Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:30 AM GMT

PDB ID	:	3IPU
Title	:	X-ray structure of benzisoxazole urea synthetic agonist bound to the LXR-alpha
Authors	:	Fradera, X.; Vu, D.; Nimz, O.; Skene, R.; Hosfield, D.; Wijnands, R.; Cooke, A.J.; Haunso, A.; King, A.; Bennet, D.J.; McGuire, R.; Uitdehaag, J.C.M.
Deposited on	:	2009-08-18
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 (i) symbol.

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

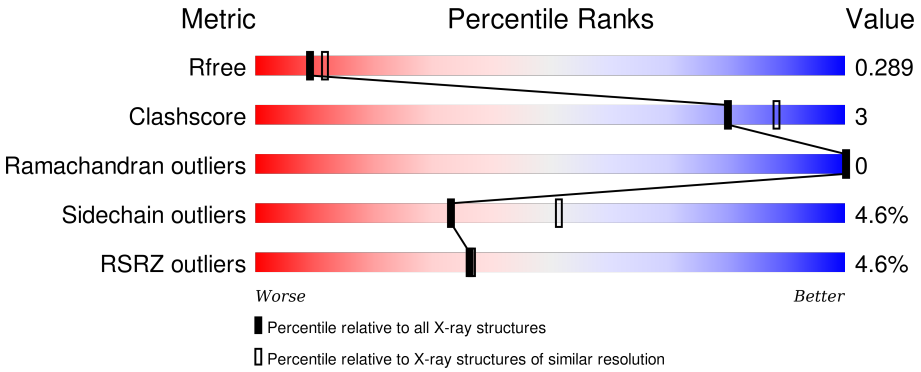
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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 <=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	4% 74% 9% • 16%
1	B	283	4% 73% 10% 17%
2	C	25	44% 16% 40%
2	D	25	4% 60% 40%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4297 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	238	Total	C	N	O	S	0	0	0
			1945	1241	344	353	7			
1	B	235	Total	C	N	O	S	12	1	0
			1927	1229	340	351	7			

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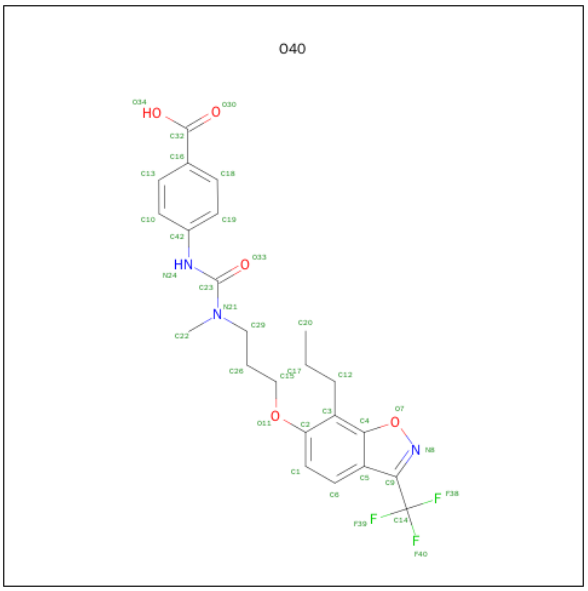
Chain	Residue	Modelled	Actual	Comment	Reference
B	173	HIS	-	EXPRESSION TAG	UNP Q13133
B	174	GLN	-	EXPRESSION TAG	UNP Q13133
B	175	HIS	-	EXPRESSION TAG	UNP Q13133
B	176	GLN	-	EXPRESSION TAG	UNP Q13133
B	177	HIS	-	EXPRESSION TAG	UNP Q13133
B	178	GLN	-	EXPRESSION TAG	UNP Q13133
B	179	GLN	-	EXPRESSION TAG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

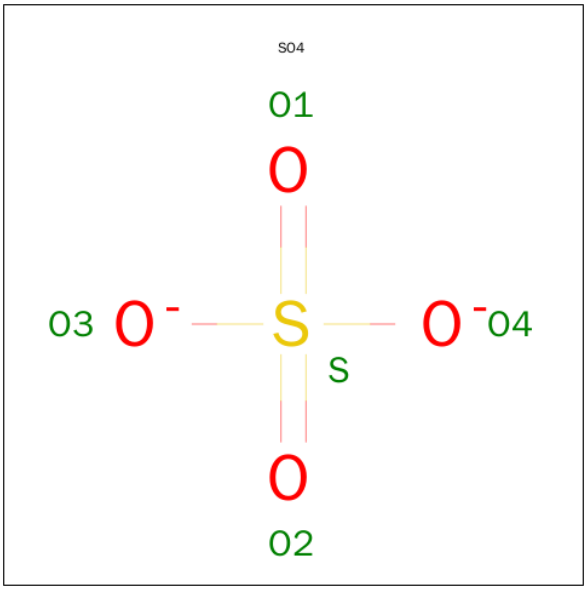
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	4	0	0
			131	82	27	22			
2	D	15	Total	C	N	O	4	0	0
			131	82	27	22			

- Molecule 3 is 4-{[METHYL(3-{[7-PROPYL-3-(TRIFLUOROMETHYL)-1,2-BENZISOXAZOL-6-YL]OXY}PROPYL)CARBAMOYL]AMINO}BENZOIC ACID (three-letter code: O40) (formula: $C_{23}H_{24}F_3N_3O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			34	23	3	3	5		
3	B	1	Total	C	F	N	O	0	0
			34	23	3	3	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

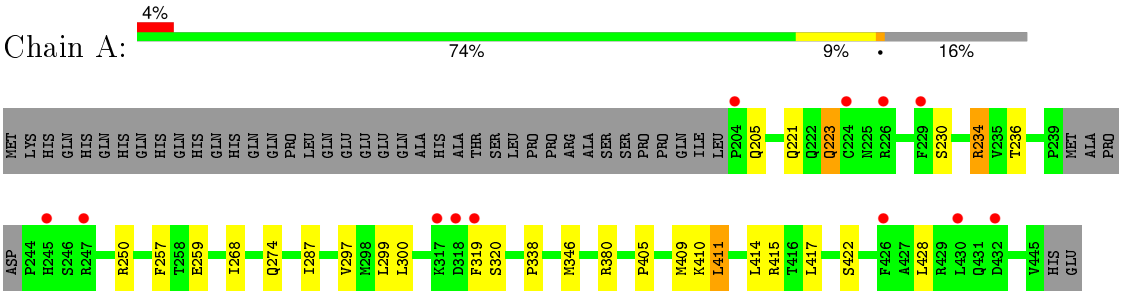
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	35	Total O 35 35	0	0
5	B	42	Total O 42 42	0	0
5	C	7	Total O 7 7	0	0
5	D	1	Total O 1 1	0	0

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.

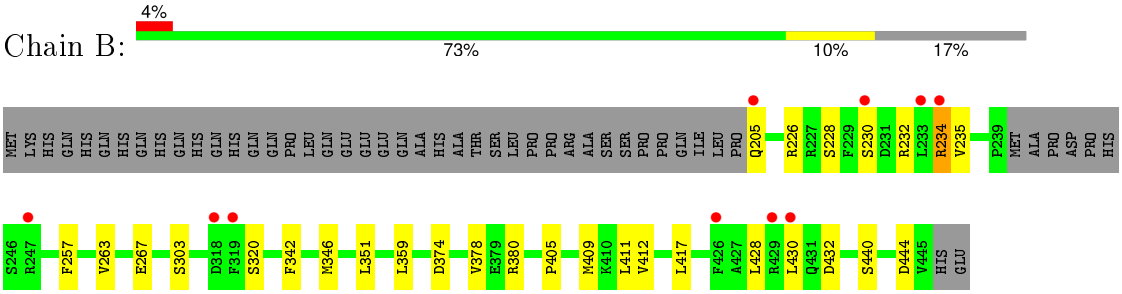
- Molecule 1: Oxysterols receptor LXR-alpha

Chain A:



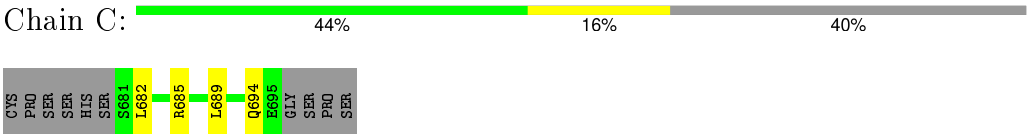
- Molecule 1: Oxysterols receptor LXR-alpha

Chain B:



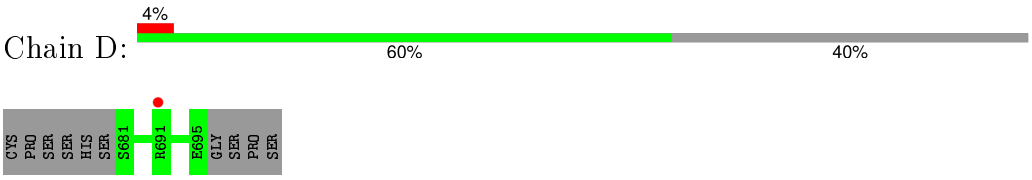
- Molecule 2: Nuclear receptor coactivator 1

Chain C:



- Molecule 2: Nuclear receptor coactivator 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	125.18Å 125.18Å 92.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.66 – 2.40 29.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.66-2.40) 90.3 (29.66-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.291 0.235 , 0.289	Depositor DCC
R_{free} test set	1375 reflections (5.46%)	DCC
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.57$, $< L^2 > = 0.41$	Xtriage
Outliers	5 of 26580 reflections (0.019%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4297	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.99 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.5903e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: O40, SO4

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	0.53	0/1987	0.59	0/2686
1	B	0.57	1/1969 (0.1%)	0.63	1/2661 (0.0%)
2	C	0.57	0/132	0.76	0/175
2	D	0.52	0/132	0.67	0/175
All	All	0.55	1/4220 (0.0%)	0.62	1/5697 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	226	ARG	CA-CB	5.41	1.65	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	226	ARG	CB-CA-C	-5.56	99.27	110.40

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	1945	0	1951	13	0
1	B	1927	0	1936	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	131	0	139	3	0
2	D	131	0	139	0	0
3	A	34	0	23	0	0
3	B	34	0	23	0	0
4	B	5	0	0	0	0
4	C	5	0	0	1	0
5	A	35	0	0	0	0
5	B	42	0	0	0	0
5	C	7	0	0	0	0
5	D	1	0	0	0	0
All	All	4297	0	4211	28	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 3.

All (28) 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:346:MET:HE2	1:A:410:LYS:HD2	1.83	0.60
2:C:694:GLN:NE2	4:C:802:SO4:O4	2.38	0.53
1:B:232:ARG:O	1:B:235:VAL:HG22	2.08	0.53
1:B:232:ARG:HG2	1:B:263:VAL:HG11	1.90	0.53
1:A:411:LEU:HD12	1:A:414:LEU:HD12	1.91	0.52
1:B:346:MET:CE	1:B:351:LEU:HD22	2.40	0.52
1:B:230:SER:O	1:B:234:ARG:HD3	2.10	0.51
1:A:236:THR:HG23	1:A:259:GLU:OE1	2.11	0.50
1:B:440:SER:OG	1:B:444:ASP:OD2	2.22	0.48
1:B:374:ASP:O	1:B:378:VAL:HG23	2.14	0.47
1:B:359:LEU:HD22	1:B:411:LEU:HD11	1.96	0.47
1:B:346:MET:HE3	1:B:351:LEU:HD22	1.97	0.46
2:C:682:LEU:HD23	2:C:685:ARG:HH22	1.81	0.46
1:A:338:PRO:HB2	1:A:417:LEU:HD21	1.98	0.45
1:B:342:PHE:HB2	1:B:417:LEU:HD11	1.99	0.45
1:B:303:SER:OG	1:B:346:MET:HG2	2.17	0.44
1:A:300:LEU:HG	1:A:414:LEU:HD11	1.99	0.44
1:A:230:SER:O	1:A:234:ARG:HD2	2.18	0.44
1:A:299:LEU:HD22	1:A:417:LEU:HD13	2.01	0.43
1:A:405:PRO:O	1:A:409:MET:HG2	2.19	0.42
1:B:405:PRO:O	1:B:409:MET:HG2	2.19	0.42
1:A:268:ILE:HG12	1:A:297:VAL:HG11	2.01	0.42
1:A:417:LEU:HA	1:A:417:LEU:HD23	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ARG:HG2	1:B:412:VAL:HG13	2.02	0.41
1:A:223:GLN:HE21	1:A:223:GLN:HA	1.86	0.41
1:B:232:ARG:CG	1:B:263:VAL:HG11	2.51	0.41
1:B:228:SER:OG	1:B:267:GLU:OE2	2.35	0.41
1:A:287:ILE:HG23	2:C:689:LEU:HD23	2.02	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	234/283 (83%)	229 (98%)	5 (2%)	0	100	100
1	B	232/283 (82%)	228 (98%)	4 (2%)	0	100	100
2	C	13/25 (52%)	12 (92%)	1 (8%)	0	100	100
2	D	13/25 (52%)	12 (92%)	1 (8%)	0	100	100
All	All	492/616 (80%)	481 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/257 (84%)	203 (94%)	13 (6%)	24	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	214/257 (83%)	206 (96%)	8 (4%)	41 62
2	C	15/24 (62%)	15 (100%)	0	100 100
2	D	15/24 (62%)	15 (100%)	0	100 100
All	All	460/562 (82%)	439 (95%)	21 (5%)	33 51

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	221	GLN
1	A	223	GLN
1	A	234	ARG
1	A	250	ARG
1	A	257	PHE
1	A	274	GLN
1	A	319	PHE
1	A	320	SER
1	A	380	ARG
1	A	411	LEU
1	A	422	SER
1	A	428	LEU
1	B	205	GLN
1	B	234	ARG
1	B	257	PHE
1	B	320	SER
1	B	380	ARG
1	B	428	LEU
1	B	430	LEU
1	B	432	ASP

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

Mol	Chain	Res	Type
1	A	205	GLN
1	A	223	GLN
1	A	266	GLN
1	B	266	GLN
1	B	307	ASN
1	B	332	GLN
1	B	375	GLN

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

4 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	$\#\|Z\| > 2$
3	O40	A	801	-	27,36,36	1.19	3 (11%)	37,51,51	2.07	8 (21%)
3	O40	B	801	-	27,36,36	1.18	3 (11%)	37,51,51	1.71	7 (18%)
4	SO4	B	802	-	4,4,4	0.33	0	6,6,6	0.17	0
4	SO4	C	802	-	4,4,4	0.23	0	6,6,6	0.45	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
3	O40	A	801	-	-	0/24/28/28	0/2/3/3
3	O40	B	801	-	-	0/24/28/28	0/2/3/3
4	SO4	B	802	-	-	0/0/0/0	0/0/0/0
4	SO4	C	802	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	O40	C23-N24	-2.78	1.32	1.36
3	B	801	O40	C42-N24	-2.60	1.36	1.41
3	B	801	O40	C23-N24	-2.27	1.32	1.36
3	A	801	O40	C42-N24	-2.14	1.37	1.41
3	B	801	O40	C2-C3	2.42	1.41	1.38
3	A	801	O40	C2-C3	2.53	1.41	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	O40	F39-C14-C9	-5.46	104.26	112.02
3	B	801	O40	F38-C14-C9	-4.89	105.07	112.02
3	A	801	O40	C9-C5-C4	-4.19	99.85	107.51
3	B	801	O40	C9-C5-C4	-4.00	100.19	107.51
3	A	801	O40	C1-C6-C5	-3.84	116.09	121.13
3	B	801	O40	C1-C6-C5	-3.73	116.23	121.13
3	A	801	O40	O33-C23-N24	-3.06	118.04	124.27
3	A	801	O40	F38-C14-C9	-3.00	107.76	112.02
3	B	801	O40	O33-C23-N24	-2.65	118.87	124.27
3	B	801	O40	O33-C23-N21	-2.21	118.33	122.18
3	A	801	O40	O33-C23-N21	-2.13	118.47	122.18
3	B	801	O40	C6-C5-C4	3.09	123.77	117.44
3	B	801	O40	C14-C9-N8	3.52	123.99	119.68
3	A	801	O40	C6-C5-C4	3.65	124.91	117.44
3	A	801	O40	C14-C9-N8	5.69	126.65	119.68

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	C	802	SO4	1	0

5.7 Other polymers (i)

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, 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	238/283 (84%)	0.05	12 (5%) 32 33	16, 28, 58, 68	0
1	B	235/283 (83%)	-0.07	10 (4%) 39 40	17, 28, 48, 54	2 (0%)
2	C	15/25 (60%)	-0.46	0 100 100	20, 25, 33, 38	1 (6%)
2	D	15/25 (60%)	-0.31	1 (6%) 21 21	22, 26, 36, 40	1 (6%)
All	All	503/616 (81%)	-0.03	23 (4%) 36 37	16, 28, 53, 68	4 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	ASP	5.1
1	A	245	HIS	4.7
1	B	318	ASP	4.1
1	B	319	PHE	3.8
1	A	319	PHE	3.7
1	A	318	ASP	3.6
1	A	317	LYS	3.5
1	A	229	PHE	3.5
1	B	233	LEU	3.0
1	A	430	LEU	3.0
1	A	426	PHE	2.7
1	B	247	ARG	2.6
2	D	691	ARG	2.6
1	B	230	SER	2.6
1	A	224	CYS	2.4
1	A	204	PRO	2.4
1	A	226	ARG	2.3
1	B	426	PHE	2.2
1	A	247	ARG	2.1
1	B	430	LEU	2.1
1	B	234	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	429	ARG	2.0
1	B	205	GLN	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
3	O40	A	801	34/34	0.86	0.18	0.33	39,41,45,48	0
3	O40	B	801	34/34	0.92	0.16	0.03	34,36,41,44	0
4	SO4	B	802	5/5	0.99	0.08	-	18,20,20,21	5
4	SO4	C	802	5/5	0.99	0.07	-	14,14,16,17	5

6.5 Other polymers (i)

There are no such residues in this entry.