

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 1, 2023 - 05:26 AM EDT

PDB ID	:	3NSQ
Title	:	Crystal structure of tetrameric RXRalpha-LBD complexed with antagonist
		danthron
Authors	:	Zhang, H.; Hu, T.; Li, L.; Zhou, R.; Chen, L.; Hu, L.; Jiang, H.; Shen, X.
Deposited on	:	2010-07-02
Resolution	:	2.60  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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	А	240	44%	30%	5%	20%		
1	В	240	45%	27%	10% •	17%		

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
2	CHZ	В	1	-	-	-	Х



#### 3NSQ

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3201 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 Retinoid X receptor, alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	1 A	193	Total	С	Ν	0	S	0	0	0
1			1526	983	264	270	9	0	0	
1	В	100	Total	С	Ν	0	S	0	0	0
ГБ	199	1573	1012	273	278	10	0	U		

• Molecule 2 is 1,8-dihydroxyanthracene-9,10-dione (three-letter code: CHZ) (formula:  $\rm C_{14}H_8O_4).$ 



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	В	1	Total 18	C 14	0 4	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	46	Total         O           46         46	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	38	Total         O           38         38	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Retinoid X receptor, alpha



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	115.03Å 99.92Å 47.20Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	14.88 - 2.60	Depositor
Resolution (A)	14.88 - 2.60	EDS
% Data completeness	95.4 (14.88-2.60)	Depositor
(in resolution range)	95.5(14.88-2.60)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.39 (at 2.61 \text{\AA})$	Xtriage
Refinement program	CNS, REFMAC $5.2.0019$	Depositor
B B.	0.265 , $0.318$	Depositor
II, II free	0.252 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	43.6	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, $60.8$	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3201	wwPDB-VP
Average B, all atoms $(Å^2)$	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.99% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: CHZ

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	Bo	nd lengths	Bond angles		
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	1.75	7/1558~(0.4%)	1.02	4/2106~(0.2%)	
1	В	1.76	11/1607~(0.7%)	0.99	2/2172~(0.1%)	
All	All	1.75	18/3165~(0.6%)	1.01	6/4278~(0.1%)	

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	269	CYS	CB-SG	-7.70	1.69	1.82
1	А	369	CYS	CB-SG	-7.45	1.69	1.82
1	В	453	GLU	CG-CD	-7.38	1.40	1.51
1	В	401	GLU	CD-OE2	-6.91	1.18	1.25
1	В	432	CYS	CB-SG	-6.74	1.70	1.82
1	А	432	CYS	CB-SG	-6.03	1.72	1.82
1	В	404	CYS	CB-SG	-5.88	1.72	1.81
1	В	401	GLU	CG-CD	-5.50	1.43	1.51
1	А	389	VAL	CB-CG1	-5.45	1.41	1.52
1	В	401	GLU	CD-OE1	-5.45	1.19	1.25
1	В	408	TYR	CD2-CE2	-5.19	1.31	1.39
1	В	354	VAL	CB-CG2	-5.16	1.42	1.52
1	В	403	TYR	CE1-CZ	-5.13	1.31	1.38
1	А	404	CYS	CB-SG	-5.10	1.73	1.81
1	А	408	TYR	CD2-CE2	-5.09	1.31	1.39
1	В	453	GLU	CB-CG	-5.04	1.42	1.52
1	А	304	GLY	C-O	-5.03	1.15	1.23
1	А	307	GLU	CD-OE2	-5.01	1.20	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	276	LEU	CB-CA-C	-8.61	93.83	110.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	455	LEU	CA-CB-CG	-7.49	98.08	115.30
1	А	277	PHE	N-CA-C	-6.13	94.44	111.00
1	А	330	LEU	CA-CB-CG	5.98	129.06	115.30
1	В	348	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	В	440	LYS	N-CA-C	-5.92	95.00	111.00

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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	А	1526	0	1567	62	1
1	В	1573	0	1613	100	2
2	В	18	0	6	1	0
3	А	46	0	0	1	0
3	В	38	0	0	4	0
All	All	3201	0	3186	161	2

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 26.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:440:LYS:C	1:B:441:LEU:HD12	1.42	1.37
1:B:440:LYS:C	1:B:441:LEU:CD1	1.96	1.32
1:B:440:LYS:O	1:B:441:LEU:CD1	1.84	1.24
1:B:440:LYS:O	1:B:441:LEU:HD13	1.10	1.22
1:B:451:LEU:O	1:B:455:LEU:HD13	1.45	1.17
1:B:441:LEU:HD12	1:B:441:LEU:N	1.59	1.08
1:B:407:LYS:HD2	1:B:408:TYR:CE1	1.95	1.02
1:A:366:GLU:OE2	1:A:414:ARG:NH2	1.92	1.01
1:B:460:GLN:O	1:B:461:MET:HG2	1.59	1.01
1:B:456:GLU:H	1:B:456:GLU:CD	1.57	0.99



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:454:MET:O	1:A:454:MET:HG3	1.63	0.96	
1:B:447:ILE:O	1:B:451:LEU:HD13	1.63	0.96	
1:A:276:LEU:O	1:A:276:LEU:HG	1.70	0.91	
1:A:310:ILE:O	1:A:314:SER:OG	1.89	0.90	
1:A:275:GLN:O	1:A:276:LEU:CB	2.21	0.89	
1:B:440:LYS:HG2	1:B:441:LEU:HD12	1.55	0.88	
1:A:316:ARG:HG2	1:A:325:LEU:HD23	1.56	0.86	
1:B:268:ILE:O	1:B:269:CYS:HB3	1.74	0.86	
1:B:460:GLN:C	1:B:461:MET:HG2	1.92	0.86	
1:B:369:CYS:O	1:B:373:ILE:HG13	1.76	0.86	
1:B:345:ILE:HD12	1:B:345:ILE:O	1.75	0.85	
1:A:366:GLU:CD	1:A:414:ARG:HH21	1.80	0.83	
1:A:275:GLN:O	1:A:276:LEU:HB3	1.78	0.82	
1:B:327:ALA:O	1:B:328:THR:HG22	1.81	0.81	
1:B:442:ILE:O	1:B:446:PRO:HD3	1.81	0.80	
1:B:322:ASP:OD1	1:B:333:HIS:ND1	2.16	0.77	
1:A:285:ARG:HD2	3:A:73:HOH:O	1.85	0.76	
1:A:454:MET:O	1:A:454:MET:CG	2.30	0.75	
1:B:451:LEU:O	1:B:455:LEU:CD1	2.31	0.74	
1:A:272:ALA:O	1:A:275:GLN:O	2.07	0.72	
1:A:326:LEU:O	1:A:327:ALA:HB3	1.89	0.71	
1:B:274:LYS:HG3	1:B:275:GLN:N	2.03	0.71	
1:B:442:ILE:O	1:B:446:PRO:CD	2.38	0.71	
1:B:326:LEU:HD12	1:B:330:LEU:CD1	2.21	0.70	
1:A:373:ILE:O	1:A:393:ARG:NH2	2.24	0.69	
1:B:326:LEU:HB2	1:B:330:LEU:HD12	1.75	0.68	
1:A:369:CYS:HB2	1:A:400:LEU:HD13	1.75	0.68	
1:B:462:THR:O	1:B:462:THR:HG22	1.94	0.68	
1:B:328:THR:HG22	1:B:330:LEU:HB2	1.77	0.67	
1:A:307:GLU:HG2	1:A:425:LEU:HG	1.76	0.66	
1:B:462:THR:O	1:B:462:THR:CG2	2.44	0.65	
1:B:318:ILE:O	1:B:318:ILE:HG22	1.96	0.65	
1:B:444:ASP:N	1:B:444:ASP:OD1	2.29	0.65	
1:B:273:ASP:OD2	1:B:273:ASP:N	2.30	0.64	
1:A:390:GLU:O	1:A:394:GLU:HG3	1.97	0.64	
1:B:460:GLN:N	1:B:460:GLN:OE1	2.30	0.64	
1:B:456:GLU:CD	1:B:456:GLU:N	2.28	0.63	
1:B:276:LEU:HD13	1:B:276:LEU:O	1.98	0.63	
1:B:440:LYS:HG2	1:B:441:LEU:CD1	2.27	0.63	
1:A:314:SER:O	1:A:354:VAL:HG22	1.98	0.63	
1:A:373:ILE:CD1	1:A:397:TYR:HB3	2.29	0.62	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:318:ILE:O	1:A:358:ARG:NH1	2.32	0.62	
1:B:288:HIS:CE1	1:B:395:LYS:HE3	2.34	0.62	
1:B:421:ARG:HH11	1:B:421:ARG:HG2	1.64	0.61	
1:B:449:THR:O	1:B:453:GLU:HG3	2.01	0.61	
1:A:373:ILE:HD11	1:A:397:TYR:HB3	1.81	0.60	
1:B:348:ARG:O	1:B:352:GLU:HB2	2.01	0.60	
1:A:414:ARG:O	1:A:418:LEU:HG	2.02	0.59	
1:A:347:ASP:O	1:A:351:THR:OG1	2.15	0.59	
1:A:276:LEU:O	1:A:276:LEU:CG	2.44	0.59	
1:A:369:CYS:CB	1:A:400:LEU:HD13	2.33	0.58	
1:B:407:LYS:HD2	1:B:408:TYR:CZ	2.39	0.58	
1:B:287:PRO:O	1:B:288:HIS:HB2	2.04	0.57	
1:B:460:GLN:O	1:B:461:MET:CG	2.46	0.57	
1:A:357:MET:HG2	1:A:362:MET:SD	2.45	0.57	
1:A:335:ASN:H	1:A:338:HIS:HD2	1.53	0.57	
1:B:362:MET:HE3	1:B:367:LEU:HA	1.85	0.57	
1:A:320:VAL:HG11	1:A:331:HIS:NE2	2.19	0.57	
1:B:443:GLY:O	1:B:447:ILE:HG12	2.05	0.57	
1:A:453:GLU:O	1:A:453:GLU:HG3	2.04	0.56	
1:B:269:CYS:C	1:B:271:ALA:N	2.54	0.56	
1:A:363:ASP:C	1:A:363:ASP:OD2	2.43	0.56	
1:B:362:MET:HE3	1:B:367:LEU:CA	2.36	0.56	
1:B:407:LYS:CD	1:B:408:TYR:CE1	2.82	0.56	
1:B:446:PRO:O	1:B:450:PHE:HB2	2.05	0.56	
1:B:268:ILE:CG2	1:B:269:CYS:N	2.69	0.55	
1:A:436:LEU:HB2	1:A:440:LYS:HE3	1.87	0.55	
1:B:268:ILE:HG22	1:B:269:CYS:N	2.20	0.55	
1:B:439:PHE:C	1:B:440:LYS:O	2.41	0.55	
1:B:394:GLU:HG2	1:B:397:TYR:CZ	2.42	0.55	
1:B:284:LYS:NZ	3:B:31:HOH:O	2.40	0.54	
1:B:348:ARG:NH2	1:B:427:SER:OG	2.41	0.54	
1:B:360:MET:CE	1:B:417:LYS:HD3	2.38	0.53	
1:B:421:ARG:NH1	3:B:22:HOH:O	2.41	0.53	
1:B:438:PHE:C	1:B:440:LYS:H	2.13	0.51	
1:B:460:GLN:N	1:B:460:GLN:CD	2.62	0.51	
1:B:326:LEU:HD22	3:B:35:HOH:O	2.11	0.51	
1:B:421:ARG:HG2	1:B:421:ARG:NH1	2.26	0.51	
1:B:456:GLU:N	1:B:456:GLU:OE1	2.30	0.51	
1:B:390:GLU:OE1	1:B:390:GLU:O	2.30	0.50	
1:B:327:ALA:O	1:B:330:LEU:CB	2.59	0.50	
1:A:348:ARG:HH11	1:A:431:LYS:HZ3	1.60	0.50	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:275:GLN:O	1:A:276:LEU:HB2	2.08	0.50
1:A:306:ASN:O	1:A:310:ILE:HG13	2.12	0.50
1:B:326:LEU:HD12	1:B:330:LEU:HD12	1.95	0.49
1:A:366:GLU:OE1	1:A:414:ARG:NE	2.36	0.49
1:B:407:LYS:CD	1:B:408:TYR:CZ	2.96	0.49
1:A:451:LEU:O	1:A:454:MET:HB3	2.12	0.49
1:B:318:ILE:O	1:B:318:ILE:CG2	2.59	0.48
1:B:360:MET:HE3	1:B:417:LYS:HD3	1.96	0.48
1:B:394:GLU:HG2	1:B:397:TYR:OH	2.14	0.48
1:A:316:ARG:CZ	1:A:327:ALA:HB2	2.43	0.48
1:A:332:VAL:HG12	1:A:333:HIS:N	2.28	0.48
1:A:306:ASN:O	1:A:310:ILE:HD12	2.13	0.48
1:A:280:VAL:O	1:A:280:VAL:HG12	2.14	0.47
1:A:360:MET:O	1:A:361:GLN:HB2	2.14	0.47
1:A:287:PRO:O	1:A:288:HIS:HB2	2.15	0.47
1:B:438:PHE:O	1:B:440:LYS:N	2.44	0.47
1:B:451:LEU:CD1	1:B:451:LEU:N	2.77	0.47
1:B:269:CYS:C	1:B:271:ALA:H	2.19	0.47
1:A:348:ARG:HH11	1:A:431:LYS:NZ	2.13	0.47
1:A:410:GLU:HG2	1:A:411:GLN:HG3	1.97	0.47
1:A:339:SER:OG	1:A:342:VAL:HG23	2.15	0.46
1:B:270:GLN:HE21	1:B:270:GLN:HB2	1.36	0.46
1:B:451:LEU:N	1:B:451:LEU:HD12	2.30	0.46
1:B:346:PHE:HA	2:B:1:CHZ:HAF	1.97	0.46
1:A:320:VAL:CG1	1:A:331:HIS:NE2	2.79	0.46
1:B:288:HIS:HE1	3:B:61:HOH:O	1.98	0.46
1:B:362:MET:CE	1:B:367:LEU:HB2	2.45	0.46
1:B:330:LEU:HD22	1:B:331:HIS:N	2.30	0.46
1:B:326:LEU:CD1	1:B:330:LEU:HD12	2.46	0.45
1:B:307:GLU:HG2	1:B:425:LEU:HG	1.97	0.45
1:A:326:LEU:HD12	1:A:330:LEU:HB3	1.98	0.45
1:A:264:PRO:HB2	1:A:447:ILE:HD13	1.98	0.45
1:B:299:ILE:HG21	1:B:383:LEU:HD13	1.99	0.45
1:A:410:GLU:O	1:A:412:PRO:HD3	2.17	0.45
1:B:276:LEU:HD13	1:B:276:LEU:C	2.37	0.45
1:A:276:LEU:HA	1:A:279:LEU:HB3	1.97	0.45
1:B:394:GLU:HA	1:B:397:TYR:CE2	2.52	0.45
1:B:304:GLY:O	1:B:308:LEU:HG	2.16	0.44
1:A:339:SER:O	1:A:340:ALA:C	2.55	0.44
1:A:373:ILE:HD11	1:A:397:TYR:CB	2.47	0.44
1:A:306:ASN:O	1:A:310:ILE:CD1	2.66	0.44



A + 1	A.t	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:327:ALA:O	1:B:330:LEU:HB3	2.18	0.44
1:B:286:ILE:N	1:B:286:ILE:HD13	2.33	0.44
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.83	0.43
1:A:416:ALA:HB3	1:B:397:TYR:CE1	2.53	0.43
1:B:327:ALA:O	1:B:328:THR:CG2	2.60	0.43
1:B:273:ASP:HA	1:B:276:LEU:CB	2.49	0.42
1:A:318:ILE:HD13	1:A:318:ILE:HG21	1.80	0.42
1:B:381:LYS:HE3	1:B:381:LYS:HB2	1.78	0.42
1:B:438:PHE:C	1:B:440:LYS:N	2.72	0.42
1:A:323:GLY:HA3	1:A:331:HIS:NE2	2.33	0.42
1:A:360:MET:CE	1:A:417:LYS:HD3	2.50	0.42
1:A:326:LEU:O	1:A:327:ALA:CB	2.56	0.42
1:B:270:GLN:C	1:B:272:ALA:H	2.23	0.42
1:B:324:ILE:HD13	1:B:324:ILE:HG21	1.66	0.42
1:A:342:VAL:HG23	1:A:342:VAL:H	1.62	0.41
1:B:442:ILE:HD12	1:B:442:ILE:HG21	1.80	0.41
1:B:414:ARG:NH1	1:B:414:ARG:HG3	2.34	0.41
1:B:353:LEU:O	1:B:357:MET:HG3	2.20	0.41
1:A:363:ASP:OD2	1:A:365:THR:N	2.54	0.41
1:A:396:VAL:O	1:A:399:SER:OG	2.35	0.41
1:B:268:ILE:O	1:B:269:CYS:CB	2.44	0.41
1:B:330:LEU:HD22	1:B:330:LEU:C	2.40	0.41
1:B:325:LEU:HD11	1:B:329:GLY:HA2	2.02	0.41
1:B:411:GLN:HE22	1:B:414:ARG:NH1	2.19	0.41
1:B:326:LEU:CD1	1:B:330:LEU:CD1	2.97	0.40
1:B:457:ALA:N	1:B:458:PRO:CD	2.84	0.40
1:B:414:ARG:HG3	1:B:414:ARG:HH11	1.85	0.40
1:A:280:VAL:HG22	1:A:301:LEU:HD13	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:CYS:SG	$1:B:270:GLN:CG[2_655]$	1.40	0.80
1:B:335:ASN:ND2	$1:B:384:SER:OG[1_556]$	1.71	0.49



### 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	Perce	$\mathbf{ntiles}$
1	А	191/240~(80%)	185~(97%)	6 (3%)	0	100	100
1	В	197/240~(82%)	188 (95%)	9~(5%)	0	100	100
All	All	388/480~(81%)	373 (96%)	15 (4%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	А	166/207~(80%)	143 (86%)	23~(14%)	3 6
1	В	171/207~(83%)	137~(80%)	34 (20%)	1 2
All	All	337/414 (81%)	280 (83%)	57 (17%)	2 3

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	277	PHE
1	А	312	SER
1	А	313	PHE
1	А	314	SER
1	А	317	SER
1	А	318	ILE
1	А	322	ASP
1	А	325	LEU



Mol	Chain	Res	Type
1	А	330	LEU
1	А	334	ARG
1	А	351	THR
1	А	363	ASP
1	А	383	LEU
1	А	384	SER
1	А	397	TYR
1	А	421	ARG
1	А	427	SER
1	А	431	LYS
1	А	442	ILE
1	А	444	ASP
1	А	451	LEU
1	А	452	MET
1	А	455	LEU
1	В	265	VAL
1	В	269	CYS
1	В	270	GLN
1	В	273	ASP
1	В	274	LYS
1	В	275	GLN
1	В	276	LEU
1	В	279	LEU
1	В	286	ILE
1	В	312	SER
1	В	313	PHE
1	В	316	ARG
1	В	320	VAL
1	В	322	ASP
1	В	325	LEU
1	В	328	THR
1	В	336	SER
1	В	339	SER
1	В	345	ILE
1	В	381	LYS
1	В	383	LEU
1	В	394	GLU
1	В	399	SER
1	В	407	LYS
1	В	427	SER
1	В	431	LYS
1	В	436	LEU



Continued from previous page...

Mol	Chain	Res	Type
1	В	440	LYS
1	В	441	LEU
1	В	442	ILE
1	В	444	ASP
1	В	450	PHE
1	В	456	GLU
1	В	461	MET

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

Mol	Chain	Res	Type
1	А	275	GLN
1	А	288	HIS
1	А	306	ASN
1	А	338	HIS
1	А	411	GLN
1	В	270	GLN
1	В	288	HIS
1	В	411	GLN

#### 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

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	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dog	Link	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
	Type		m nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2						
2	CHZ	В	1	-	20,20,20	1.86	4 (20%)	30,30,30	0.69	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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CHZ	В	1	-	-	-	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1	CHZ	CAP-CAM	-4.36	1.39	1.48
2	В	1	CHZ	CAO-CAM	-4.26	1.39	1.48
2	В	1	CHZ	CAQ-CAN	-3.45	1.39	1.47
2	В	1	CHZ	CAR-CAN	-3.45	1.39	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1	CHZ	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,  $95^{th}$  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		$OWAB(Å^2)$	Q<0.9
1	А	193/240~(80%)	-0.21	2 (1%) 82	80	21, 38, 59, 64	0
1	В	199/240~(82%)	0.03	7 (3%) 44	36	20, 37, 64, 71	0
All	All	392/480~(81%)	-0.09	9 (2%) 60	54	20, 38, 60, 71	0

All (9) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	В	329	GLY	5.8
1	В	264	PRO	5.2
1	В	266	THR	4.6
1	В	328	THR	4.4
1	В	265	VAL	3.5
1	А	335	ASN	2.7
1	В	267	ASN	2.7
1	А	327	ALA	2.1
1	В	439	PHE	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 monosaccharides 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. The B-factors column lists the minimum,



median,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	CHZ	В	1	18/18	0.53	0.51	72,72,73,73	18

## 6.5 Other polymers (i)

There are no such residues in this entry.

