



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:35 PM GMT

PDB ID : 1PQ9
Title : HUMAN LXR BETA HORMONE RECEPTOR COMPLEXED WITH
T0901317 COMPLEX
Authors : Farnegardh, M.; Bonn, T.; Sun, S.; Ljunggren, J.; Ahola, H.; Wilhelmsson, A.;
Gustafsson, J.-A.; Carlquist, M.
Deposited on : 2003-06-18
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

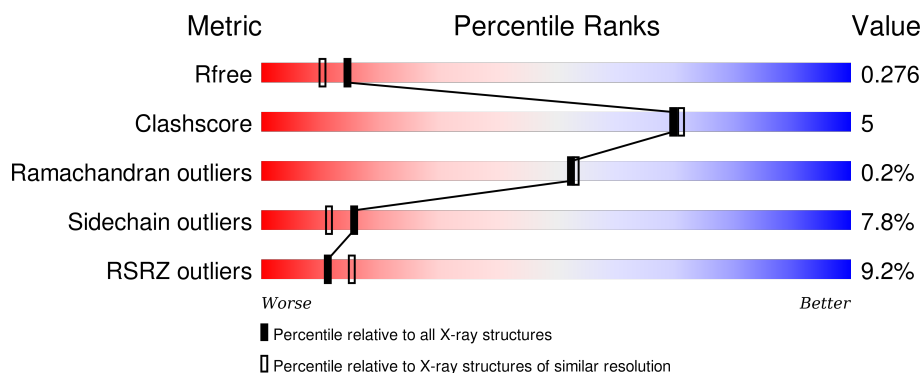
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	253	
1	B	253	
1	C	253	
1	D	253	

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	BNS	C	3500	-	-	-	X
2	BNS	D	4500	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7779 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.

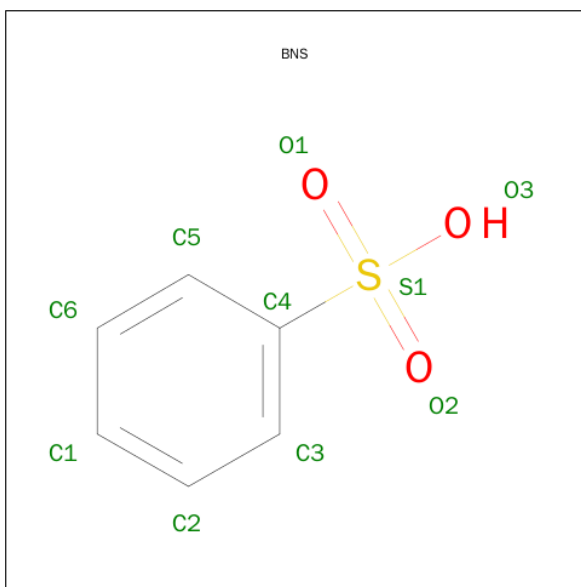
- Molecule 1 is a protein called Oxysterols receptor LXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1891	1210	331	343	7			
1	B	238	Total	C	N	O	S	0	0	0
			1925	1230	337	351	7			
1	C	231	Total	C	N	O	S	0	0	0
			1884	1204	333	340	7			
1	D	219	Total	C	N	O	S	0	0	0
			1774	1133	313	321	7			

There are 16 discrepancies between the modelled and reference sequences:

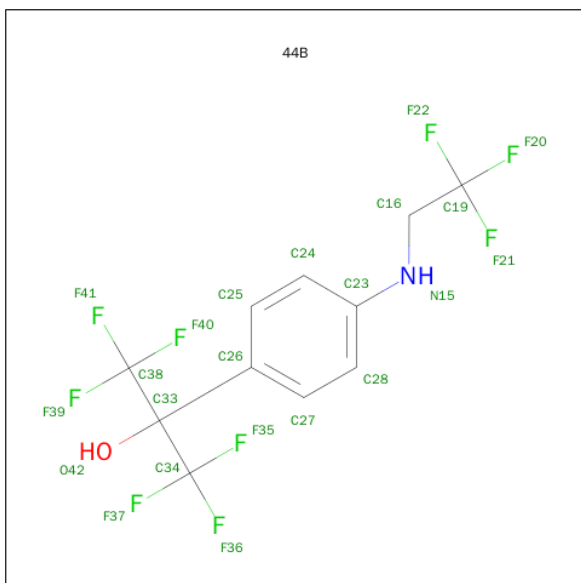
Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLY	-	CLONING ARTIFACT	UNP P55055
A	210	SER	-	CLONING ARTIFACT	UNP P55055
A	211	HIS	-	CLONING ARTIFACT	UNP P55055
A	212	MET	-	CLONING ARTIFACT	UNP P55055
B	209	GLY	-	CLONING ARTIFACT	UNP P55055
B	210	SER	-	CLONING ARTIFACT	UNP P55055
B	211	HIS	-	CLONING ARTIFACT	UNP P55055
B	212	MET	-	CLONING ARTIFACT	UNP P55055
C	209	GLY	-	CLONING ARTIFACT	UNP P55055
C	210	SER	-	CLONING ARTIFACT	UNP P55055
C	211	HIS	-	CLONING ARTIFACT	UNP P55055
C	212	MET	-	CLONING ARTIFACT	UNP P55055
D	209	GLY	-	CLONING ARTIFACT	UNP P55055
D	210	SER	-	CLONING ARTIFACT	UNP P55055
D	211	HIS	-	CLONING ARTIFACT	UNP P55055
D	212	MET	-	CLONING ARTIFACT	UNP P55055

- Molecule 2 is BENZENESULFONIC ACID (three-letter code: BNS) (formula: C₆H₆O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			9	6	2	1		
2	B	1	Total	C	O	S	0	0
			9	6	2	1		
2	C	1	Total	C	O	S	0	0
			9	6	2	1		
2	D	1	Total	C	O	S	0	0
			9	6	2	1		

- Molecule 3 is 1,1,1,3,3,3-HEXAFLUORO-2-{4-[(2,2,2-TRIFLUOROETHYL)AMINO]PHE
NYL}PROPAN-2-OL (three-letter code: 44B) (formula: C₁₁H₈F₉NO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			22	11	9	1	1		
3	B	1	Total	C	F	N	O	0	0
			22	11	9	1	1		
3	C	1	Total	C	F	N	O	0	0
			22	11	9	1	1		
3	D	1	Total	C	F	N	O	0	0
			22	11	9	1	1		

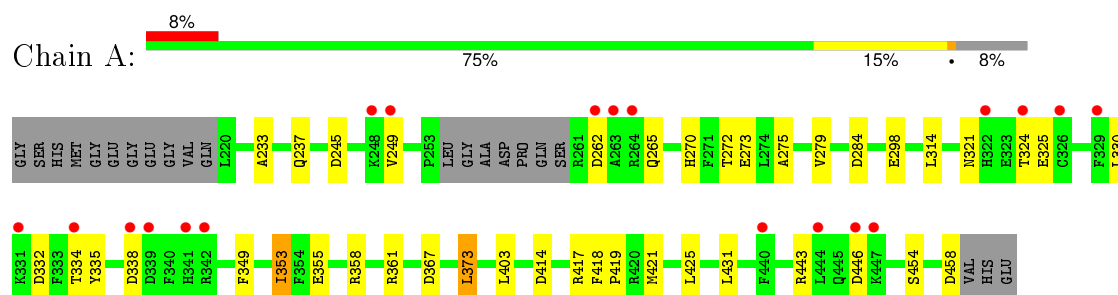
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	73	Total	O	0	0
			73	73		
4	C	52	Total	O	0	0
			52	52		
4	D	21	Total	O	0	0
			21	21		

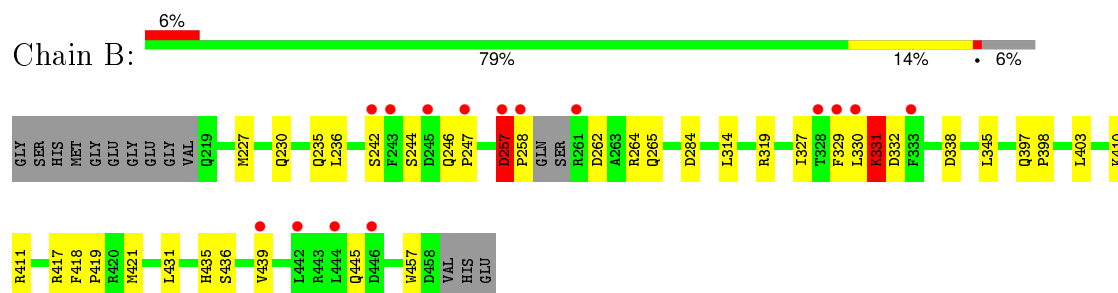
3 Residue-property plots

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.

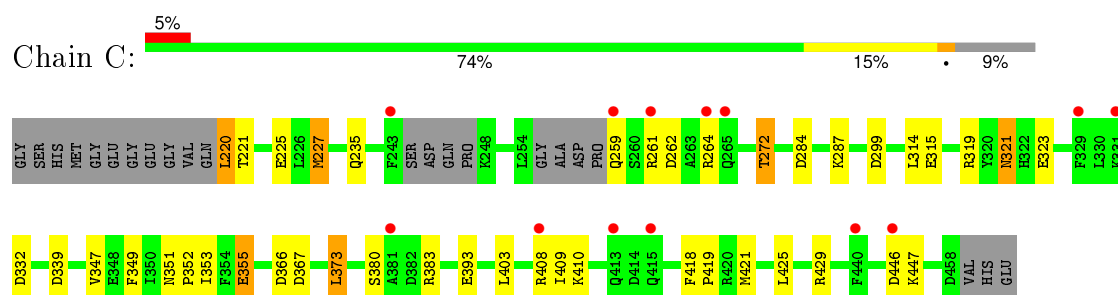
• Molecule 1: Oxysterols receptor LXR-beta



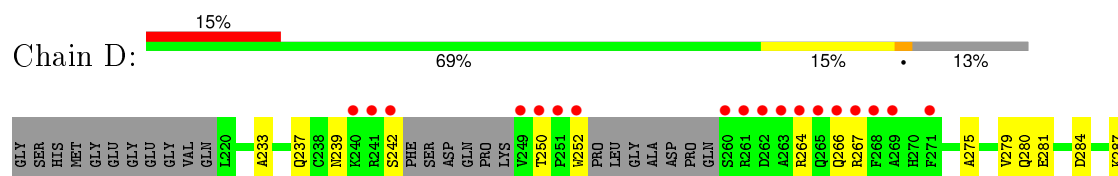
• Molecule 1: Oxysterols receptor LXR-beta

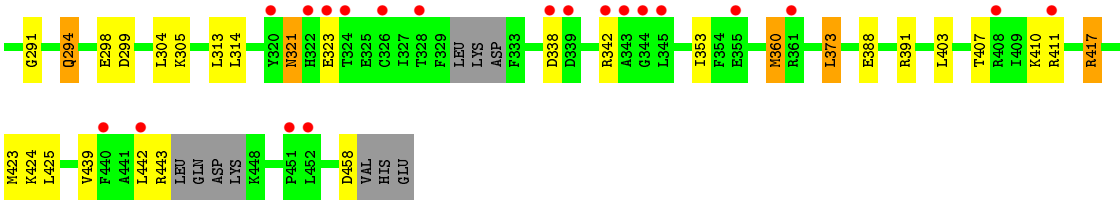


• Molecule 1: Oxysterols receptor LXR-beta



• Molecule 1: Oxysterols receptor LXR-beta





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.87Å 103.61Å 176.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.84 – 2.10 55.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (55.84-2.10) 99.7 (55.84-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.28	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.214 , 0.254 0.272 , 0.276	Depositor DCC
R_{free} test set	3227 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 63700 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7779	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BNS, 44B

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	0.62	0/1928	0.80	8/2607 (0.3%)
1	B	0.66	0/1963	0.82	4/2656 (0.2%)
1	C	0.68	1/1919 (0.1%)	0.84	10/2591 (0.4%)
1	D	0.59	0/1804	0.75	4/2436 (0.2%)
All	All	0.64	1/7614 (0.0%)	0.80	26/10290 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	272	THR	CB-CG2	-5.35	1.34	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	MET	CG-SD-CE	-8.11	87.23	100.20
1	B	284	ASP	CB-CG-OD2	7.41	124.97	118.30
1	B	338	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	332	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	446	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	446	ASP	CB-CG-OD2	5.76	123.48	118.30
1	C	339	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	366	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	262	ASP	CB-CG-OD2	5.56	123.31	118.30
1	D	458	ASP	CB-CG-OD2	5.53	123.27	118.30
1	D	299	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	332	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	284	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	338	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	257	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	332	ASP	CB-CG-OD2	5.27	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	262	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	429	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	299	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	245	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	284	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	458	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	338	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	367	ASP	CB-CG-OD2	5.05	122.84	118.30
1	C	284	ASP	CB-CG-OD2	5.03	122.82	118.30
1	C	367	ASP	CB-CG-OD2	5.00	122.80	118.30

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	1891	0	1913	12	0
1	B	1925	0	1936	16	0
1	C	1884	0	1905	18	0
1	D	1774	0	1788	19	0
2	A	9	0	5	1	0
2	B	9	0	5	1	0
2	C	9	0	5	2	0
2	D	9	0	5	1	0
3	A	22	0	8	1	0
3	B	22	0	8	0	0
3	C	22	0	8	2	0
3	D	22	0	8	1	0
4	A	35	0	0	0	0
4	B	73	0	0	0	0
4	C	52	0	0	0	0
4	D	21	0	0	0	0
All	All	7779	0	7594	69	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 5.

All (69) 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:C:352:PRO:HA	1:C:355:GLU:HG3	1.49	0.94
1:D:233:ALA:O	1:D:237:GLN:HG3	1.87	0.74
1:D:360:MET:HE1	1:D:424:LYS:HD2	1.72	0.72
2:C:3500:BNS:O1	3:C:3501:44B:N15	2.25	0.70
1:C:351:ASN:O	1:C:355:GLU:HG2	1.93	0.69
1:C:315:GLU:OE1	1:C:319:ARG:NH1	2.27	0.68
1:C:352:PRO:HA	1:C:355:GLU:CG	2.23	0.67
1:D:242:SER:OG	1:D:281:GLU:OE2	2.10	0.66
1:A:403:LEU:HD21	1:A:421:MET:HE2	1.81	0.63
1:A:349:PHE:CE1	1:A:353:ILE:HD11	2.36	0.60
1:A:373:LEU:HD22	1:A:425:LEU:HD21	1.85	0.59
1:B:246:GLN:NE2	1:B:330:LEU:O	2.35	0.59
1:B:257:ASP:CB	1:B:258:PRO:CD	2.82	0.57
1:C:321:ASN:HD21	1:C:323:GLU:HB3	1.70	0.56
1:D:250:THR:CG2	1:D:266:GLN:HE21	2.19	0.56
1:D:321:ASN:C	1:D:321:ASN:HD22	2.10	0.55
1:D:252:TRP:CZ2	1:D:267:ARG:HD3	2.42	0.54
1:A:321:ASN:ND2	1:A:324:THR:OG1	2.34	0.54
1:C:403:LEU:HD21	1:C:421:MET:HE2	1.89	0.54
1:B:257:ASP:CB	1:B:258:PRO:HD2	2.38	0.53
1:C:221:THR:O	1:C:225:GLU:HG3	2.09	0.53
1:C:409:ILE:O	1:C:410:LYS:C	2.48	0.51
1:C:373:LEU:HD22	1:C:425:LEU:HD21	1.92	0.51
1:B:418:PHE:HB3	1:B:419:PRO:HD3	1.93	0.50
1:B:257:ASP:HB3	1:B:258:PRO:CD	2.42	0.50
1:D:410:LYS:HD3	1:D:411:ARG:HG3	1.93	0.50
1:D:410:LYS:HZ1	1:D:411:ARG:HE	1.58	0.50
1:A:355:GLU:HG3	1:A:358:ARG:NH1	2.26	0.49
1:A:349:PHE:O	1:A:353:ILE:HD13	2.12	0.49
1:D:291:GLY:O	1:D:294:GLN:HG2	2.13	0.48
1:A:249:VAL:HG13	1:A:273:GLU:HB2	1.96	0.48
1:D:373:LEU:HD22	1:D:425:LEU:HD21	1.95	0.48
1:B:329:PHE:CZ	2:B:2500:BNS:O1	2.67	0.47
1:D:360:MET:CE	1:D:424:LYS:HD2	2.43	0.47
1:B:246:GLN:HB3	1:B:247:PRO:HD3	1.96	0.47
1:B:410:LYS:HG2	1:B:411:ARG:HG2	1.95	0.47
1:A:270:HIS:NE2	1:A:335:TYR:OH	2.38	0.47
1:C:351:ASN:O	1:C:355:GLU:CG	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:PHE:HB3	1:A:419:PRO:HD3	1.97	0.46
1:D:410:LYS:NZ	1:D:411:ARG:HE	2.13	0.45
1:C:349:PHE:CZ	1:C:353:ILE:HD11	2.52	0.45
1:C:352:PRO:CA	1:C:355:GLU:HG3	2.35	0.45
2:C:3500:BNS:O1	3:C:3501:44B:C23	2.64	0.45
1:B:257:ASP:HB3	1:B:258:PRO:HD2	1.99	0.45
1:A:414:ASP:OD2	1:A:417:ARG:HB2	2.17	0.44
1:B:330:LEU:O	1:B:331:LYS:HB2	2.17	0.44
1:D:403:LEU:O	1:D:407:THR:HG23	2.18	0.44
1:B:403:LEU:HD21	1:B:421:MET:HE2	2.00	0.43
1:C:418:PHE:HB3	1:C:419:PRO:HD3	1.99	0.43
1:D:388:GLU:CD	1:D:391:ARG:HD3	2.39	0.43
1:C:220:LEU:HD13	1:C:225:GLU:HG2	2.00	0.42
1:B:435:HIS:HE1	1:B:457:TRP:CD2	2.38	0.42
2:D:4500:BNS:O2	3:D:4501:44B:N15	2.47	0.42
1:B:330:LEU:O	1:B:331:LYS:CB	2.67	0.42
1:D:321:ASN:HD21	1:D:323:GLU:HB2	1.85	0.42
2:A:1500:BNS:S1	3:A:1501:44B:N15	2.92	0.42
1:A:275:ALA:O	1:A:279:VAL:HG23	2.19	0.41
1:B:397:GLN:HB3	1:B:398:PRO:HD3	2.02	0.41
1:B:436:SER:HA	1:B:439:VAL:HG22	2.01	0.41
1:C:353:ILE:HD13	1:C:353:ILE:HG21	1.83	0.41
1:C:380:SER:O	1:C:383:ARG:HG2	2.19	0.41
1:C:349:PHE:CE2	1:C:353:ILE:HD11	2.56	0.41
1:B:417:ARG:O	1:B:421:MET:HG3	2.21	0.41
1:D:417:ARG:HH11	1:D:417:ARG:HG2	1.86	0.41
1:D:313:LEU:CD2	1:D:353:ILE:HD12	2.51	0.40
1:D:304:LEU:HD23	1:D:304:LEU:HA	1.86	0.40
1:A:233:ALA:O	1:A:237:GLN:HG3	2.21	0.40
1:C:418:PHE:HB3	1:C:419:PRO:CD	2.52	0.40
1:D:275:ALA:O	1:D:279:VAL:HG23	2.22	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	228/253 (90%)	224 (98%)	4 (2%)	0	100	100
1	B	234/253 (92%)	229 (98%)	3 (1%)	2 (1%)	21	15
1	C	225/253 (89%)	221 (98%)	4 (2%)	0	100	100
1	D	209/253 (83%)	202 (97%)	7 (3%)	0	100	100
All	All	896/1012 (88%)	876 (98%)	18 (2%)	2 (0%)	52	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	257	ASP
1	B	331	LYS

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	206/222 (93%)	193 (94%)	13 (6%)	22	18
1	B	208/222 (94%)	191 (92%)	17 (8%)	14	10
1	C	204/222 (92%)	188 (92%)	16 (8%)	16	11
1	D	191/222 (86%)	174 (91%)	17 (9%)	12	8
All	All	809/888 (91%)	746 (92%)	63 (8%)	16	11

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	GLN
1	A	272	THR
1	A	298	GLU
1	A	314	LEU
1	A	325	GLU
1	A	330	LEU

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Mol	Chain	Res	Type
1	A	334	THR
1	A	353	ILE
1	A	361	ARG
1	A	373	LEU
1	A	431	LEU
1	A	443	ARG
1	A	454	SER
1	B	227	MET
1	B	230	GLN
1	B	235	GLN
1	B	236	LEU
1	B	242	SER
1	B	244	SER
1	B	257	ASP
1	B	262	ASP
1	B	264	ARG
1	B	265	GLN
1	B	314	LEU
1	B	319	ARG
1	B	327	ILE
1	B	331	LYS
1	B	345	LEU
1	B	431	LEU
1	B	445	GLN
1	C	220	LEU
1	C	227	MET
1	C	235	GLN
1	C	259	GLN
1	C	261	ARG
1	C	264	ARG
1	C	272	THR
1	C	287	LYS
1	C	314	LEU
1	C	321	ASN
1	C	347	VAL
1	C	355	GLU
1	C	373	LEU
1	C	393	GLU
1	C	408	ARG
1	C	447	LYS
1	D	239	ASN
1	D	264	ARG

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Mol	Chain	Res	Type
1	D	280	GLN
1	D	287	LYS
1	D	294	GLN
1	D	298	GLU
1	D	305	LYS
1	D	314	LEU
1	D	321	ASN
1	D	342	ARG
1	D	360	MET
1	D	373	LEU
1	D	417	ARG
1	D	423	MET
1	D	439	VAL
1	D	442	LEU
1	D	443	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	GLN
1	A	300	GLN
1	A	321	ASN
1	A	396	GLN
1	B	239	ASN
1	B	246	GLN
1	B	288	GLN
1	C	230	GLN
1	C	259	GLN
1	C	321	ASN
1	C	346	GLN
1	D	239	ASN
1	D	266	GLN
1	D	280	GLN
1	D	294	GLN
1	D	321	ASN

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 ⓘ

8 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	BNS	A	1500	-	7,9,10	2.04	3 (42%)	10,11,14	1.12	1 (10%)
3	44B	A	1501	-	21,22,22	1.56	4 (19%)	34,36,36	1.58	7 (20%)
2	BNS	B	2500	-	7,9,10	1.97	2 (28%)	10,11,14	0.75	0
3	44B	B	2501	-	21,22,22	1.73	6 (28%)	34,36,36	1.51	3 (8%)
2	BNS	C	3500	-	7,9,10	2.15	2 (28%)	10,11,14	0.53	0
3	44B	C	3501	-	21,22,22	1.73	5 (23%)	34,36,36	2.08	4 (11%)
2	BNS	D	4500	-	7,9,10	2.14	2 (28%)	10,11,14	0.99	1 (10%)
3	44B	D	4501	-	21,22,22	1.88	7 (33%)	34,36,36	1.55	7 (20%)

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	BNS	A	1500	-	-	0/4/4/6	0/1/1/1
3	44B	A	1501	-	-	0/30/30/30	0/1/1/1
2	BNS	B	2500	-	-	0/4/4/6	0/1/1/1
3	44B	B	2501	-	-	0/30/30/30	0/1/1/1
2	BNS	C	3500	-	-	0/4/4/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	44B	C	3501	-	-	0/30/30/30	0/1/1/1
2	BNS	D	4500	-	-	0/4/4/6	0/1/1/1
3	44B	D	4501	-	-	0/30/30/30	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	BNS	C4-S1	-2.19	1.76	1.80
3	B	2501	44B	C24-C25	2.00	1.42	1.38
3	A	1501	44B	C25-C26	2.05	1.42	1.39
3	D	4501	44B	C28-C27	2.17	1.42	1.38
3	D	4501	44B	C33-C26	2.19	1.57	1.53
3	C	3501	44B	C28-C27	2.24	1.42	1.38
3	B	2501	44B	C28-C23	2.24	1.42	1.39
3	A	1501	44B	C38-C33	2.25	1.59	1.54
3	D	4501	44B	C38-C33	2.27	1.59	1.54
3	C	3501	44B	C24-C23	2.42	1.43	1.39
2	A	1500	BNS	C3-C4	2.45	1.42	1.38
3	B	2501	44B	C24-C23	2.48	1.43	1.39
2	B	2500	BNS	C3-C4	2.52	1.42	1.38
2	A	1500	BNS	C5-C4	2.62	1.42	1.38
3	D	4501	44B	C28-C23	2.62	1.43	1.39
2	C	3500	BNS	C3-C4	2.65	1.42	1.38
2	D	4500	BNS	C3-C4	2.81	1.42	1.38
2	B	2500	BNS	C5-C4	2.95	1.43	1.38
2	D	4500	BNS	C5-C4	3.05	1.43	1.38
2	C	3500	BNS	C5-C4	3.22	1.43	1.38
3	D	4501	44B	C25-C26	3.29	1.44	1.39
3	C	3501	44B	C25-C26	3.30	1.44	1.39
3	A	1501	44B	C27-C26	3.33	1.44	1.39
3	B	2501	44B	C25-C26	3.43	1.44	1.39
3	D	4501	44B	C23-N15	3.49	1.48	1.38
3	C	3501	44B	C27-C26	3.50	1.44	1.39
3	A	1501	44B	C23-N15	3.56	1.49	1.38
3	B	2501	44B	C27-C26	3.61	1.44	1.39
3	B	2501	44B	C23-N15	3.66	1.49	1.38
3	D	4501	44B	C27-C26	4.14	1.45	1.39
3	C	3501	44B	C23-N15	4.18	1.51	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3501	44B	F22-C19-C16	-10.00	103.75	112.27
3	B	2501	44B	F22-C19-C16	-6.27	106.93	112.27
3	D	4501	44B	F22-C19-C16	-4.66	108.30	112.27
3	A	1501	44B	F20-C19-C16	-4.56	108.39	112.27
3	A	1501	44B	F22-C19-C16	-3.93	108.92	112.27
3	B	2501	44B	C38-C33-C34	-3.02	107.91	110.55
3	D	4501	44B	C38-C33-C34	-2.82	108.09	110.55
3	D	4501	44B	F21-C19-C16	-2.82	109.87	112.27
3	A	1501	44B	C38-C33-C26	-2.73	106.58	110.88
3	D	4501	44B	C24-C23-N15	-2.51	116.26	121.06
3	C	3501	44B	C38-C33-C26	-2.22	107.38	110.88
2	D	4500	BNS	O1-S1-C4	-2.22	99.48	104.38
3	D	4501	44B	C25-C26-C33	-2.20	115.49	120.52
3	C	3501	44B	C38-C33-C34	-2.11	108.70	110.55
3	A	1501	44B	C38-C33-C34	-2.08	108.73	110.55
3	D	4501	44B	C38-C33-C26	-2.04	107.67	110.88
3	A	1501	44B	F41-C38-C33	2.04	116.15	111.92
3	A	1501	44B	F20-C19-F22	2.05	114.25	106.43
3	A	1501	44B	F21-C19-C16	2.39	114.31	112.27
2	A	1500	BNS	O2-S1-C4	2.72	110.41	104.38
3	D	4501	44B	C27-C26-C33	2.74	126.78	120.52
3	B	2501	44B	F21-C19-C16	3.13	114.94	112.27
3	C	3501	44B	F21-C19-C16	4.02	115.69	112.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	BNS	1	0
3	A	1501	44B	1	0
2	B	2500	BNS	1	0
2	C	3500	BNS	2	0
3	C	3501	44B	2	0
2	D	4500	BNS	1	0
3	D	4501	44B	1	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	232/253 (91%)	0.78	19 (8%)	14 20	9, 20, 32, 36	0
1	B	238/253 (94%)	0.68	15 (6%)	23 31	8, 19, 40, 51	0
1	C	231/253 (91%)	0.66	13 (5%)	28 36	7, 19, 35, 57	0
1	D	219/253 (86%)	0.95	38 (17%)	2 3	11, 19, 30, 43	0
All	All	920/1012 (90%)	0.76	85 (9%)	11 15	7, 19, 34, 57	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	PHE	6.8
1	A	263	ALA	6.4
1	D	241	ARG	5.9
1	D	263	ALA	5.7
1	B	243	PHE	5.3
1	B	258	PRO	5.2
1	D	252	TRP	5.0
1	C	243	PHE	4.8
1	D	262	ASP	4.8
1	A	264	ARG	4.8
1	A	262	ASP	4.8
1	D	260	SER	4.7
1	D	451	PRO	4.5
1	B	333	PHE	4.5
1	A	322	HIS	4.3
1	C	331	LYS	4.3
1	A	446	ASP	4.3
1	D	266	GLN	4.3
1	D	345	LEU	4.2
1	A	324	THR	4.2
1	D	361	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	264	ARG	4.0
1	B	247	PRO	4.0
1	B	330	LEU	3.9
1	A	440	PHE	3.9
1	D	343	ALA	3.8
1	B	257	ASP	3.7
1	D	440	PHE	3.7
1	A	444	LEU	3.7
1	A	341	HIS	3.7
1	B	446	ASP	3.6
1	C	261	ARG	3.5
1	D	249	VAL	3.4
1	D	261	ARG	3.4
1	C	259	GLN	3.4
1	D	344	GLY	3.3
1	A	249	VAL	3.3
1	D	242	SER	3.3
1	D	452	LEU	3.2
1	C	440	PHE	3.2
1	A	248	LYS	3.1
1	C	413	GLN	3.1
1	D	251	PRO	3.1
1	D	411	ARG	3.1
1	B	242	SER	3.1
1	D	240	LYS	3.0
1	C	329	PHE	2.8
1	A	447	LYS	2.8
1	A	331	LYS	2.8
1	A	342	ARG	2.7
1	D	250	THR	2.7
1	A	326	CYS	2.6
1	D	320	TYR	2.6
1	D	267	ARG	2.6
1	D	322	HIS	2.5
1	C	264	ARG	2.5
1	D	342	ARG	2.5
1	D	339	ASP	2.5
1	A	334	THR	2.5
1	D	324	THR	2.4
1	C	381	ALA	2.4
1	D	328	THR	2.4
1	D	268	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	271	PHE	2.4
1	D	265	GLN	2.4
1	A	338	ASP	2.3
1	A	329	PHE	2.3
1	C	265	GLN	2.3
1	C	415	GLN	2.2
1	D	323	GLU	2.2
1	B	328	THR	2.2
1	B	439	VAL	2.2
1	B	442	LEU	2.2
1	D	326	CYS	2.2
1	C	446	ASP	2.2
1	D	269	ALA	2.2
1	D	355	GLU	2.1
1	D	338	ASP	2.1
1	D	408	ARG	2.1
1	B	261	ARG	2.0
1	C	408	ARG	2.0
1	D	442	LEU	2.0
1	B	444	LEU	2.0
1	B	245	ASP	2.0
1	A	339	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BNS	D	4500	9/10	0.79	0.42	6.58	46,46,50,51	0
2	BNS	C	3500	9/10	0.87	0.27	2.71	48,49,54,55	0
2	BNS	B	2500	9/10	0.81	0.23	0.72	48,50,53,53	0
2	BNS	A	1500	9/10	0.92	0.18	0.56	33,34,39,39	0
3	44B	C	3501	22/22	0.95	0.15	0.07	15,21,27,28	0
3	44B	D	4501	22/22	0.92	0.17	0.06	12,18,25,26	0
3	44B	B	2501	22/22	0.94	0.11	-1.22	13,17,28,29	0
3	44B	A	1501	22/22	0.94	0.11	-1.28	9,14,25,26	0

6.5 Other polymers

There are no such residues in this entry.