WORLDWIDE

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:36 AM GMT

PDB ID	:	3FAL
Title	:	humanRXR alpha & mouse LXR alpha complexed with Retenoic acid and GSK2186
Authors	:	Chao, E.Y.; Caravella, J.A.; Watson, M.A.; Campobasso, N.; Ghisletti, S.; Billin, A.N.; Galardi, C.; Willson, T.M.; Zuercher, W.J.; Collins, J.L.
Deposited on	:	2008-11-17
Resolution	:	2.36 Å(reported)

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 (i)

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

The reported resolution of this entry is 2.36 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.
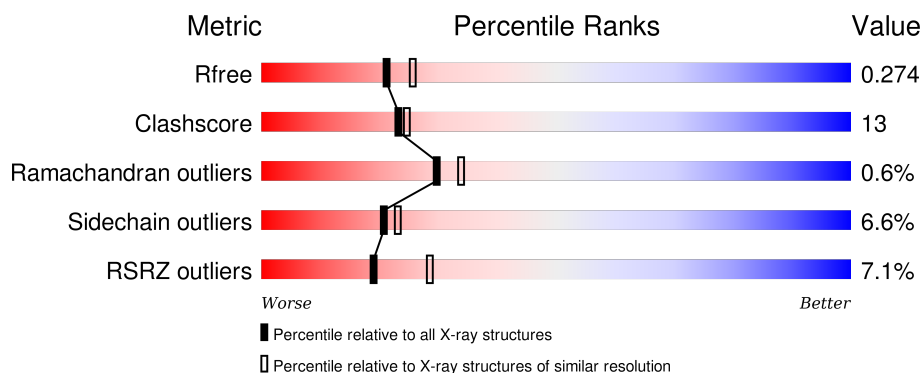
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	242	13% / 50% 28% • 19%
1	C	242	% / 64% 15% • 18%
2	B	266	2% / 66% 22% • 11%
2	D	266	8% / 62% 27% • 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7094 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total 1529	C 977	N 268	O 274	S 10	0	0	0
1	C	198	Total 1539	C 983	N 270	O 276	S 10	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	MET	-	EXPRESSION TAG	UNP P19793
A	222	LYS	-	EXPRESSION TAG	UNP P19793
A	223	LYS	-	EXPRESSION TAG	UNP P19793
A	224	GLY	-	EXPRESSION TAG	UNP P19793
C	221	MET	-	EXPRESSION TAG	UNP P19793
C	222	LYS	-	EXPRESSION TAG	UNP P19793
C	223	LYS	-	EXPRESSION TAG	UNP P19793
C	224	GLY	-	EXPRESSION TAG	UNP P19793

- Molecule 2 is a protein called Oxysterols receptor LXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total 1936	C 1235	N 339	O 355	S 7	0	0	0
2	D	242	Total 1964	C 1253	N 343	O 361	S 7	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	180	MET	-	EXPRESSION TAG	UNP Q9Z0Y9
B	181	ARG	-	EXPRESSION TAG	UNP Q9Z0Y9
B	182	GLY	-	EXPRESSION TAG	UNP Q9Z0Y9
B	183	SER	-	EXPRESSION TAG	UNP Q9Z0Y9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	184	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
B	185	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
B	186	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
B	187	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
B	188	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
B	189	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
B	190	GLY	-	EXPRESSION TAG	UNP Q9Z0Y9
B	191	MET	-	EXPRESSION TAG	UNP Q9Z0Y9
B	192	ALA	-	EXPRESSION TAG	UNP Q9Z0Y9
B	193	SER	-	EXPRESSION TAG	UNP Q9Z0Y9
B	194	LEU	-	EXPRESSION TAG	UNP Q9Z0Y9
B	195	VAL	-	EXPRESSION TAG	UNP Q9Z0Y9
B	196	PRO	-	EXPRESSION TAG	UNP Q9Z0Y9
B	197	ARG	-	EXPRESSION TAG	UNP Q9Z0Y9
B	198	GLY	-	EXPRESSION TAG	UNP Q9Z0Y9
B	199	SER	-	EXPRESSION TAG	UNP Q9Z0Y9
B	399	PRO	ARG	SEE REMARK 999	UNP Q9Z0Y9
D	180	MET	-	EXPRESSION TAG	UNP Q9Z0Y9
D	181	ARG	-	EXPRESSION TAG	UNP Q9Z0Y9
D	182	GLY	-	EXPRESSION TAG	UNP Q9Z0Y9
D	183	SER	-	EXPRESSION TAG	UNP Q9Z0Y9
D	184	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
D	185	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
D	186	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
D	187	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
D	188	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
D	189	HIS	-	EXPRESSION TAG	UNP Q9Z0Y9
D	190	GLY	-	EXPRESSION TAG	UNP Q9Z0Y9
D	191	MET	-	EXPRESSION TAG	UNP Q9Z0Y9
D	192	ALA	-	EXPRESSION TAG	UNP Q9Z0Y9
D	193	SER	-	EXPRESSION TAG	UNP Q9Z0Y9
D	194	LEU	-	EXPRESSION TAG	UNP Q9Z0Y9
D	195	VAL	-	EXPRESSION TAG	UNP Q9Z0Y9
D	196	PRO	-	EXPRESSION TAG	UNP Q9Z0Y9
D	197	ARG	-	EXPRESSION TAG	UNP Q9Z0Y9
D	198	GLY	-	EXPRESSION TAG	UNP Q9Z0Y9
D	199	SER	-	EXPRESSION TAG	UNP Q9Z0Y9
D	399	PRO	ARG	SEE REMARK 999	UNP Q9Z0Y9

- Molecule 3 is RETINOIC ACID (three-letter code: REA) (formula: $C_{20}H_{28}O_2$).

REA
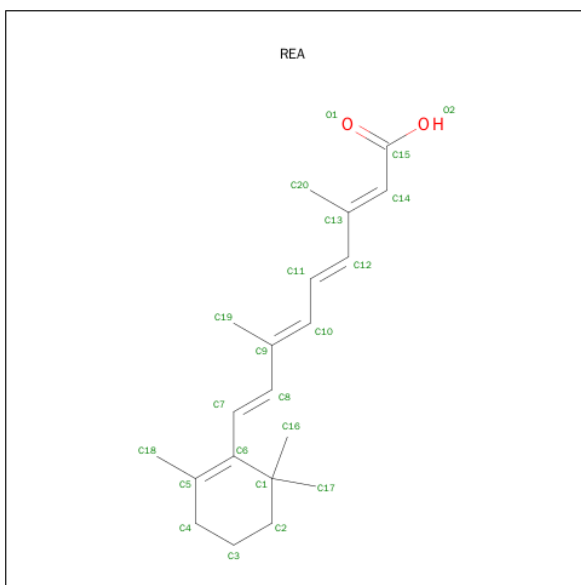
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	20	2		
3	C	1	Total	C	O	0	0
			22	20	2		

- Molecule 4 is 2-{4-[BUTYL(3-CHLORO-4,5-DIMETHOXYBENZYL)AMINO]PHENYL}-1,1,1,3,3,3-HEXAFLUOROPROPAN-2-OL (three-letter code: LO2) (formula: $C_{22}H_{24}ClF_6NO_3$).

LO2
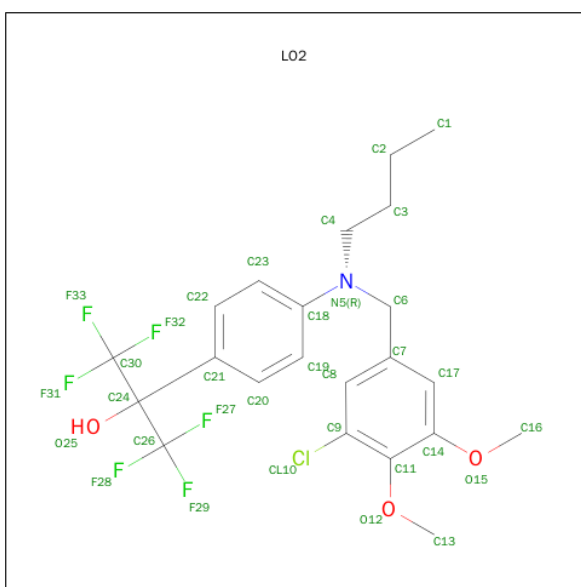
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	Cl	F	N	O	0	0
			33	22	1	6	1	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
4	D	1	33	22	1	6	1	3	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	5	Total 5	O 5	0	0
5	C	4	Total 4	O 4	0	0
5	D	7	Total 7	O 7	0	0

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.
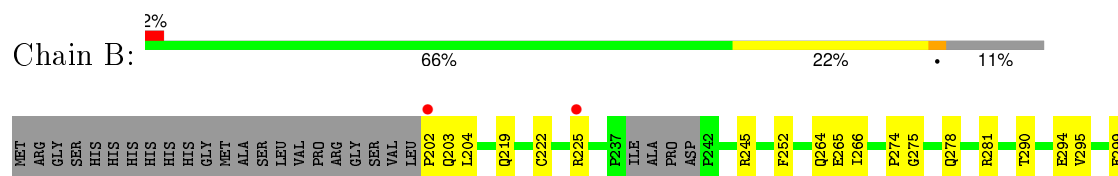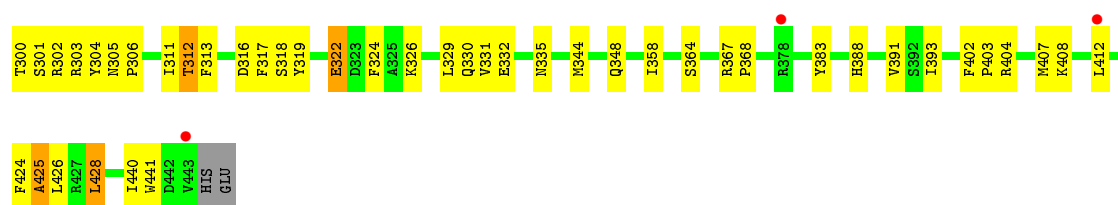
- Molecule 1: Retinoic acid receptor RXR-alpha
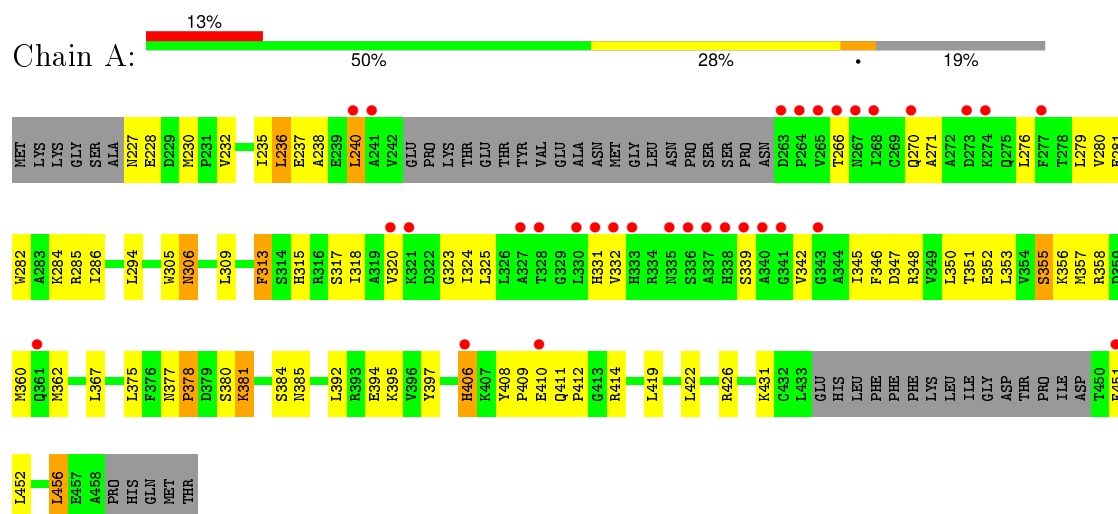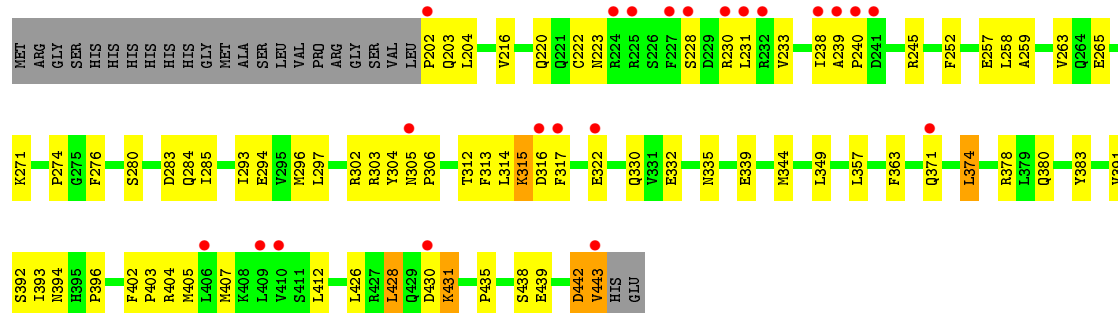
Chain A:

- Molecule 1: Retinoic acid receptor RXR-alpha

Chain C:

- Molecule 2: Oxysterols receptor LXR-alpha

Chain B:
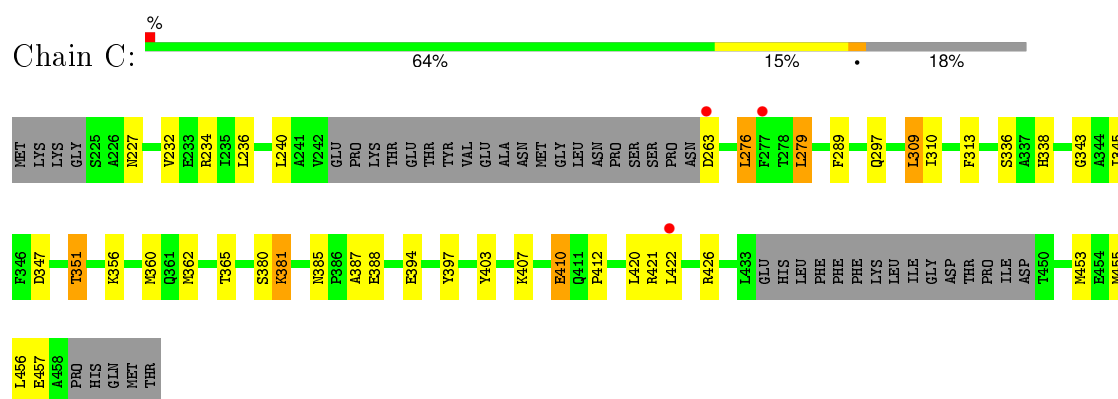
• Molecule 2: Oxysterols receptor LXR-alpha

4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.21Å 90.00Å 101.31Å 90.00° 111.88° 90.00°	Depositor
Resolution (Å)	42.34 – 2.36 42.34 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.5 (42.34-2.36) 98.5 (42.34-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.18 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.219 , 0.278 0.220 , 0.274	Depositor DCC
R_{free} test set	2106 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning [2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	0 of 41749 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7094	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LO2, REA

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	0.34	0/1555	0.51	0/2100
1	C	0.42	0/1565	0.58	0/2114
2	B	0.47	0/1976	0.57	1/2673 (0.0%)
2	D	0.52	0/2006	0.56	1/2718 (0.0%)
All	All	0.45	0/7102	0.56	2/9605 (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})
2	B	202	PRO	N-CA-CB	7.24	111.99	103.30
2	D	202	PRO	N-CA-CB	7.02	111.72	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1529	0	1565	56	0
1	C	1539	0	1572	30	0
2	B	1936	0	1939	47	0
2	D	1964	0	1966	63	0
3	A	22	0	27	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	22	0	27	3	0
4	B	33	0	24	4	0
4	D	33	0	24	5	0
5	B	5	0	0	0	0
5	C	4	0	0	0	0
5	D	7	0	0	0	0
All	All	7094	0	7144	190	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 13.

The worst 5 of 190 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)
3:A:501:REA:H201	3:A:501:REA:O2	1.67	0.92
2:D:203:GLN:HA	2:D:393:ILE:HD11	1.52	0.88
4:B:1:LO2:H13A	4:B:1:LO2:O15	1.72	0.88
3:C:501:REA:O2	3:C:501:REA:H201	1.73	0.86
1:C:227:ASN:HD21	1:C:232:VAL:HB	1.39	0.84

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	190/242 (78%)	176 (93%)	14 (7%)	0	100	100
1	C	192/242 (79%)	186 (97%)	6 (3%)	0	100	100
2	B	234/266 (88%)	226 (97%)	7 (3%)	1 (0%)	39	46
2	D	240/266 (90%)	228 (95%)	8 (3%)	4 (2%)	11	9
All	All	856/1016 (84%)	816 (95%)	35 (4%)	5 (1%)	30	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	425	ALA
2	D	315	LYS
2	D	431	LYS
2	D	228	SER
2	D	442	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	164/208 (79%)	145 (88%)	19 (12%)	7	6
1	C	164/208 (79%)	145 (88%)	19 (12%)	7	6
2	B	215/239 (90%)	209 (97%)	6 (3%)	51	65
2	D	218/239 (91%)	212 (97%)	6 (3%)	51	65
All	All	761/894 (85%)	711 (93%)	50 (7%)	21	23

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	322	GLU
1	C	240	LEU
2	D	374	LEU
2	B	388	HIS
1	C	234	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	348	GLN
2	D	335	ASN
1	C	335	ASN
1	A	385	ASN
1	C	227	ASN

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)

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	REA	A	501	-	19,22,22	1.15	1 (5%)	26,30,30	1.65	6 (23%)
4	LO2	B	1	-	34,34,34	0.84	0	50,51,51	1.45	4 (8%)
3	REA	C	501	-	19,22,22	1.11	1 (5%)	26,30,30	1.58	5 (19%)
4	LO2	D	1	-	34,34,34	0.86	1 (2%)	50,51,51	1.56	4 (8%)

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	REA	A	501	-	-	0/13/32/32	0/1/1/1
4	LO2	B	1	-	-	0/40/40/40	0/2/2/2
3	REA	C	501	-	-	0/13/32/32	0/1/1/1
4	LO2	D	1	-	-	0/40/40/40	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	REA	C1-C6	-3.26	1.49	1.53
3	C	501	REA	C1-C6	-3.00	1.49	1.53
4	D	1	LO2	C24-C21	-2.07	1.50	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1	LO2	C16-O15-C14	-8.08	105.28	117.54
4	B	1	LO2	C16-O15-C14	-6.34	107.93	117.54
3	C	501	REA	C7-C8-C9	-4.46	119.41	126.22
4	D	1	LO2	C4-N5-C18	-3.81	115.36	121.10
3	A	501	REA	C18-C5-C6	-3.62	121.05	124.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	REA	4	0
4	B	1	LO2	4	0
3	C	501	REA	3	0
4	D	1	LO2	5	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	196/242 (80%)	1.00	32 (16%)	2	4	26, 51, 66, 80	0
1	C	198/242 (81%)	0.38	3 (1%)	76	85	18, 30, 47, 58	0
2	B	238/266 (89%)	0.38	5 (2%)	67	79	20, 32, 52, 71	0
2	D	242/266 (90%)	0.66	22 (9%)	11	18	20, 34, 69, 91	0
All	All	874/1016 (86%)	0.60	62 (7%)	19	28	18, 35, 62, 91	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	202	PRO	7.4
2	D	238	ILE	6.5
2	D	443	VAL	6.2
2	D	231	LEU	6.2
2	D	230	ARG	6.0

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	REA	A	501	22/22	0.86	0.20	0.10	44,51,55,56	0
3	REA	C	501	22/22	0.94	0.14	-0.16	25,31,38,41	0
4	LO2	B	1	33/33	0.95	0.13	-0.49	21,27,35,45	0
4	LO2	D	1	33/33	0.96	0.13	-0.82	27,34,41,55	0

6.5 Other polymers (i)

There are no such residues in this entry.