

Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 04:54 PM EDT

PDB ID	:	3OZJ
Title	:	Crystal structure of human retinoic X receptor alpha complexed with bigelovin
		and coactivator SRC-1
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Deposited on	:	2010-09-25
Resolution	:	2.10 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
buster-report	:	1.1.7(2018)
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 2.10 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 $(\#Entries)$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range({\rm \AA})}) \end{array}$
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	Quali	ty of chain		
1	А	238	47%	34%	9%	10%
1	С	238	47%	38%	5%	10%
2	В	11	64%	27%		9%
2	D	11	45%	45%		9%

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	BGV	А	1	-	-	Х	-
3	BGV	С	1	-	-	Х	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3692 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 Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	215	Total 1697	C 1088	N 291	O 308	S 10	0	0	0
1	С	215	Total 1711	C 1098	N 295	O 308	S 10	6	2	0

• Molecule 2 is a protein called SRC-1, peptide of Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
2	В	10	Total	С	Ν	0	0	0	0		
			89	57	19	13					
2	Л	Л	D	11	Total	С	Ν	0	0	0	0
2	D	D 11		63	21	14	0	0	0		

• Molecule 3 is (3aR,4S,4aR,7aR,8R,9aS)-4a,8-dimethyl-3-methylidene-2,5-dioxo-2,3,3a,4,4a,5,7a,8,9,9a-decahydroazuleno[6,5-b]furan-4-yl acetate (three-letter code: BGV) (formula: $C_{17}H_{20}O_5$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C O 22 17 5	0	0
3	С	1	Total C O 22 17 5	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	26	TotalO2626	0	0
4	В	1	Total O 1 1	0	0
4	С	25	TotalO2525	0	0
4	D	1	Total O 1 1	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: Retinoic acid receptor RXR-alpha







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	65.40Å 66.59Å 111.73Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	33.29 - 2.10	Depositor
Resolution (A)	33.30 - 2.10	EDS
% Data completeness	88.5 (33.29-2.10)	Depositor
(in resolution range)	86.7 (33.30-2.10)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.08 (at 2.10 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
D D	0.245 , (Not available)	Depositor
Λ, Λ_{free}	0.239 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	24.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 22.2	EDS
L-test for twinning ²	$< L > = 0.42, < L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.080 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3692	wwPDB-VP
Average B, all atoms $(Å^2)$	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: BGV

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.88	16/1731~(0.9%)	1.08	3/2342~(0.1%)	
1	С	1.89	19/1753~(1.1%)	1.08	2/2372~(0.1%)	
2	В	1.35	0/90	1.08	0/119	
2	D	1.30	0/99	1.18	0/130	
All	All	1.86	35/3673~(1.0%)	1.08	5/4963~(0.1%)	

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	432	CYS	CB-SG	-10.22	1.64	1.82
1	С	269	CYS	CB-SG	-8.25	1.68	1.82
1	С	369	CYS	CB-SG	-7.13	1.70	1.82
1	С	307	GLU	CD-OE1	-7.09	1.17	1.25
1	С	453	GLU	CD-OE2	-6.92	1.18	1.25
1	С	338[A]	HIS	N-CA	-6.64	1.33	1.46
1	С	338[B]	HIS	N-CA	-6.64	1.33	1.46
1	С	403	TYR	CD2-CE2	-6.21	1.30	1.39
1	А	305	TRP	CE3-CZ3	-6.19	1.27	1.38
1	С	366	GLU	CD-OE1	-6.18	1.18	1.25
1	А	269	CYS	CB-SG	-6.15	1.71	1.82
1	А	403	TYR	CD2-CE2	-5.93	1.30	1.39
1	А	369	CYS	CB-SG	-5.79	1.72	1.81
1	А	404	CYS	CB-SG	-5.77	1.72	1.81
1	А	401	GLU	CD-OE2	-5.66	1.19	1.25
1	С	239	GLU	CD-OE1	-5.65	1.19	1.25
1	С	389	VAL	CB-CG2	-5.61	1.41	1.52
1	А	380	SER	CB-OG	-5.58	1.35	1.42
1	А	415	PHE	CD1-CE1	-5.58	1.28	1.39
1	А	323	GLY	C-O	-5.45	1.15	1.23
1	А	233	GLU	CD-OE2	-5.43	1.19	1.25
1	С	366	GLU	CD-OE2	-5.39	1.19	1.25



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)
1	С	396	VAL	CB-CG2	-5.38	1.41	1.52
1	А	349	VAL	CB-CG2	-5.37	1.41	1.52
1	А	307	GLU	CD-OE1	-5.29	1.19	1.25
1	С	312	SER	CB-OG	-5.28	1.35	1.42
1	А	397	TYR	CD2-CE2	-5.25	1.31	1.39
1	А	410	GLU	CD-OE1	-5.22	1.20	1.25
1	С	410	GLU	CD-OE1	-5.21	1.20	1.25
1	С	432	CYS	CB-SG	-5.16	1.73	1.81
1	С	228	GLU	CD-OE1	-5.10	1.20	1.25
1	С	403	TYR	CD1-CE1	-5.09	1.31	1.39
1	С	283	ALA	CA-CB	-5.08	1.41	1.52
1	C	352	GLU	CD-OE1	-5.07	1.20	1.25
1	А	434	GLU	CG-CD	-5.04	1.44	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	419	LEU	CA-CB-CG	5.50	127.96	115.30
1	С	276	LEU	CA-CB-CG	5.38	127.66	115.30
1	А	404	CYS	CA-CB-SG	5.28	123.50	114.00
1	А	443	GLY	N-CA-C	5.17	126.03	113.10
1	А	418	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	А	1697	0	1727	87	0
1	С	1711	0	1741	82	0
2	В	89	0	95	2	0
2	D	98	0	111	4	0
3	А	22	0	20	23	0
3	C	22	0	20	14	0
4	А	26	0	0	1	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
4	В	1	0	0	0	0		
4	С	25	0	0	0	0		
4	D	1	0	0	0	0		
All	All	3692	0	3714	179	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 24.

All (179) 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 (Å)	overlap (Å)	
1:C:439:PHE:CE2	3:C:1:BGV:HAC	1.70	1.26	
3:A:1:BGV:HAR	3:A:1:BGV:HAD	1.23	1.19	
1:A:304:GLY:O	1:A:308:LEU:HD12	1.53	1.08	
1:C:439:PHE:HE2	3:C:1:BGV:CAC	1.68	1.06	
3:A:1:BGV:HAD	3:A:1:BGV:CAR	1.81	1.05	
1:C:231:PRO:HB2	1:C:234:ARG:HG3	1.39	1.02	
1:A:320:VAL:CG2	1:A:323:GLY:O	2.11	0.98	
1:A:320:VAL:HG21	1:A:323:GLY:O	1.64	0.97	
1:A:392:LEU:O	1:A:396:VAL:HG23	1.64	0.97	
1:C:439:PHE:HE2	3:C:1:BGV:HAC	0.78	0.93	
1:A:264:PRO:HA	1:A:267:ASN:HD22	1.34	0.91	
1:C:273:ASP:OD1	1:C:450:PHE:HB3	1.75	0.87	
1:C:439:PHE:CE2	3:C:1:BGV:CAC	2.52	0.83	
1:C:333:HIS:CD2	1:C:335:ASN:H	1.98	0.82	
1:C:407:LYS:HG2	1:C:408:TYR:CE1	2.14	0.81	
1:A:316:ARG:HD2	1:A:325:LEU:O	1.81	0.81	
1:C:302:ARG:HH12	1:C:458:PRO:HG3	1.46	0.81	
1:A:436:LEU:HG	3:A:1:BGV:HACB	1.62	0.80	
1:C:238:ALA:O	1:C:242:VAL:HG22	1.82	0.80	
1:C:436:LEU:HD23	3:C:1:BGV:HACB	1.64	0.79	
1:C:391:ALA:HA	1:C:394:GLU:OE1	1.83	0.79	
1:A:321:LYS:HA	1:A:321:LYS:HE3	1.65	0.79	
1:C:416:ALA:O	1:C:420:LEU:HD12	1.82	0.79	
1:C:436:LEU:HD21	3:C:1:BGV:HAJ	1.64	0.79	
1:C:347:ASP:O	1:C:351:THR:HG23	1.84	0.77	
3:A:1:BGV:CAR	3:A:1:BGV:CAD	2.60	0.77	
1:C:333:HIS:HD2	1:C:335:ASN:H	1.33	0.77	
1:A:380:SER:HB2	1:A:383:LEU:HD22	1.67	0.77	
1:C:373:ILE:O	1:C:393:ARG:NH2	2.18	0.76	
1:A:320:VAL:HG23	1:A:323:GLY:O	1.84	0.76	



	le al pagem	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:C:273:ASP:OD1	1:C:450:PHE:CB	2.33	0.76		
1:A:436:LEU:HG	3:A:1:BGV:CAC	2.15	0.76		
1:A:238:ALA:O	1:A:282:TRP:HD1	1.70	0.75		
1:A:268:ILE:HG21	3:A:1:BGV:HADA	1.69	0.75		
1:C:333:HIS:CD2	1:C:334:ARG:N	2.55	0.75		
1:C:236:LEU:CD2	1:C:236:LEU:O	2.36	0.74		
1:C:348:ARG:O	1:C:352:GLU:HB2	1.88	0.73		
1:A:435:HIS:O	1:A:438:PHE:N	2.21	0.73		
1:C:376:PHE:O	1:C:378:PRO:HD3	1.88	0.72		
1:A:268:ILE:HG21	3:A:1:BGV:CAD	2.20	0.72		
1:C:432:CYS:SG	3:C:1:BGV:CAN	2.78	0.72		
1:C:435:HIS:HB3	3:C:1:BGV:HAI	1.71	0.71		
1:A:313:PHE:HE2	3:A:1:BGV:HAA	1.56	0.71		
1:A:239:GLU:OE2	1:A:282:TRP:NE1	2.25	0.69		
1:C:333:HIS:HD2	1:C:334:ARG:N	1.91	0.69		
1:A:438:PHE:O	1:A:442:ILE:HG22	1.92	0.68		
1:A:447:ILE:HG23	1:A:451:LEU:HD23	1.74	0.68		
1:C:306:ASN:ND2	1:C:433:LEU:HG	2.09	0.68		
1:C:444:ASP:OD1	1:C:445:THR:N	2.27	0.67		
1:C:447:ILE:HG23	1:C:451:LEU:HD23	1.76	0.67		
1:A:436:LEU:HD13	1:A:455:LEU:HD21	1.78	0.66		
1:C:316:ARG:HG2	1:C:316:ARG:O	1.94	0.66		
1:C:436:LEU:CD2	3:C:1:BGV:HACB	2.26	0.66		
1:A:436:LEU:CG	3:A:1:BGV:HACB	2.26	0.65		
1:C:452:MET:O	1:C:456:GLU:HG3	1.97	0.65		
1:C:236:LEU:O	1:C:236:LEU:HD22	1.98	0.64		
1:C:236:LEU:O	1:C:236:LEU:HD23	1.97	0.64		
1:A:313:PHE:CE2	3:A:1:BGV:HAA	2.32	0.64		
1:C:431:LYS:HE3	1:C:435:HIS:CE1	2.34	0.63		
1:A:304:GLY:C	1:A:308:LEU:HD12	2.19	0.62		
3:A:1:BGV:HAR	3:A:1:BGV:CAD	2.16	0.61		
1:A:457:ALA:O	1:A:458:PRO:C	2.39	0.61		
1:A:240:LEU:O	1:A:243:GLU:HG2	2.01	0.61		
2:B:3:LYS:HB3	2:B:7:ARG:NH1	2.15	0.61		
1:A:298:VAL:O	1:A:302:ARG:HG3	2.00	0.60		
2:D:10:GLN:O	2:D:11:ASP:HB3	2.03	0.59		
1:C:302:ARG:NH2	1:C:456:GLU:O	2.36	0.59		
1:A:348:ARG:O	1:A:352:GLU:HB2	2.03	0.58		
1:C:394:GLU:HA	1:C:397:TYR:CE2	2.38	0.58		
1:A:281:GLU:HA	1:A:281:GLU:OE2	2.03	0.58		
1:A:238:ALA:O	1:A:282:TRP:CD1	2.55	0.57		



	is as pagem	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:C:373:ILE:HD11	1:C:397:TYR:HB3	1.86	0.57		
1:A:306:ASN:OD1	1:A:433:LEU:HG	2.05	0.56		
1:C:306:ASN:HD21	1:C:433:LEU:HG	1.69	0.56		
1:A:448:ASP:O	1:A:452:MET:HB2	2.05	0.56		
1:C:403:TYR:CD2	1:C:403:TYR:C	2.79	0.56		
1:A:264:PRO:C	1:A:266:THR:H	2.09	0.55		
1:C:276:LEU:HD21	1:C:305:TRP:HE3	1.72	0.55		
1:C:302:ARG:NH1	1:C:458:PRO:HG3	2.20	0.55		
1:C:333:HIS:CD2	1:C:334:ARG:H	2.23	0.55		
1:C:275:GLN:OE1	1:C:275:GLN:HA	2.06	0.54		
1:C:296:ASP:OD2	1:C:384:SER:OG	2.22	0.54		
1:A:335:ASN:N	1:A:335:ASN:OD1	2.39	0.54		
1:A:410:GLU:HG2	1:A:411:GLN:HG3	1.90	0.54		
1:A:268:ILE:CG2	3:A:1:BGV:CAD	2.85	0.54		
1:C:438:PHE:O	1:C:442:ILE:HG12	2.08	0.54		
1:A:300:LEU:HD13	1:A:375:LEU:O	2.07	0.53		
1:A:432:CYS:O	3:A:1:BGV:HACA	2.08	0.53		
1:A:401:GLU:HG2	1:A:405:LYS:HD3	1.90	0.53		
1:C:393:ARG:O	1:C:397:TYR:CD2	2.62	0.53		
1:C:231:PRO:CB	1:C:234:ARG:HG3	2.27	0.53		
1:C:391:ALA:O	1:C:394:GLU:HB2	2.08	0.53		
1:C:300:LEU:HD22	1:C:375:LEU:O	2.08	0.53		
1:A:268:ILE:CG2	3:A:1:BGV:HADA	2.38	0.52		
1:C:435:HIS:CB	3:C:1:BGV:HAI	2.40	0.52		
1:A:265:VAL:CG1	1:A:265:VAL:O	2.57	0.52		
1:A:436:LEU:HD21	3:A:1:BGV:HAJ	1.92	0.52		
1:C:411:GLN:HG3	1:C:414:ARG:HB2	1.91	0.52		
3:C:1:BGV:HAB	3:C:1:BGV:HAAA	1.91	0.51		
1:C:401:GLU:HB2	1:C:415:PHE:CZ	2.44	0.51		
1:A:264:PRO:C	1:A:266:THR:N	2.63	0.51		
1:C:391:ALA:O	1:C:394:GLU:N	2.45	0.50		
1:A:436:LEU:CD2	3:A:1:BGV:HACB	2.41	0.50		
1:C:407:LYS:HG2	1:C:408:TYR:CZ	2.47	0.50		
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.47	0.50		
1:C:277:PHE:CD1	1:C:450:PHE:HD1	2.29	0.50		
1:A:385:ASN:ND2	1:A:388:GLU:HB2	2.27	0.50		
1:C:401:GLU:HB2	1:C:415:PHE:CE2	2.46	0.49		
1:A:265:VAL:O	1:A:265:VAL:HG12	2.10	0.49		
1:A:263:ASP:OD1	1:A:264:PRO:HD2	2.12	0.49		
1:A:236:LEU:HD13	1:A:365:THR:OG1	2.13	0.49		
$1:\overline{C:298:VAL:HG21}$	2:D:6:HIS:NE2	2.28	0.49		



	A h C	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:432:CYS:SG	3:C:1:BGV:CAP	3.00	0.49	
1:C:242:VAL:HG11	1:C:282:TRP:HB2	1.95	0.49	
1:C:333:HIS:HD2	1:C:335:ASN:N	2.05	0.49	
1:C:452:MET:O	1:C:456:GLU:CG	2.61	0.49	
1:A:436:LEU:HG	3:A:1:BGV:HACA	1.95	0.49	
3:C:1:BGV:HAAA	3:C:1:BGV:OAK	2.13	0.48	
1:A:332:VAL:O	1:A:332:VAL:HG12	2.12	0.48	
1:A:370:LEU:O	1:A:374:VAL:HG23	2.14	0.48	
1:C:422:LEU:N	1:C:423:PRO:CD	2.76	0.48	
1:A:442:ILE:HG12	1:A:442:ILE:O	2.13	0.48	
1:C:442:ILE:HD13	1:C:442:ILE:N	2.29	0.48	
1:A:409:PRO:HD2	1:A:410:GLU:OE1	2.13	0.48	
1:A:428:ILE:O	1:A:432:CYS:HB2	2.12	0.48	
1:A:379:ASP:CG	1:C:421:ARG:HH22	2.18	0.48	
1:C:438:PHE:CE1	1:C:442:ILE:HD11	2.48	0.48	
1:C:236:LEU:CD2	1:C:236:LEU:C	2.81	0.47	
1:C:308:LEU:HD21	1:C:371:ARG:O	2.15	0.47	
1:A:290:SER:O	1:A:292:LEU:N	2.47	0.47	
1:A:304:GLY:O	1:A:308:LEU:CD1	2.44	0.47	
1:C:277:PHE:CE1	1:C:450:PHE:HD1	2.32	0.47	
1:A:243:GLU:O	1:A:244:PRO:C	2.53	0.47	
1:A:310:ILE:HD13	1:A:428:ILE:HG22	1.98	0.46	
1:A:400:LEU:O	1:A:403:TYR:HB3	2.15	0.46	
1:A:234:ARG:NH2	4:A:27:HOH:O	2.49	0.46	
1:C:457:ALA:HA	1:C:458:PRO:HD3	1.75	0.46	
1:C:243:GLU:O	1:C:244:PRO:C	2.52	0.45	
1:A:262:ASN:CG	1:A:262:ASN:O	2.55	0.45	
1:A:297:GLN:OE1	2:B:9:LEU:HD22	2.16	0.45	
1:A:400:LEU:HD21	1:A:418:LEU:HD13	1.98	0.45	
1:C:280:VAL:HG13	1:C:301:LEU:HD11	1.98	0.45	
1:A:372:ALA:O	1:A:376:PHE:CD1	2.70	0.45	
1:A:287:PRO:O	1:A:288:HIS:HB2	2.18	0.44	
1:C:442:ILE:HG22	1:C:444:ASP:HB3	2.00	0.44	
2:D:9:LEU:HD23	2:D:9:LEU:HA	1.86	0.44	
1:A:420:LEU:HD13	1:C:393:ARG:HD3	1.98	0.44	
1:A:453:GLU:O	1:A:456:GLU:HB2	2.18	0.44	
3:A:1:BGV:HAU	3:A:1:BGV:HAS	1.11	0.44	
1:C:356:LYS:HA	1:C:356:LYS:HD3	1.59	0.44	
1:A:268:ILE:CG2	3:A:1:BGV:HAR	2.48	0.44	
1:A:311:ALA:HB2	1:A:425:LEU:HD11	1.98	0.44	
1:A:268:ILE:HG22	3:A:1:BGV:HAR	1.99	0.43	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:268:ILE:HG12	1:A:326:LEU:HD21	1.99	0.43	
1:C:362:MET:HG3	1:C:418:LEU:HD21	1.99	0.43	
3:C:1:BGV:HAU	3:C:1:BGV:HAS	1.17	0.43	
1:A:268:ILE:CG2	3:A:1:BGV:HAD	2.49	0.43	
1:A:237:GLU:C	1:A:239:GLU:H	2.22	0.43	
1:A:268:ILE:HG21	3:A:1:BGV:HAT	2.01	0.43	
1:C:317:SER:OG	1:C:324:ILE:HG22	2.19	0.43	
1:C:315:HIS:C	1:C:317:SER:H	2.22	0.42	
1:C:263:ASP:O	1:C:264:PRO:C	2.53	0.42	
1:A:415:PHE:O	1:A:419:LEU:HG	2.20	0.42	
1:C:294:LEU:O	1:C:297:GLN:HB2	2.19	0.42	
1:A:435:HIS:O	1:A:436:LEU:C	2.58	0.42	
2:D:3:LYS:HE2	2:D:3:LYS:HB2	1.75	0.42	
1:A:231:PRO:O	1:A:235:ILE:HG13	2.20	0.42	
1:A:342:VAL:O	1:A:342:VAL:HG23	2.19	0.41	
1:C:300:LEU:HD23	1:C:300:LEU:HA	1.81	0.41	
1:A:290:SER:HA	1:A:297:GLN:NE2	2.35	0.41	
1:C:279:LEU:O	1:C:279:LEU:HG	2.18	0.41	
1:C:262:ASN:OD1	1:C:262:ASN:N	2.52	0.41	
1:A:287:PRO:O	1:A:288:HIS:CB	2.68	0.41	
1:A:235:ILE:O	1:A:235:ILE:HG22	2.19	0.41	
1:A:380:SER:O	1:A:383:LEU:HB2	2.21	0.41	
1:A:313:PHE:CE2	3:A:1:BGV:CAA	3.02	0.41	
1:A:422:LEU:N	1:A:423:PRO:CD	2.84	0.40	
1:A:372:ALA:O	1:A:376:PHE:HD1	2.04	0.40	
1:A:243:GLU:O	1:A:243:GLU:HG3	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	Perce	ntiles
1	А	211/238~(89%)	204 (97%)	7 (3%)	0	100	100
1	С	213/238~(90%)	207~(97%)	6 (3%)	0	100	100
2	В	8/11~(73%)	8 (100%)	0	0	100	100
2	D	9/11~(82%)	7 (78%)	2(22%)	0	100	100
All	All	441/498 (89%)	426 (97%)	15 (3%)	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 side chain 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	Pe	erce	entiles
1	А	185/205~(90%)	164 (89%)	21 (11%)		5	3
1	С	187/205~(91%)	169~(90%)	18 (10%)		8	5
2	В	10/11~(91%)	10 (100%)	0	1	00	100
2	D	11/11~(100%)	9~(82%)	2(18%)		1	1
All	All	393/432~(91%)	352 (90%)	41 (10%)		7	4

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	242	VAL
1	А	244	PRO
1	А	263	ASP
1	А	270	GLN
1	А	281	GLU
1	А	306	ASN
1	А	321	LYS
1	А	325	LEU
1	А	334	ARG
1	А	335	ASN
1	А	355	SER
1	A	363	ASP
1	А	383	LEU



Mol	Chain	Res	Type
1	А	397	TYR
1	А	421	ARG
1	А	433	LEU
1	А	435	HIS
1	А	442	ILE
1	А	448	ASP
1	А	450	PHE
1	А	456	GLU
1	С	227	ASN
1	С	229	ASP
1	С	236	LEU
1	С	262	ASN
1	С	266	THR
1	С	275	GLN
1	С	313	PHE
1	С	321	LYS
1	С	325	LEU
1	С	330	LEU
1	С	336	SER
1	С	356	LYS
1	С	388	GLU
1	С	389	VAL
1	С	403	TYR
1	С	433	LEU
1	С	444	ASP
1	С	450	PHE
2	D	2	HIS
2	D	11	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	267	ASN
1	С	270	GLN
1	С	297	GLN
1	С	306	ASN
1	С	333	HIS
1	С	335	ASN
2	D	2	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 monosaccharides 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	Turne	Chain	Dec	Tink	Bond lengths			Bond angles		
	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	BGV	А	1	-	23,24,24	4.02	13 (56%)	31,38,38	<mark>3.39</mark>	16 (51%)
3	BGV	С	1	-	23,24,24	4.88	15 (65%)	31,38,38	4.39	22 (70%)

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
3	BGV	А	1	-	-	3/4/55/55	0/3/3/3
3	BGV	С	1	-	-	2/4/55/55	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	С	1	BGV	CAV-CAO	-12.50	1.41	1.54



Mol	Chain	\mathbf{Res}	Type	Atoms		Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
3	А	1	BGV	CAH-CAO	-10.14	1.28	1.46
3	С	1	BGV	CAV-CAS	-9.53	1.43	1.55
3	С	1	BGV	CAH-CAO	-8.89	1.30	1.46
3	А	1	BGV	CAV-CAO	-7.48	1.46	1.54
3	А	1	BGV	CAV-CAS	-7.24	1.46	1.55
3	А	1	BGV	CAP-CAN	-6.34	1.37	1.48
3	С	1	BGV	CAS-CAQ	-5.98	1.43	1.55
3	С	1	BGV	CAJ-CAR	-5.48	1.41	1.51
3	А	1	BGV	OAL-CAR	-5.35	1.38	1.46
3	С	1	BGV	CAP-CAN	-5.19	1.39	1.48
3	С	1	BGV	OAK-CAT	-4.88	1.36	1.45
3	С	1	BGV	OAL-CAR	-4.50	1.39	1.46
3	С	1	BGV	CAJ-CAQ	-4.21	1.49	1.54
3	С	1	BGV	CAA-CAN	4.09	1.39	1.32
3	А	1	BGV	OAL-CAP	-4.07	1.29	1.36
3	А	1	BGV	CAU-CAR	-4.01	1.48	1.54
3	С	1	BGV	CAU-CAR	-3.79	1.48	1.54
3	С	1	BGV	OAK-CAM	-3.60	1.27	1.35
3	А	1	BGV	CAS-CAQ	-3.25	1.48	1.55
3	А	1	BGV	CAV-CAT	-2.67	1.48	1.53
3	А	1	BGV	CAA-CAN	2.62	1.37	1.32
3	А	1	BGV	CAJ-CAQ	-2.61	1.50	1.54
3	С	1	BGV	OAL-CAP	-2.59	1.32	1.36
3	A	1	BGV	CAJ-CAR	-2.50	1.46	1.51
3	А	1	BGV	OAK-CAM	-2.33	1.29	1.35
3	С	1	BGV	CAV-CAT	2.29	1.56	1.53
3	С	1	BGV	CAD-CAV	-2.08	1.50	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	С	1	BGV	CAJ-CAQ-CAS	-10.52	99.91	111.17
3	С	1	BGV	CAT-OAK-CAM	-9.21	104.35	117.81
3	С	1	BGV	CAJ-CAR-CAU	-8.38	94.46	116.54
3	С	1	BGV	CAD-CAV-CAO	-8.15	90.31	103.98
3	А	1	BGV	CAJ-CAR-CAU	-7.85	95.84	116.54
3	А	1	BGV	OAL-CAR-CAJ	-7.79	93.08	107.96
3	А	1	BGV	CAV-CAS-CAQ	-7.22	106.59	117.29
3	С	1	BGV	OAK-CAM-CAB	6.44	122.94	111.09
3	С	1	BGV	CAS-CAI-CAH	-6.11	106.14	112.75
3	А	1	BGV	CAR-CAU-CAN	-5.53	96.21	102.43
3	С	1	BGV	CAD-CAV-CAT	4.94	119.58	112.51



Mol	Chain	\mathbf{Res}	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	С	1	BGV	CAV-CAS-CAQ	-4.75	110.25	117.29
3	С	1	BGV	CAU-CAN-CAA	-4.74	122.98	130.52
3	С	1	BGV	OAF-CAO-CAV	-4.69	120.40	124.76
3	А	1	BGV	CAU-CAN-CAA	-4.68	123.08	130.52
3	А	1	BGV	CAT-OAK-CAM	4.58	124.50	117.81
3	А	1	BGV	OAK-CAT-CAU	4.32	117.89	105.99
3	С	1	BGV	CAR-CAU-CAN	-3.79	98.16	102.43
3	А	1	BGV	OAK-CAM-CAB	3.61	117.74	111.09
3	А	1	BGV	CAD-CAV-CAT	-3.50	107.50	112.51
3	А	1	BGV	OAF-CAO-CAH	-3.50	122.30	127.74
3	С	1	BGV	OAK-CAT-CAU	3.14	114.62	105.99
3	С	1	BGV	CAA-CAN-CAP	3.08	126.34	122.11
3	А	1	BGV	OAF-CAO-CAV	-3.05	121.92	124.76
3	А	1	BGV	CAA-CAN-CAP	3.05	126.30	122.11
3	С	1	BGV	CAV-CAS-CAI	2.83	104.82	102.58
3	С	1	BGV	CAC-CAQ-CAS	-2.50	107.09	111.91
3	С	1	BGV	OAL-CAR-CAJ	-2.49	103.20	107.96
3	А	1	BGV	CAU-CAN-CAP	2.42	110.62	107.33
3	С	1	BGV	OAL-CAP-CAN	-2.41	107.39	109.44
3	А	1	BGV	OAL-CAP-OAG	2.30	123.96	121.25
3	С	1	BGV	CAI-CAH-CAO	2.23	111.93	109.85
3	С	1	BGV	OAL-CAP-OAG	2.22	123.88	121.25
3	С	1	BGV	OAK-CAM-OAE	-2.13	118.73	122.96
3	С	1	BGV	CAQ-CAJ-CAR	-2.13	109.40	115.20
3	А	1	BGV	CAS-CAI-CAH	-2.05	110.53	112.75
3	С	1	BGV	CAU-CAN-CAP	2.03	110.08	107.33
3	А	1	BGV	CAJ-CAQ-CAS	-2.02	109.00	111.17

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	1	BGV	CAB-CAM-OAK-CAT
3	А	1	BGV	CAU-CAT-OAK-CAM
3	С	1	BGV	CAB-CAM-OAK-CAT
3	А	1	BGV	OAE-CAM-OAK-CAT
3	С	1	BGV	OAE-CAM-OAK-CAT

There are no ring outliers.

2 monomers are involved in 37 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	1	BGV	23	0
3	С	1	BGV	14	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and similar rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	$\langle RSRZ \rangle$	#RSRZ>2		Z>2	$OWAB(Å^2)$	Q<0.9
1	А	215/238~(90%)	-0.73	0	100	100	6, 19, 32, 45	0
1	С	215/238~(90%)	-0.74	0	100	100	8, 20, 32, 41	3 (1%)
2	В	10/11~(90%)	-0.81	0	100	100	13, 17, 23, 24	0
2	D	11/11 (100%)	-0.62	0	100	100	17, 22, 27, 33	0
All	All	451/498 (90%)	-0.74	0	100	100	6, 19, 32, 45	3 (0%)

There are no RSRZ outliers to report.

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
3	BGV	А	1	22/22	0.95	0.20	$25,\!32,\!33,\!34$	0
3	BGV	С	1	22/22	0.96	0.19	28,31,34,35	0

The following is a graphical depiction of the model fit to experimental electron density of all



instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

There are no such residues in this entry.

