



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:36 PM GMT

PDB ID : 1PQ6
Title : HUMAN LXR BETA HORMONE RECEPTOR / GW3965 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 : 2.40 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

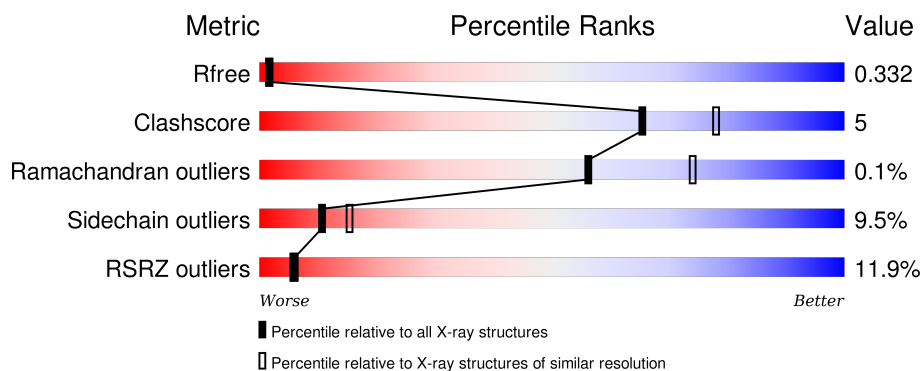
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	 2% 73% 16% • 8%
1	B	253	 3% 79% 14% • 5%
1	C	253	 17% 66% 15% • 18%
1	D	253	 21% 66% 21% • 10%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IPA	A	1501	-	-	-	X
3	IPA	B	2501	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7673 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.

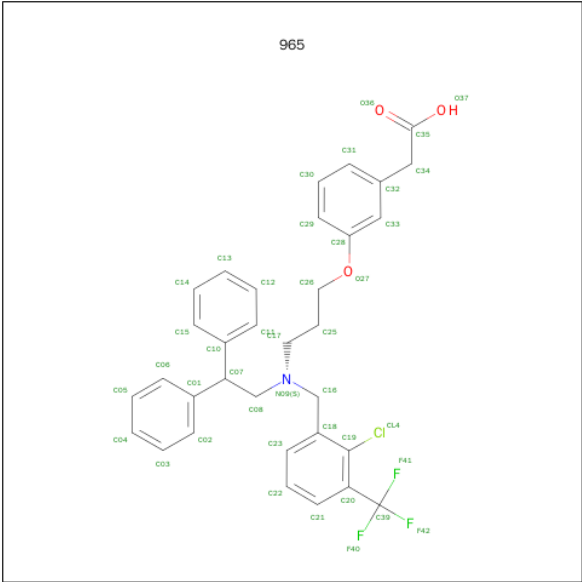
- Molecule 1 is a protein called Oxysterols receptor LXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1879	1203	330	339	7			
1	B	241	Total	C	N	O	S	0	0	0
			1950	1246	341	356	7			
1	C	208	Total	C	N	O	S	0	0	0
			1698	1082	300	309	7			
1	D	227	Total	C	N	O	S	0	0	0
			1848	1188	323	330	7			

There are 16 discrepancies between the modelled and reference sequences:

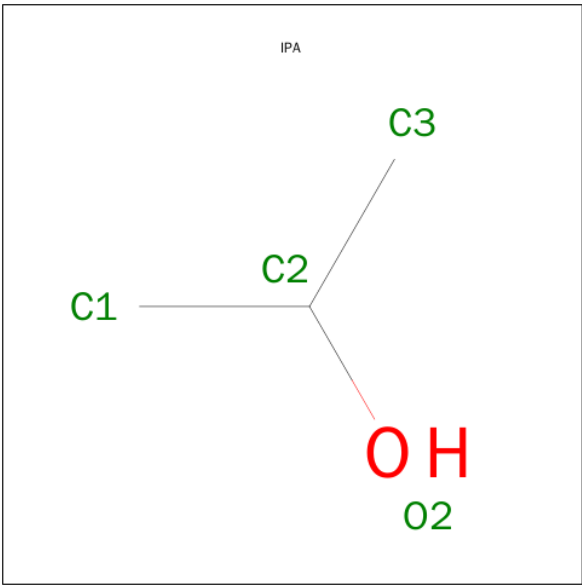
Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLY	-	CLONING ARTIFACT	UNP P55055
A	210	SER	-	CLONING ARTIFACT	UNP P55055
A	211	HIS	-	CLONING ARTIFACT	UNP P55055
A	212	MET	-	CLONING ARTIFACT	UNP P55055
B	209	GLY	-	CLONING ARTIFACT	UNP P55055
B	210	SER	-	CLONING ARTIFACT	UNP P55055
B	211	HIS	-	CLONING 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 [3-(3-{[2-CHLORO-3-(TRIFLUOROMETHYL)BENZYL](2,2-DIPHENYLETHYL)AMINO}PROPOXY)PHENYL]ACETIC ACID (three-letter code: 965) (formula: C₃₃H₃₁ClF₃NO₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			41	33	1	3	1	3		
2	B	1	Total	C	Cl	F	N	O	0	0
			41	33	1	3	1	3		
2	D	1	Total	C	Cl	F	N	O	0	0
			41	33	1	3	1	3		

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	3	1		

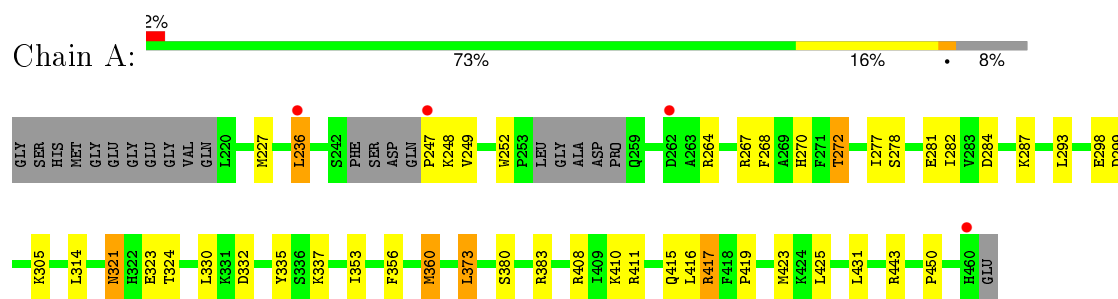
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	69	Total	O	0	0
			69	69		
4	C	19	Total	O	0	0
			19	19		
4	D	28	Total	O	0	0
			28	28		

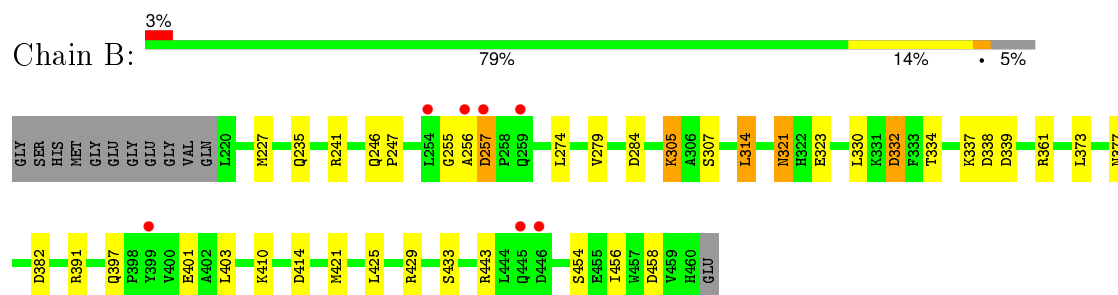
3 Residue-property plots [i](#)

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.

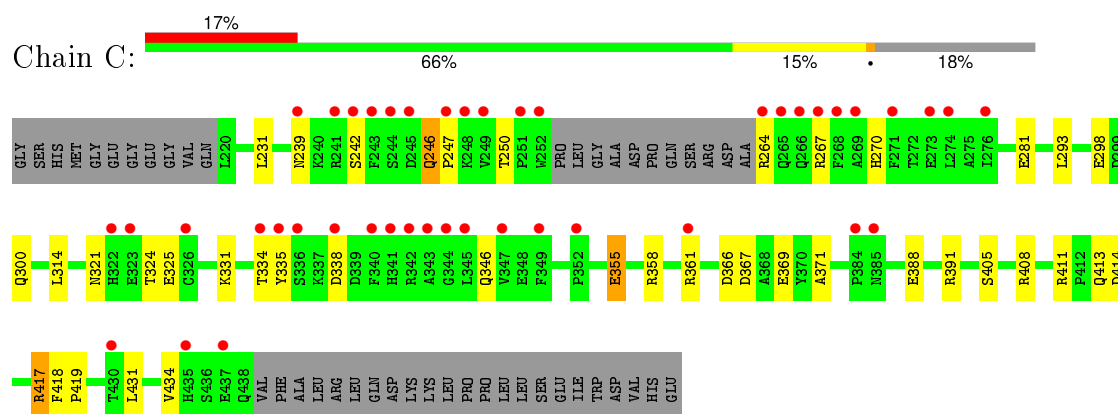
• Molecule 1: Oxysterols receptor LXR-beta



• Molecule 1: Oxysterols receptor LXR-beta

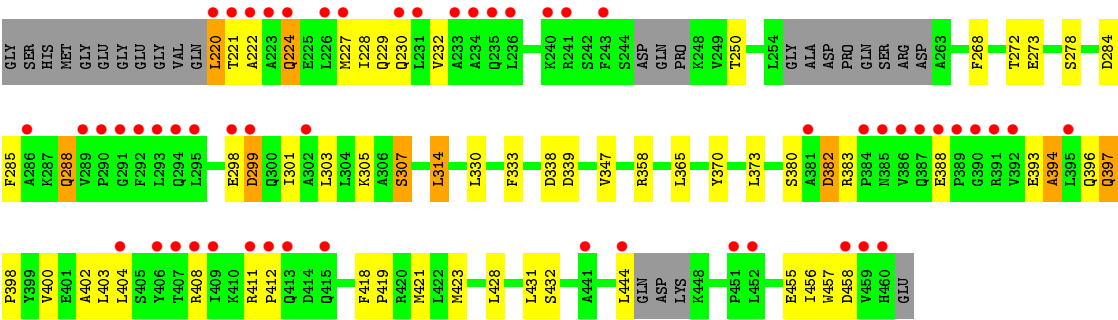


• Molecule 1: Oxysterols receptor LXR-beta



• 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	58.72Å 98.93Å 175.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.71 – 2.40 55.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (87.71-2.40) 98.4 (55.69-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.207 , 0.262 0.289 , 0.332	Depositor DCC
R_{free} test set	2021 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 40275 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7673	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 965, IPA

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	0.68	1/1914 (0.1%)	0.81	2/2587 (0.1%)
1	B	0.64	0/1989	0.85	9/2693 (0.3%)
1	C	0.56	1/1729 (0.1%)	0.75	4/2334 (0.2%)
1	D	0.89	6/1882 (0.3%)	0.92	7/2542 (0.3%)
All	All	0.71	8/7514 (0.1%)	0.84	22/10156 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	299	ASP	CG-OD2	21.94	1.75	1.25
1	D	299	ASP	CG-OD1	9.55	1.47	1.25
1	D	222	ALA	C-O	8.32	1.39	1.23
1	D	229	GLN	C-O	6.54	1.35	1.23
1	D	299	ASP	CB-CG	6.44	1.65	1.51
1	D	394	ALA	C-O	5.96	1.34	1.23
1	A	360	MET	SD-CE	-5.65	1.46	1.77
1	C	325	GLU	C-O	5.04	1.32	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	299	ASP	CB-CG-OD1	-21.07	99.34	118.30
1	D	299	ASP	CB-CG-OD2	12.24	129.32	118.30
1	D	358	ARG	NE-CZ-NH2	-9.15	115.73	120.30
1	A	284	ASP	CB-CG-OD2	8.24	125.71	118.30
1	D	358	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	339	ASP	CB-CG-OD2	6.53	124.17	118.30
1	B	391	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	C	366	ASP	CB-CG-OD2	6.19	123.88	118.30
1	D	284	ASP	CB-CG-OD2	5.97	123.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	LEU	CA-CB-CG	5.62	128.21	115.30
1	B	382	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	284	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	332	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	367	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	382	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	414	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	338	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	299	ASP	CB-CG-OD2	5.15	122.93	118.30
1	D	339	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	414	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	458	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	338	ASP	CB-CG-OD2	5.03	122.83	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	1879	0	1902	21	0
1	B	1950	0	1968	20	0
1	C	1698	0	1716	11	0
1	D	1848	0	1883	24	0
2	A	41	0	30	1	0
2	B	41	0	30	1	0
2	D	41	0	30	1	0
3	A	4	0	8	2	0
3	B	4	0	8	0	0
4	A	51	0	0	0	0
4	B	69	0	0	1	0
4	C	19	0	0	0	0
4	D	28	0	0	0	0
All	All	7673	0	7575	76	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 (76) 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:D:299:ASP:OD2	1:D:299:ASP:CG	1.75	1.25
1:C:242:SER:OG	1:C:281:GLU:OE2	1.97	0.82
1:A:415:GLN:NE2	1:B:401:GLU:OE1	2.20	0.73
1:A:356:PHE:CZ	1:A:360:MET:CE	2.72	0.73
1:D:303:LEU:O	1:D:307:SER:HB2	1.95	0.67
1:A:419:PRO:O	1:A:423:MET:HG2	1.94	0.65
1:A:270:HIS:NE2	1:A:335:TYR:OH	2.25	0.65
1:B:321:ASN:C	1:B:321:ASN:HD22	2.04	0.61
1:A:356:PHE:CZ	1:A:360:MET:HE2	2.37	0.59
1:B:403:LEU:HD21	1:B:421:MET:HE2	1.82	0.59
1:D:228:ILE:O	1:D:232:VAL:HG23	2.02	0.58
1:D:419:PRO:O	1:D:423:MET:HG2	2.03	0.58
1:B:279:VAL:HG11	1:B:456:ILE:HD11	1.85	0.58
1:A:278:SER:HB2	2:A:1500:965:C32	2.35	0.57
1:A:321:ASN:HD22	1:A:324:THR:H	1.53	0.56
1:C:369:GLU:OE1	1:C:417:ARG:NH2	2.38	0.56
1:B:403:LEU:HD11	1:B:421:MET:HE1	1.87	0.55
1:A:272:THR:HG23	1:A:450:PRO:HG3	1.87	0.55
1:B:307:SER:HB2	1:B:377:ASN:ND2	2.22	0.54
1:C:418:PHE:HB3	1:C:419:PRO:HD3	1.89	0.54
1:D:224:GLN:HG2	1:D:402:ALA:HB2	1.88	0.54
1:B:321:ASN:ND2	1:B:323:GLU:H	2.06	0.53
1:C:250:THR:O	1:C:270:HIS:ND1	2.42	0.53
1:D:268:PHE:O	1:D:272:THR:HG23	2.10	0.52
1:A:380:SER:O	1:A:383:ARG:HG2	2.10	0.52
1:B:321:ASN:HD22	1:B:323:GLU:H	1.57	0.51
1:D:250:THR:OG1	1:D:273:GLU:OE2	2.28	0.51
1:B:274:LEU:HD22	1:B:330:LEU:HD11	1.93	0.51
1:C:388:GLU:OE1	1:C:391:ARG:HD2	2.11	0.51
1:D:314:LEU:HD13	1:D:428:LEU:HD11	1.93	0.50
1:D:403:LEU:HD11	1:D:421:MET:HE1	1.94	0.49
1:B:255:GLY:C	1:B:257:ASP:N	2.66	0.49
1:D:299:ASP:OD2	1:D:388:GLU:OE1	2.31	0.49
1:D:394:ALA:O	1:D:398:PRO:CD	2.61	0.48
1:C:231:LEU:HB3	1:C:371:ALA:HB1	1.96	0.48
1:A:281:GLU:HB3	3:A:1501:IPA:H31	1.96	0.48
1:A:287:LYS:HD2	1:A:293:LEU:HD21	1.96	0.47
1:D:220:LEU:HD22	1:D:224:GLN:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:ALA:O	1:D:398:PRO:HD3	2.15	0.46
1:A:277:ILE:HG21	1:A:330:LEU:HD21	1.99	0.45
1:B:255:GLY:C	1:B:257:ASP:H	2.19	0.45
1:D:285:PHE:O	1:D:288:GLN:HG2	2.17	0.44
1:B:373:LEU:HD22	1:B:425:LEU:HD21	1.98	0.44
1:B:257:ASP:CG	1:B:257:ASP:O	2.56	0.44
1:C:246:GLN:N	1:C:247:PRO:CD	2.81	0.44
1:B:246:GLN:HE22	1:B:332:ASP:HB2	1.83	0.44
1:A:287:LYS:CD	1:A:293:LEU:HD21	2.47	0.44
2:B:2500:965:H251	2:B:2500:965:H161	1.87	0.44
1:D:397:GLN:HB3	1:D:398:PRO:HD3	1.99	0.44
1:D:404:LEU:HD13	1:D:418:PHE:CD2	2.53	0.43
1:C:270:HIS:NE2	1:C:335:TYR:OH	2.51	0.43
1:B:307:SER:HB2	1:B:377:ASN:HD22	1.84	0.43
1:A:282:ILE:HA	3:A:1501:IPA:H33	2.00	0.43
1:A:411:ARG:HD3	1:A:417:ARG:HG3	2.00	0.43
1:D:330:LEU:HD12	1:D:333:PHE:CE1	2.54	0.43
1:D:365:LEU:HB2	1:D:370:TYR:CE1	2.54	0.42
1:D:298:GLU:HA	1:D:301:ILE:HD12	2.02	0.42
1:A:236:LEU:HD12	1:A:236:LEU:O	2.20	0.42
1:D:418:PHE:HB3	1:D:419:PRO:HD3	2.01	0.42
1:B:257:ASP:OD2	1:B:257:ASP:O	2.38	0.42
1:B:305:LYS:NZ	4:B:57:HOH:O	2.52	0.41
1:D:365:LEU:HD13	1:D:421:MET:HE3	2.03	0.41
1:D:456:ILE:HG22	1:D:457:TRP:CD1	2.55	0.41
2:D:3500:965:F42	2:D:3500:965:CL4	2.65	0.41
1:C:293:LEU:HA	1:C:300:GLN:NE2	2.36	0.41
1:C:355:GLU:HG3	1:C:358:ARG:NH1	2.36	0.41
1:A:416:LEU:CD1	1:B:397:GLN:HG3	2.51	0.41
1:D:396:GLN:O	1:D:400:VAL:HG23	2.21	0.41
1:A:268:PHE:O	1:A:272:THR:HB	2.21	0.41
1:C:321:ASN:ND2	1:C:324:THR:HG23	2.36	0.41
1:A:247:PRO:HD2	1:A:277:ILE:HD12	2.03	0.40
1:D:380:SER:O	1:D:383:ARG:HG2	2.21	0.40
1:A:373:LEU:HD22	1:A:425:LEU:HD21	2.03	0.40
1:B:246:GLN:N	1:B:247:PRO:CD	2.83	0.40
1:A:252:TRP:CH2	1:A:267:ARG:HD3	2.56	0.40
1:B:429:ARG:HD3	1:B:429:ARG:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/253 (89%)	221 (98%)	5 (2%)	0	100	100
1	B	239/253 (94%)	232 (97%)	6 (2%)	1 (0%)	39	56
1	C	204/253 (81%)	199 (98%)	5 (2%)	0	100	100
1	D	219/253 (87%)	209 (95%)	10 (5%)	0	100	100
All	All	888/1012 (88%)	861 (97%)	26 (3%)	1 (0%)	56	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	256	ALA

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	203/222 (91%)	183 (90%)	20 (10%)	10	14
1	B	212/222 (96%)	198 (93%)	14 (7%)	21	32
1	C	185/222 (83%)	167 (90%)	18 (10%)	10	15
1	D	201/222 (90%)	177 (88%)	24 (12%)	6	8
All	All	801/888 (90%)	725 (90%)	76 (10%)	11	15

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	MET
1	A	236	LEU
1	A	248	LYS
1	A	249	VAL
1	A	264	ARG
1	A	272	THR
1	A	298	GLU
1	A	305	LYS
1	A	314	LEU
1	A	321	ASN
1	A	323	GLU
1	A	332	ASP
1	A	337	LYS
1	A	353	ILE
1	A	373	LEU
1	A	408	ARG
1	A	410	LYS
1	A	417	ARG
1	A	431	LEU
1	A	443	ARG
1	B	227	MET
1	B	235	GLN
1	B	241	ARG
1	B	257	ASP
1	B	305	LYS
1	B	314	LEU
1	B	321	ASN
1	B	334	THR
1	B	337	LYS
1	B	361	ARG
1	B	410	LYS
1	B	433	SER
1	B	443	ARG
1	B	454	SER
1	C	239	ASN
1	C	246	GLN
1	C	264	ARG
1	C	267	ARG
1	C	298	GLU
1	C	314	LEU
1	C	331	LYS
1	C	334	THR
1	C	346	GLN

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Mol	Chain	Res	Type
1	C	355	GLU
1	C	361	ARG
1	C	405	SER
1	C	408	ARG
1	C	411	ARG
1	C	413	GLN
1	C	417	ARG
1	C	431	LEU
1	C	434	VAL
1	D	220	LEU
1	D	221	THR
1	D	224	GLN
1	D	227	MET
1	D	230	GLN
1	D	278	SER
1	D	288	GLN
1	D	305	LYS
1	D	307	SER
1	D	314	LEU
1	D	338	ASP
1	D	347	VAL
1	D	373	LEU
1	D	382	ASP
1	D	393	GLU
1	D	397	GLN
1	D	408	ARG
1	D	411	ARG
1	D	412	PRO
1	D	431	LEU
1	D	432	SER
1	D	444	LEU
1	D	455	GLU
1	D	458	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	265	GLN
1	A	300	GLN
1	A	321	ASN
1	A	377	ASN

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Mol	Chain	Res	Type
1	A	415	GLN
1	B	230	GLN
1	B	321	ASN
1	B	346	GLN
1	B	377	ASN
1	B	445	GLN
1	C	246	GLN
1	C	266	GLN
1	C	300	GLN
1	C	321	ASN
1	C	387	GLN
1	C	397	GLN
1	D	237	GLN
1	D	300	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	965	A	1500	-	40,44,44	1.68	3 (7%)	51,60,60	1.42	5 (9%)
3	IPA	A	1501	-	3,3,3	0.45	0	3,3,3	0.38	0
2	965	B	2500	-	40,44,44	1.84	3 (7%)	51,60,60	1.59	7 (13%)
3	IPA	B	2501	-	3,3,3	0.38	0	3,3,3	0.38	0
2	965	D	3500	-	40,44,44	1.57	3 (7%)	51,60,60	1.64	6 (11%)

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	965	A	1500	-	-	0/31/33/33	0/4/4/4
3	IPA	A	1501	-	-	0/0/0/0	0/0/0/0
2	965	B	2500	-	-	0/31/33/33	0/4/4/4
3	IPA	B	2501	-	-	0/0/0/0	0/0/0/0
2	965	D	3500	-	-	0/31/33/33	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3500	965	C19-CL4	2.69	1.78	1.72
2	A	1500	965	C19-CL4	2.86	1.78	1.72
2	B	2500	965	C19-CL4	3.92	1.81	1.72
2	D	3500	965	C19-C20	5.37	1.46	1.39
2	A	1500	965	C19-C20	6.05	1.47	1.39
2	B	2500	965	C19-C20	6.59	1.48	1.39
2	D	3500	965	C19-C18	7.18	1.46	1.39
2	A	1500	965	C19-C18	7.42	1.47	1.39
2	B	2500	965	C19-C18	8.31	1.48	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3500	965	F41-C39-C20	-3.91	105.81	112.68
2	A	1500	965	F41-C39-C20	-3.11	107.20	112.68
2	D	3500	965	C25-C17-N09	-3.02	106.30	113.89
2	B	2500	965	F41-C39-C20	-3.01	107.38	112.68
2	B	2500	965	C35-C34-C32	-2.81	107.17	112.73
2	B	2500	965	F42-C39-C20	-2.29	108.66	112.68
2	D	3500	965	C35-C34-C32	-2.14	108.50	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2500	965	C17-N09-C08	2.50	118.38	112.25
2	D	3500	965	C21-C20-C39	2.63	123.79	118.15
2	B	2500	965	C16-N09-C17	2.71	116.94	111.28
2	A	1500	965	C21-C20-C39	2.72	123.98	118.15
2	A	1500	965	C17-N09-C08	3.28	120.30	112.25
2	A	1500	965	C16-N09-C17	3.33	118.23	111.28
2	B	2500	965	C18-C16-N09	4.36	120.43	112.79
2	D	3500	965	C17-N09-C08	5.22	125.06	112.25
2	A	1500	965	C16-N09-C08	6.11	119.27	111.27
2	D	3500	965	C16-N09-C08	6.25	119.46	111.27
2	B	2500	965	C16-N09-C08	6.58	119.88	111.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	965	1	0
3	A	1501	IPA	2	0
2	B	2500	965	1	0
2	D	3500	965	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 ⓘ

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%)	0.63	4 (1%) 73 72	11, 22, 34, 47	0
1	B	241/253 (95%)	0.69	7 (2%) 55 54	14, 23, 36, 49	0
1	C	208/253 (82%)	1.15	43 (20%) 1 1	12, 21, 38, 42	0
1	D	227/253 (89%)	1.24	54 (23%) 1 1	10, 24, 39, 50	0
All	All	908/1012 (89%)	0.92	108 (11%) 6 6	10, 23, 37, 50	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	223	ALA	7.6
1	C	267	ARG	6.9
1	D	295	LEU	6.8
1	D	412	PRO	6.8
1	C	340	PHE	5.9
1	D	230	GLN	5.6
1	D	289	VAL	5.4
1	D	241	ARG	5.3
1	D	220	LEU	5.1
1	D	391	ARG	5.0
1	C	274	LEU	5.0
1	C	435	HIS	4.9
1	D	386	VAL	4.9
1	C	243	PHE	4.7
1	D	460	HIS	4.5
1	C	343	ALA	4.3
1	C	264	ARG	4.3
1	D	221	THR	4.3
1	C	247	PRO	4.2
1	C	245	ASP	4.2
1	D	451	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	444	LEU	4.1
1	C	266	GLN	4.0
1	C	344	GLY	3.9
1	C	249	VAL	3.9
1	C	322	HIS	3.9
1	C	342	ARG	3.9
1	C	349	PHE	3.8
1	C	345	LEU	3.7
1	D	388	GLU	3.7
1	C	361	ARG	3.7
1	D	224	GLN	3.6
1	D	384	PRO	3.6
1	D	236	LEU	3.5
1	C	437	GLU	3.5
1	D	226	LEU	3.5
1	C	338	ASP	3.5
1	D	413	GLN	3.5
1	D	298	GLU	3.4
1	D	441	ALA	3.4
1	C	335	TYR	3.4
1	D	291	GLY	3.4
1	D	390	GLY	3.2
1	C	336	SER	3.2
1	D	240	LYS	3.2
1	D	411	ARG	3.2
1	D	286	ALA	3.2
1	C	252	TRP	3.2
1	D	387	GLN	3.2
1	D	415	GLN	3.1
1	D	407	THR	3.1
1	A	460	HIS	3.1
1	C	384	PRO	3.1
1	C	268	PHE	3.0
1	C	265	GLN	3.0
1	D	299	ASP	3.0
1	D	459	VAL	2.9
1	C	271	PHE	2.9
1	D	243	PHE	2.9
1	D	406	TYR	2.9
1	C	251	PRO	2.9
1	C	341	HIS	2.9
1	B	254	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	269	ALA	2.9
1	D	292	PHE	2.8
1	D	290	PRO	2.8
1	D	395	LEU	2.7
1	D	404	LEU	2.7
1	D	235	GLN	2.7
1	D	408	ARG	2.7
1	D	409	ILE	2.7
1	C	239	ASN	2.7
1	D	233	ALA	2.7
1	D	389	PRO	2.7
1	D	392	VAL	2.6
1	D	294	GLN	2.6
1	C	248	LYS	2.6
1	D	231	LEU	2.6
1	C	326	CYS	2.6
1	D	234	ALA	2.6
1	B	445	GLN	2.6
1	D	222	ALA	2.6
1	A	236	LEU	2.5
1	C	430	THR	2.5
1	C	323	GLU	2.5
1	C	334	THR	2.5
1	C	276	ILE	2.5
1	B	446	ASP	2.4
1	C	273	GLU	2.4
1	C	385	ASN	2.4
1	B	256	ALA	2.4
1	D	452	LEU	2.3
1	C	242	SER	2.3
1	C	352	PRO	2.3
1	B	399	TYR	2.3
1	C	241	ARG	2.3
1	D	381	ALA	2.3
1	D	227	MET	2.2
1	D	385	ASN	2.2
1	D	293	LEU	2.2
1	D	458	ASP	2.1
1	D	302	ALA	2.1
1	A	262	ASP	2.1
1	A	247	PRO	2.1
1	C	347	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	257	ASP	2.0
1	B	259	GLN	2.0
1	C	244	SER	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(Å ²)	Q<0.9
3	IPA	A	1501	4/4	0.94	0.39	6.73	45,45,46,47	0
3	IPA	B	2501	4/4	0.96	0.29	4.07	37,38,39,41	0
2	965	B	2500	41/41	0.88	0.22	1.21	13,21,43,52	0
2	965	A	1500	41/41	0.90	0.21	0.62	16,23,41,48	0
2	965	D	3500	41/41	0.89	0.20	0.43	9,17,39,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.