1:A:270:VAL:HA	1:A:444:PHE:CE2	2.50	0.47
1:A:352:ASP:O	1:A:356:THR:HG23	2.15	0.47
1:A:415:GLU:H	1:A:415:GLU:CD	2.17	0.47
2:B:218:VAL:H	2:B:299:ASN:ND2	2.13	0.47
2:B:184:VAL:HG13	2:B:185:GLY:N	2.30	0.47
1:A:247:VAL:HG13	1:A:247:VAL:O	2.15	0.47
1:A:383:PRO:HB3	1:A:395:GLU:HB2	1.98	0.46
1:A:236:PRO:HB2	1:A:239:LYS:HB2	1.97	0.46
1:A:411:HIS:O	1:A:414:PRO:HD3	2.14	0.46
1:A:431:ARG:O	1:A:435:LEU:HG	2.16	0.46
2:B:402:ILE:O	2:B:405:SER:HB3	2.16	0.46
1:A:232:ASN:ND2	1:A:238:GLU:OE2	2.49	0.46
1:A:452:ILE:HG22	1:A:453:ASP:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LYS:HB3	1:A:386:LYS:HE2	1.59	0.46
2:B:221:ASP:HB3	2:B:224:LEU:HB2	1.98	0.45
2:B:234:LYS:HE2	5:B:119:HOH:O	2.15	0.45
1:A:323:ILE:HG23	1:A:363:ARG:CB	2.45	0.45
4:A:700:OLA:H111	4:A:700:OLA:H81	1.83	0.45
2:B:379:MET:HA	2:B:379:MET:CE	2.48	0.44
2:B:367:ARG:HG3	2:B:367:ARG:HH11	1.81	0.44
2:B:415:GLU:HG2	2:B:415:GLU:H	1.55	0.44
2:B:414:LEU:HD12	2:B:414:LEU:HA	1.80	0.44
2:B:238:LYS:HE2	2:B:241:GLU:OE1	2.17	0.44
1:A:425:LEU:C	1:A:428:PRO:HD2	2.38	0.44
2:B:250:THR:O	2:B:257:GLN:NE2	2.50	0.44
2:B:325:GLU:CD	2:B:366:ARG:HH11	2.21	0.44
2:B:353:GLU:HB3	2:B:354:PRO:HD3	1.99	0.44
2:B:360:LYS:HA	2:B:374:PHE:CD2	2.53	0.44
1:A:267:ASN:HD21	1:A:272:ASN:HD21	1.65	0.43
1:A:241:LEU:O	1:A:241:LEU:HD12	2.18	0.43
1:A:339:ARG:HH11	1:A:339:ARG:HG3	1.83	0.43
2:B:305:LEU:O	2:B:309:VAL:HG23	2.18	0.43
1:A:402:TYR:OH	2:B:379:MET:HG3	2.19	0.43
2:B:293:ASN:H	2:B:296:GLN:NE2	2.16	0.43
1:A:291:ILE:HA	1:A:292:PRO:HD2	1.86	0.43
2:B:342:LEU:HD12	2:B:342:LEU:HA	1.91	0.43
2:B:339:ARG:HG2	2:B:339:ARG:NH1	2.34	0.43
1:A:285:VAL:HB	5:A:92:HOH:O	2.17	0.43
1:A:267:ASN:ND2	1:A:267:ASN:C	2.70	0.43
2:B:340:GLN:HE21	2:B:340:GLN:HB2	1.63	0.43
1:A:408:TYR:OH	1:A:412:LYS:HD2	2.19	0.42
1:A:298:PRO:O	1:A:302:GLN:HG3	2.19	0.42
1:A:399:GLU:HG2	2:B:372:HIS:CB	2.50	0.42
2:B:199:PHE:CE2	2:B:272:ARG:HB3	2.53	0.42
2:B:182:PRO:CD	2:B:184:VAL:HG12	2.49	0.42
2:B:335:ILE:O	2:B:335:ILE:HG22	2.19	0.42
1:A:243:ALA:HB2	1:A:290:ARG:HB2	2.00	0.42
2:B:217:ARG:HD3	2:B:298:HIS:CG	2.55	0.42
1:A:426:ARG:HD3	1:A:426:ARG:HA	1.68	0.42
2:B:242:PHE:O	2:B:245:GLN:HB2	2.20	0.42
1:A:301:ASP:OD1	1:A:389:SER:HB3	2.20	0.41
1:A:381:PHE:O	1:A:383:PRO:HD3	2.20	0.41
2:B:182:PRO:HD2	2:B:184:VAL:CG1	2.49	0.41
2:B:203:CYS:HB3	5:B:27:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:VAL:CG2	1:A:460:LEU:HD12	2.50	0.41
2:B:193:LYS:O	2:B:197:GLU:HB2	2.21	0.41
2:B:361:VAL:CG2	2:B:362:TYR:N	2.83	0.41
1:A:286:GLU:O	1:A:290:ARG:HG3	2.20	0.41
2:B:229:SER:HA	3:B:600:BMS:H29	2.03	0.41
1:A:422:LYS:HB2	1:A:422:LYS:NZ	2.36	0.41
2:B:351:LEU:HD23	2:B:351:LEU:HA	1.91	0.41
2:B:394:ARG:O	2:B:397:THR:HB	2.21	0.40
2:B:319:LEU:HB3	2:B:321:MET:HG3	2.03	0.40
1:A:237:VAL:HG13	1:A:370:THR:CG2	2.51	0.40
1:A:341:SER:O	1:A:344:SER:HB3	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	213/233 (91%)	198 (93%)	13 (6%)	2 (1%)	21	37
2	B	228/235 (97%)	218 (96%)	10 (4%)	0	100	100
All	All	441/468 (94%)	416 (94%)	23 (5%)	2 (0%)	34	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	VAL
1	A	292	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	185/199 (93%)	155 (84%)	30 (16%)	3	5
2	B	207/211 (98%)	173 (84%)	34 (16%)	3	5
All	All	392/410 (96%)	328 (84%)	64 (16%)	3	5

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	GLU
1	A	239	LYS
1	A	247	VAL
1	A	267	ASN
1	A	273	ILE
1	A	279	LYS
1	A	284	LEU
1	A	286	GLU
1	A	299	LEU
1	A	314	LEU
1	A	341	SER
1	A	344	SER
1	A	353	ARG
1	A	355	LEU
1	A	358	LEU
1	A	369	LYS
1	A	386	LYS
1	A	388	LEU
1	A	389	SER
1	A	400	LYS
1	A	415	GLU
1	A	426	ARG
1	A	430	LEU
1	A	432	SER
1	A	436	LYS
1	A	445	LYS
1	A	449	ASP

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Mol	Chain	Res	Type
1	A	453	ASP
1	A	457	MET
1	A	461	GLU
2	B	189	GLU
2	B	205	LEU
2	B	214	SER
2	B	230	GLU
2	B	234	LYS
2	B	236	ILE
2	B	250	THR
2	B	252	LEU
2	B	253	THR
2	B	254	ILE
2	B	265	CYS
2	B	284	MET
2	B	292	LEU
2	B	305	LEU
2	B	308	LEU
2	B	329	LEU
2	B	339	ARG
2	B	340	GLN
2	B	342	LEU
2	B	344	GLN
2	B	350	MET
2	B	351	LEU
2	B	353	GLU
2	B	376	LYS
2	B	378	LEU
2	B	385	ARG
2	B	386	SER
2	B	393	GLU
2	B	395	VAL
2	B	400	MET
2	B	401	GLU
2	B	409	LEU
2	B	412	GLU
2	B	415	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN

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Mol	Chain	Res	Type
1	A	302	GLN
1	A	340	ASN
2	B	204	GLN
2	B	257	GLN
2	B	296	GLN
2	B	299	ASN
2	B	340	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 ⓘ

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	$\# Z  > 2$
4	OLA	A	700	-	16,19,19	1.54	2 (12%)	16,19,19	0.92	0
3	BMS	B	600	-	35,38,38	5.61	28 (80%)	51,56,56	2.09	13 (25%)

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
4	OLA	A	700	-	-	0/15/17/17	0/0/0/0
3	BMS	B	600	-	1/1/4/5	0/12/32/32	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	BMS	C16-C15	-7.22	1.42	1.55
3	B	600	BMS	C21-C15	-4.16	1.40	1.53
3	B	600	BMS	C9-C8	-3.98	1.41	1.50
4	A	700	OLA	C8-C9	2.04	1.59	1.50
3	B	600	BMS	C26-C23	2.09	1.45	1.41
3	B	600	BMS	C23-N2	2.19	1.41	1.37
3	B	600	BMS	O3-C8	2.53	1.28	1.23
3	B	600	BMS	C11-C15	2.63	1.56	1.51
3	B	600	BMS	C17-C18	2.80	1.61	1.53
3	B	600	BMS	C18-C12	2.90	1.58	1.53
3	B	600	BMS	C14-C13	3.14	1.44	1.38
3	B	600	BMS	C7-C6	4.13	1.46	1.38
3	B	600	BMS	C7-C2	4.35	1.48	1.39
3	B	600	BMS	C4-C5	4.49	1.46	1.39
3	B	600	BMS	C22-N2	4.93	1.40	1.31
3	B	600	BMS	C10-C9	5.03	1.46	1.39
4	A	700	OLA	C10-C9	5.17	1.61	1.31
3	B	600	BMS	C6-C5	5.36	1.48	1.39
3	B	600	BMS	C3-C2	5.59	1.51	1.39
3	B	600	BMS	C27-C26	5.89	1.50	1.36
3	B	600	BMS	C28-C29	5.98	1.50	1.36
3	B	600	BMS	C4-C3	6.13	1.49	1.38
3	B	600	BMS	C10-C11	6.79	1.51	1.39
3	B	600	BMS	C25-C21	7.02	1.48	1.37
3	B	600	BMS	C14-C9	7.12	1.51	1.39
3	B	600	BMS	C28-C27	7.19	1.56	1.38
3	B	600	BMS	C13-C12	7.51	1.50	1.39
3	B	600	BMS	C22-C21	10.32	1.52	1.38
3	B	600	BMS	C11-C12	11.48	1.55	1.40
3	B	600	BMS	C24-C23	13.87	1.61	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	BMS	C18-C12-C11	-3.83	118.11	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	BMS	C24-C23-N2	-2.65	118.31	122.08
3	B	600	BMS	C21-C25-C24	-2.64	118.07	121.54
3	B	600	BMS	C29-C24-C25	-2.46	117.85	122.08
3	B	600	BMS	C29-C24-C23	2.05	121.63	118.44
3	B	600	BMS	C16-C15-C21	2.42	115.04	111.16
3	B	600	BMS	C3-C2-C1	2.61	123.96	120.45
3	B	600	BMS	C25-C21-C22	2.62	119.65	116.78
3	B	600	BMS	C25-C21-C15	3.17	125.37	120.25
3	B	600	BMS	C22-N2-C23	3.43	120.86	116.95
3	B	600	BMS	C17-C16-C15	4.21	121.97	110.77
3	B	600	BMS	C16-C15-C11	5.10	121.31	108.85
3	B	600	BMS	C21-C15-C11	7.73	123.65	113.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	600	BMS	C15

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	OLA	1	0
3	B	600	BMS	1	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, 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	217/233 (93%)	-0.14	5 (2%) 64 67	27, 46, 67, 82	0
2	B	232/235 (98%)	-0.15	8 (3%) 49 54	26, 41, 71, 79	0
All	All	449/468 (95%)	-0.15	13 (2%) 55 60	26, 43, 69, 82	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	SER	5.9
2	B	404	GLY	5.4
2	B	403	PRO	4.1
2	B	416	ASN	3.9
1	A	230	SER	3.4
2	B	182	PRO	3.0
1	A	462	ALA	2.7
2	B	400	MET	2.7
1	A	386	LYS	2.5
1	A	461	GLU	2.5
2	B	408	PRO	2.3
1	A	411	HIS	2.2
2	B	405	SER	2.2

### 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, 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	OLA	A	700	20/20	0.95	0.21	1.80	30,35,39,39	0
3	BMS	B	600	34/34	0.95	0.17	0.98	28,32,39,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.