Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:30 AM GMT

PDB ID	:	3IPS
Title	:	X-ray structure of benzisoxazole synthetic agonist bound to the LXR-alpha
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Deposited on	:	2009-08-18
Resolution	:	2.26 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 (i) symbol.

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

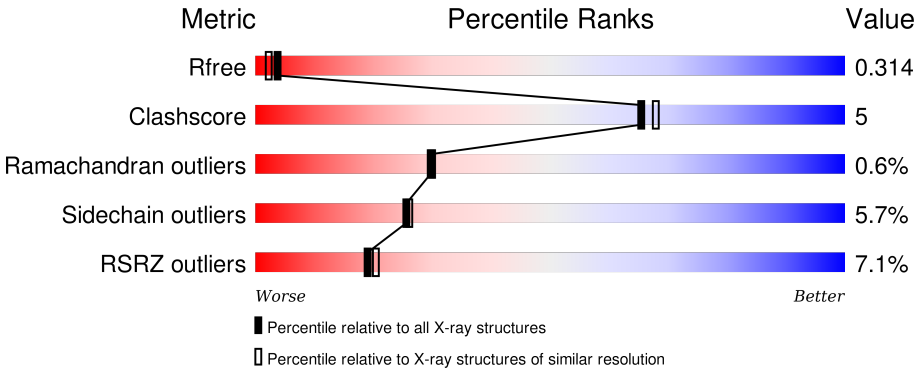
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 <=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	283	7%, 65%, 12%, 21%
1	B	283	5%, 64%, 15%, 20%
2	C	25	52%, 8%, 40%
2	D	25	48%, 12%, 40%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4047 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-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	1	0
			1831	1174	317	334	6			
1	B	226	Total	C	N	O	S	5	0	0
			1844	1182	321	335	6			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	MET	-	EXPRESSION TAG	UNP Q13133
A	166	LYS	-	EXPRESSION TAG	UNP Q13133
A	167	HIS	-	EXPRESSION TAG	UNP Q13133
A	168	GLN	-	EXPRESSION TAG	UNP Q13133
A	169	HIS	-	EXPRESSION TAG	UNP Q13133
A	170	GLN	-	EXPRESSION TAG	UNP Q13133
A	171	HIS	-	EXPRESSION TAG	UNP Q13133
A	172	GLN	-	EXPRESSION TAG	UNP Q13133
A	173	HIS	-	EXPRESSION TAG	UNP Q13133
A	174	GLN	-	EXPRESSION TAG	UNP Q13133
A	175	HIS	-	EXPRESSION TAG	UNP Q13133
A	176	GLN	-	EXPRESSION TAG	UNP Q13133
A	177	HIS	-	EXPRESSION TAG	UNP Q13133
A	178	GLN	-	EXPRESSION TAG	UNP Q13133
A	179	GLN	-	EXPRESSION TAG	UNP Q13133
A	180	PRO	-	EXPRESSION TAG	UNP Q13133
A	181	LEU	-	EXPRESSION TAG	UNP Q13133
B	165	MET	-	EXPRESSION TAG	UNP Q13133
B	166	LYS	-	EXPRESSION TAG	UNP Q13133
B	167	HIS	-	EXPRESSION TAG	UNP Q13133
B	168	GLN	-	EXPRESSION TAG	UNP Q13133
B	169	HIS	-	EXPRESSION TAG	UNP Q13133
B	170	GLN	-	EXPRESSION TAG	UNP Q13133
B	171	HIS	-	EXPRESSION TAG	UNP Q13133
B	172	GLN	-	EXPRESSION TAG	UNP Q13133

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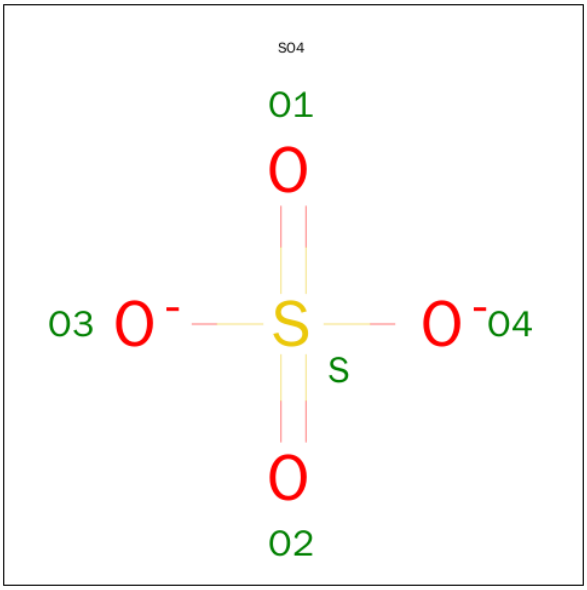
Chain	Residue	Modelled	Actual	Comment	Reference
B	173	HIS	-	EXPRESSION TAG	UNP Q13133
B	174	GLN	-	EXPRESSION TAG	UNP Q13133
B	175	HIS	-	EXPRESSION TAG	UNP Q13133
B	176	GLN	-	EXPRESSION TAG	UNP Q13133
B	177	HIS	-	EXPRESSION TAG	UNP Q13133
B	178	GLN	-	EXPRESSION TAG	UNP Q13133
B	179	GLN	-	EXPRESSION TAG	UNP Q13133
B	180	PRO	-	EXPRESSION TAG	UNP Q13133
B	181	LEU	-	EXPRESSION TAG	UNP Q13133

- Molecule 2 is a protein called Nuclear receptor coactivator 1.

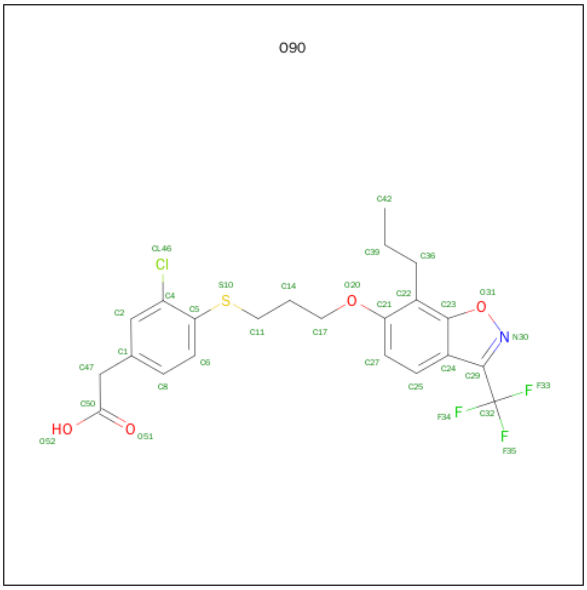
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	0	0	0
			131	82	27	22			
2	D	15	Total	C	N	O	0	1	0
			139	87	30	22			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	1
			10	8	2		
3	D	1	Total	O	S	0	1
			10	8	2		

- Molecule 4 is {3-CHLORO-4-[(3-{[7-PROPYL-3-(TRIFLUOROMETHYL)-1,2-BENZISOXAZOL-6-YL]OXY}PROPYL)SULFANYL]PHENYL}ACETIC ACID (three-letter code: O90) (formula: $C_{22}H_{21}ClF_3NO_4S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	S	0	0
			32	22	1	3	1	4	1		
4	B	1	Total	C	Cl	F	N	O	S	0	0
			32	22	1	3	1	4	1		

- Molecule 5 is water.

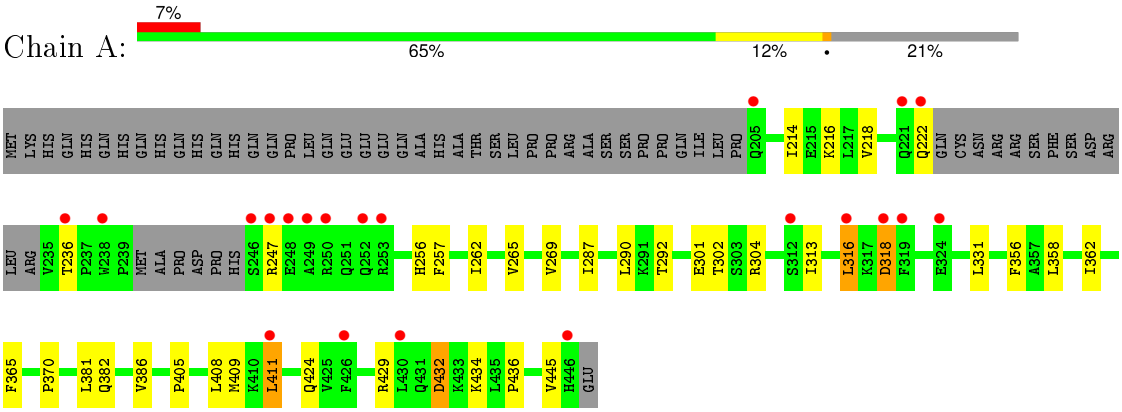
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	11	Total	O	0	0
			11	11		
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		

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.

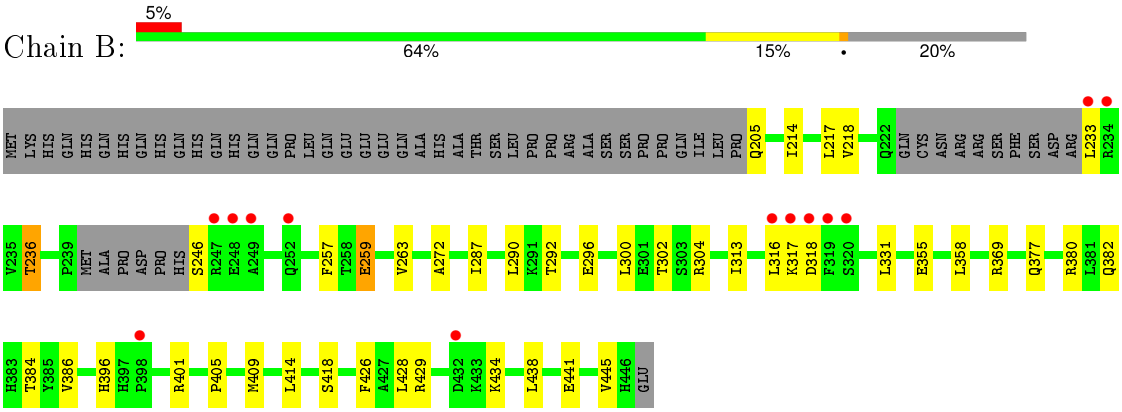
- Molecule 1: Oxysterols receptor LXR-alpha

Chain A:



- Molecule 1: Oxysterols receptor LXR-alpha

Chain B:



- Molecule 2: Nuclear receptor coactivator 1

Chain C:

- Molecule 2: Nuclear receptor coactivator 1

Chain D:

CYS
PRO
SER
SER
HIS
SER
S681
R685
I688
L689
E695
GLY
SER
PRO
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	123.05Å 123.05Å 91.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.30 – 2.26 39.30 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.30-2.26) 99.2 (39.30-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.255 , 0.315 0.259 , 0.314	Depositor DCC
R_{free} test set	1682 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 30.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 33236 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4047	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, O90

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	0.61	0/1872	0.68	0/2532
1	B	0.63	0/1882	0.75	2/2545 (0.1%)
2	C	0.58	0/132	0.72	0/175
2	D	0.71	0/143	0.85	0/189
All	All	0.62	0/4029	0.72	2/5441 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	317	LYS	CB-CA-C	-9.74	90.92	110.40
1	B	317	LYS	N-CA-CB	-6.21	99.42	110.60

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	1831	0	1837	19	0
1	B	1844	0	1853	21	0
2	C	131	0	139	4	0
2	D	139	0	152	2	0
3	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10	0	0	0	0
4	A	32	0	20	0	0
4	B	32	0	20	1	0
5	A	5	0	0	0	0
5	B	11	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	4047	0	4021	40	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 (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:THR:HG23	1:A:313:ILE:HD13	1.69	0.74
1:A:358:LEU:O	1:A:362:ILE:HD12	1.93	0.68
1:B:217:LEU:HD12	1:B:358:LEU:HD23	1.76	0.68
1:A:218:VAL:O	1:A:222:GLN:HG3	1.98	0.64
1:B:292:THR:HG21	1:B:369:ARG:HD2	1.80	0.63
1:B:355:GLU:OE2	1:B:396:HIS:ND1	2.30	0.55
1:B:296:GLU:HB3	1:B:414:LEU:HD13	1.90	0.53
1:A:405:PRO:O	1:A:409:MET:HG2	2.08	0.53
1:A:290:LEU:CD1	2:C:693:LEU:HD21	2.40	0.52
1:B:438:LEU:HD12	1:B:438:LEU:O	2.09	0.52
1:A:365:PHE:CE1	1:A:381:LEU:HD13	2.45	0.52
1:B:300:LEU:HG	1:B:414:LEU:HD11	1.92	0.51
1:B:441:GLU:OE1	2:D:688:ILE:HD12	2.11	0.51
1:B:377:GLN:OE1	1:B:377:GLN:HA	2.12	0.49
1:B:292:THR:CG2	1:B:369:ARG:HD2	2.42	0.49
1:A:265:VAL:O	1:A:269:VAL:HG23	2.12	0.49
1:A:382:GLN:O	1:A:386:VAL:HG23	2.13	0.49
1:B:405:PRO:O	1:B:409:MET:HG2	2.14	0.48
1:B:287:ILE:HG23	2:D:689:LEU:HD23	1.96	0.47
1:A:316:LEU:CD1	1:A:318:ASP:HB3	2.44	0.47
1:B:316:LEU:HA	4:B:1:O90:O51	2.15	0.47
1:A:290:LEU:HD11	2:C:693:LEU:HD21	1.96	0.46
1:A:292:THR:HG21	1:A:370:PRO:HD2	1.97	0.46
1:A:214:ILE:O	1:A:218:VAL:HG23	2.15	0.46
1:A:262:ILE:HD11	1:A:436:PRO:HB2	1.97	0.46
1:B:380:ARG:O	1:B:384:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ILE:O	1:B:218:VAL:HG23	2.16	0.45
1:B:302:THR:CG2	1:B:313:ILE:HD13	2.47	0.45
1:A:301:GLU:O	1:A:304:ARG:HB2	2.18	0.43
1:B:259:GLU:O	1:B:263:VAL:HG23	2.17	0.43
1:B:236:THR:OG1	1:B:259:GLU:OE1	2.37	0.43
1:A:408:LEU:O	1:A:411:LEU:HB2	2.19	0.42
1:A:304:ARG:HG3	1:A:356:PHE:CZ	2.55	0.42
1:B:217:LEU:CD1	1:B:358:LEU:HD23	2.49	0.41
1:A:287:ILE:HG23	2:C:689:LEU:HD23	2.02	0.41
1:B:382:GLN:O	1:B:386:VAL:HG23	2.20	0.41
1:B:426:PHE:O	1:B:429:ARG:HB2	2.21	0.41
1:A:269:VAL:HG13	2:C:693:LEU:HD23	2.03	0.41
1:A:236:THR:O	1:A:256:HIS:ND1	2.52	0.41
1:B:272:ALA:HB2	1:B:290:LEU:HD21	2.03	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	219/283 (77%)	210 (96%)	7 (3%)	2 (1%)	21 18
1	B	220/283 (78%)	213 (97%)	6 (3%)	1 (0%)	34 34
2	C	13/25 (52%)	12 (92%)	1 (8%)	0	100 100
2	D	14/25 (56%)	13 (93%)	1 (7%)	0	100 100
All	All	466/616 (76%)	448 (96%)	15 (3%)	3 (1%)	30 30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	318	ASP

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Mol	Chain	Res	Type
1	A	318	ASP
1	A	432	ASP

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	A	203/257 (79%)	192 (95%)	11 (5%)	27 29
1	B	204/257 (79%)	191 (94%)	13 (6%)	22 21
2	C	15/24 (62%)	15 (100%)	0	100 100
2	D	16/24 (67%)	14 (88%)	2 (12%)	6 3
All	All	438/562 (78%)	412 (94%)	26 (6%)	25 24

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	247	ARG
1	A	257	PHE
1	A	316	LEU
1	A	331	LEU
1	A	411	LEU
1	A	424	GLN
1	A	429	ARG
1	A	432	ASP
1	A	434	LYS
1	A	445	VAL
1	B	205	GLN
1	B	233	LEU
1	B	236	THR
1	B	246	SER
1	B	257	PHE
1	B	259	GLU
1	B	304	ARG
1	B	331	LEU

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Mol	Chain	Res	Type
1	B	401	ARG
1	B	418	SER
1	B	428	LEU
1	B	434	LYS
1	B	445	VAL
2	D	685[A]	ARG
2	D	685[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	GLN
1	B	251	GLN
1	B	332	GLN
1	B	390	HIS
1	B	421	HIS

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

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	O90	A	1	-	25,34,34	1.05	2 (8%)	35,48,48	1.79	9 (25%)
3	SO4	A	2[A]	-	4,4,4	0.31	0	6,6,6	0.30	0
3	SO4	A	2[B]	-	4,4,4	0.23	0	6,6,6	0.22	0
4	O90	B	1	-	25,34,34	0.99	1 (4%)	35,48,48	1.76	11 (31%)
3	SO4	D	1[A]	-	4,4,4	0.36	0	6,6,6	0.35	0
3	SO4	D	1[B]	-	4,4,4	0.28	0	6,6,6	0.20	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
4	O90	A	1	-	-	0/19/21/21	0/2/3/3
3	SO4	A	2[A]	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2[B]	-	-	0/0/0/0	0/0/0/0
4	O90	B	1	-	-	0/19/21/21	0/2/3/3
3	SO4	D	1[A]	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1[B]	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	O90	C2-C1	2.07	1.43	1.39
4	A	1	O90	C21-C22	2.24	1.41	1.38
4	B	1	O90	C21-C22	2.92	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1	O90	C29-C24-C23	-3.63	100.87	107.51
4	A	1	O90	C5-C4-CL46	-3.37	113.84	119.80
4	B	1	O90	C29-C24-C23	-3.12	101.81	107.51
4	A	1	O90	O20-C21-C22	-2.99	112.33	116.11
4	B	1	O90	C27-C25-C24	-2.92	117.29	121.13
4	B	1	O90	F33-C32-C29	-2.59	108.35	112.02
4	B	1	O90	O20-C21-C27	-2.57	118.64	124.01
4	B	1	O90	O20-C17-C14	-2.31	99.44	108.39
4	A	1	O90	C47-C1-C8	-2.26	113.99	120.90
4	A	1	O90	C4-C2-C1	-2.05	119.04	120.36
4	A	1	O90	C27-C25-C24	-2.04	118.45	121.13
4	B	1	O90	C36-C22-C23	2.11	125.42	120.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1	O90	C25-C24-C23	2.18	121.91	117.44
4	B	1	O90	C50-C47-C1	2.60	117.89	112.73
4	B	1	O90	C39-C36-C22	2.72	117.66	112.84
4	A	1	O90	C47-C1-C2	3.35	127.62	120.69
4	A	1	O90	C50-C47-C1	3.83	120.33	112.73
4	B	1	O90	C32-C29-N30	3.98	124.56	119.68
4	A	1	O90	C2-C4-CL46	4.25	125.05	118.50
4	B	1	O90	C17-O20-C21	4.38	128.39	117.64

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
4	B	1	O90	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, 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	A	224/283 (79%)	0.54	21 (9%) 11 12	24, 43, 72, 87	0
1	B	226/283 (79%)	0.35	13 (5%) 26 29	27, 39, 62, 78	1 (0%)
2	C	15/25 (60%)	-0.16	0 100 100	35, 38, 45, 49	0
2	D	15/25 (60%)	0.34	0 100 100	31, 36, 47, 52	0
All	All	480/616 (77%)	0.42	34 (7%) 19 20	24, 40, 68, 87	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	GLU	6.8
1	B	234	ARG	5.5
1	A	319	PHE	5.3
1	A	247	ARG	4.9
1	A	318	ASP	4.5
1	A	238	TRP	4.3
1	A	205	GLN	4.3
1	A	252	GLN	4.2
1	B	249	ALA	3.8
1	B	233	LEU	3.8
1	B	319	PHE	3.7
1	B	247	ARG	3.7
1	B	316	LEU	3.6
1	B	398	PRO	3.2
1	A	236	THR	3.1
1	A	430	LEU	3.0
1	A	411	LEU	2.9
1	B	318	ASP	2.8
1	A	250	ARG	2.8
1	A	316	LEU	2.7
1	A	312	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	317	LYS	2.5
1	A	246	SER	2.4
1	B	320	SER	2.4
1	A	222	GLN	2.4
1	A	249	ALA	2.3
1	B	432	ASP	2.3
1	A	221[A]	GLN	2.2
1	B	252	GLN	2.2
1	A	446	HIS	2.2
1	A	324	GLU	2.1
1	B	248	GLU	2.0
1	A	426	PHE	2.0
1	A	253	ARG	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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	O90	A	1	32/32	0.84	0.18	0.81	59,62,66,66	0
4	O90	B	1	32/32	0.87	0.18	0.08	61,63,68,70	0
3	SO4	D	1[B]	5/5	1.00	0.15	-	406,406,406,406	5
3	SO4	A	2[A]	5/5	0.99	0.15	-	40,40,41,42	5
3	SO4	A	2[B]	5/5	0.99	0.15	-	412,412,412,412	5
3	SO4	D	1[A]	5/5	1.00	0.15	-	34,35,35,36	5

6.5 Other polymers (i)

There are no such residues in this entry.