Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:27 PM GMT

PDB ID	:	4F2A
Title	:	Crystal structure of cholestryl esters transfer protein in complex with inhibitors
Authors	:	Liu, S.; Qiu, X.
Deposited on	:	2012-05-07
Resolution	:	3.11 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:

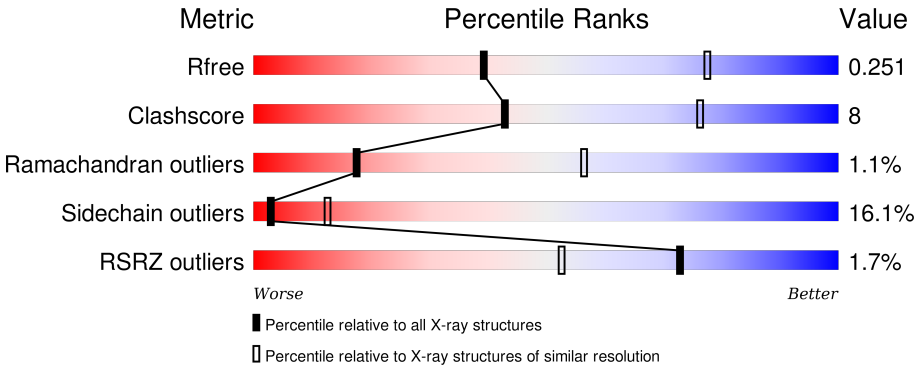
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.11 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	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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	476	2% 68% 28%

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
3	2OB	A	605	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2OB	A	606	-	-	-	X
4	PCW	A	607	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3967 atoms, of which 21 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 Cholesteryl ester transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3712	2390	603	702	17			

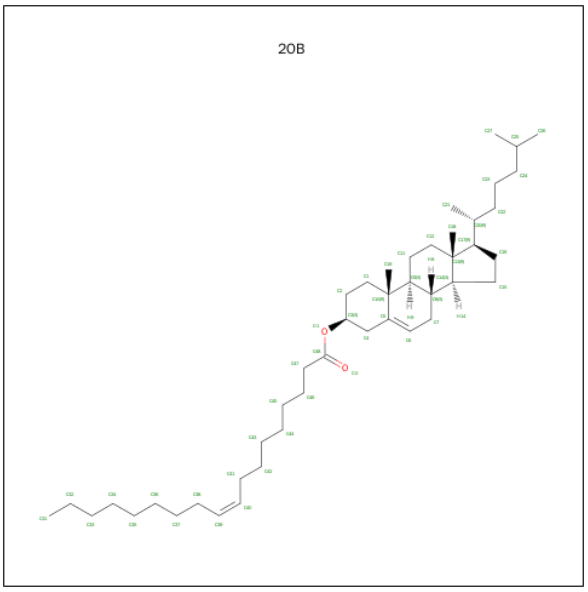
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	CYS	ENGINEERED MUTATION	UNP P11597
A	88	ASP	ASN	ENGINEERED MUTATION	UNP P11597
A	131	ALA	CYS	ENGINEERED MUTATION	UNP P11597
A	240	ASP	ASN	ENGINEERED MUTATION	UNP P11597
A	341	ASP	ASN	ENGINEERED MUTATION	UNP P11597
A	405	ILE	VAL	ENGINEERED MUTATION	UNP P11597

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

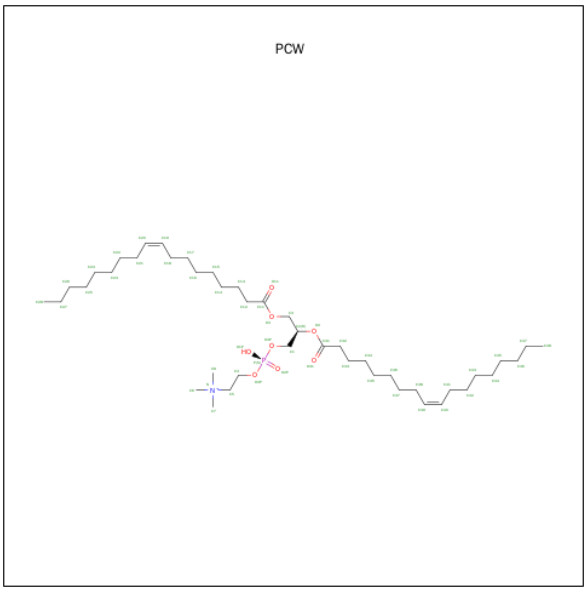
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 3 is CHOLESTERYL OLEATE (three-letter code: 2OB) (formula: $C_{45}H_{78}O_2$).



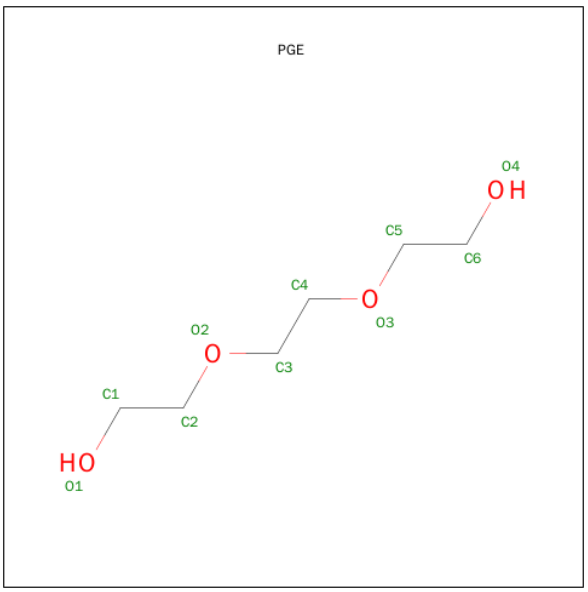
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 35 33 2	0	0
3	A	1	Total C O 47 45 2	0	0

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 54 44 1 8 1	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

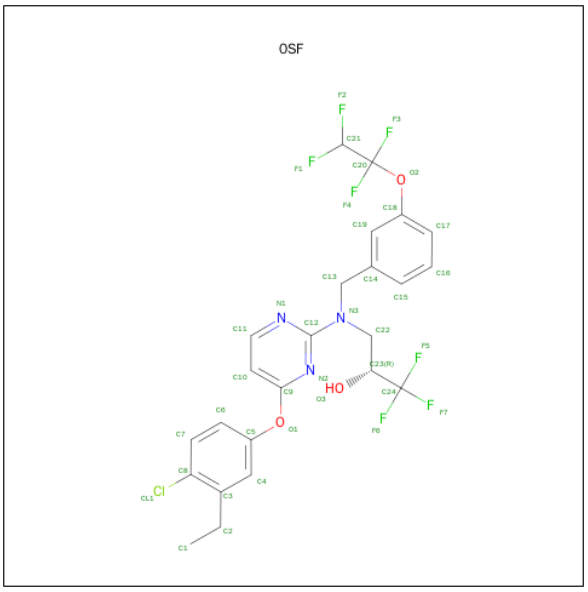


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is (2R)-3-{[4-(4-CHLORO-3-ETHYLPHENOXY)PYRIMIDIN-2-YL][3-(1,1,2,2-TETRAFLUOROETHOXY)BENZYL]AMINO}-1,1,1-TRIFLUOROPROPAN-2-OL (three-letter code: 0SF) (formula: $C_{24}H_{21}ClF_7N_3O_3$).



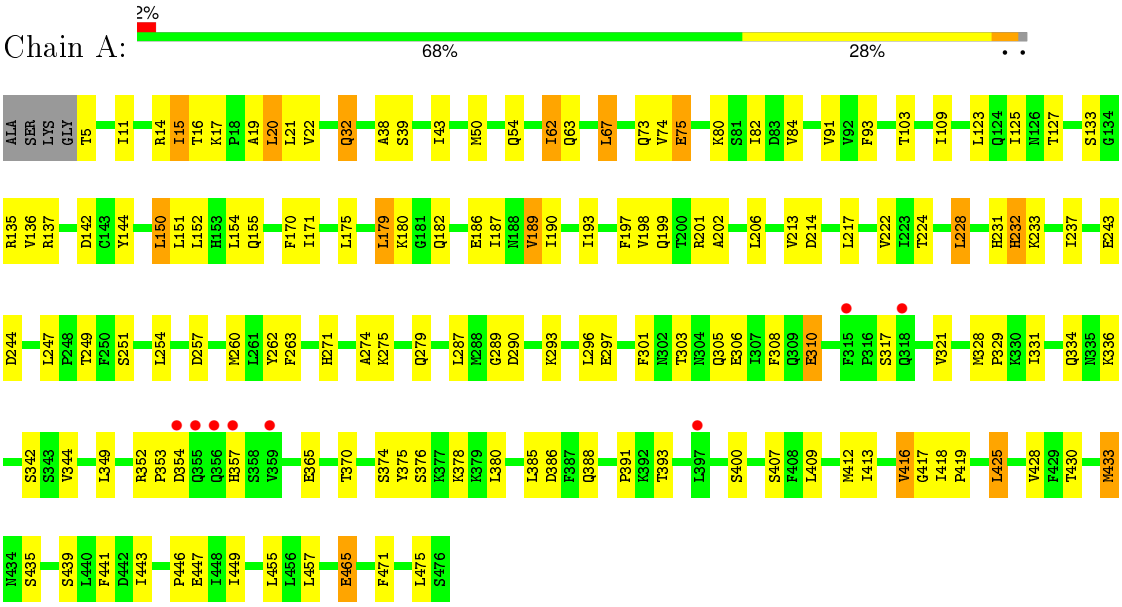
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	F	H	N	O		
7	A	1	59	24	1	7	21	3	3	21	0

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: Cholesteryl ester transfer protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.77Å 69.92Å 187.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.88 – 3.11 38.68 – 3.11	Depositor EDS
% Data completeness (in resolution range)	75.5 (38.88-3.11) 75.9 (38.68-3.11)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.183 , 0.239 0.203 , 0.251	Depositor DCC
R_{free} test set	614 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	68.4	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 72.0	EDS
Estimated twinning fraction	0.032 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 12746 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3967	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: PGE, NAG, CL, 2OB, 0SF, PCW, FUC, MAN

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	0.51	0/3790	0.78	0/5138

There are no bond length outliers.

There are no bond angle outliers.

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	3712	0	3724	64	0
2	A	49	0	43	0	0
3	A	82	0	131	6	0
4	A	54	0	84	4	0
5	A	10	0	14	0	0
6	A	1	0	0	0	0
7	A	38	21	21	2	0
All	All	3946	21	4017	65	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 8.

All (65) 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:198:VAL:HG11	3:A:605:2OB:H191	1.68	0.74
4:A:607:PCW:O31	4:A:607:PCW:H12	1.90	0.70
1:A:305:GLN:HB2	1:A:308:PHE:HD1	1.57	0.68
1:A:222:VAL:HG23	1:A:231:HIS:HE1	1.61	0.66
1:A:38:ALA:HB1	1:A:182:GLN:HB3	1.76	0.66
1:A:417:GLY:HA2	3:A:606:2OB:H361	1.79	0.65
1:A:136:VAL:H	1:A:199:GLN:HE22	1.44	0.64
1:A:15:ILE:HD12	1:A:19:ALA:HB3	1.79	0.63
1:A:14:ARG:HB3	1:A:262:TYR:HB2	1.82	0.62
1:A:412:MET:O	1:A:416:VAL:HG23	2.01	0.61
1:A:62:ILE:HD12	1:A:62:ILE:H	1.65	0.59
1:A:15:ILE:CD1	1:A:19:ALA:HB3	2.31	0.59
1:A:428:VAL:HG11	4:A:607:PCW:H32	1.84	0.59
1:A:233:LYS:HA	1:A:247:LEU:HD21	1.85	0.58
1:A:32:GLN:HG3	1:A:67:LEU:HD22	1.85	0.58
1:A:263:PHE:HB2	1:A:457:LEU:HB2	1.84	0.58
1:A:425:LEU:HD13	4:A:607:PCW:H121	1.86	0.57
1:A:352:ARG:HB3	1:A:353:PRO:HD2	1.86	0.57
1:A:305:GLN:HB2	1:A:308:PHE:CD1	2.40	0.54
1:A:425:LEU:CD1	4:A:607:PCW:H31	2.38	0.54
1:A:93:PHE:CZ	1:A:179:LEU:HD21	2.43	0.54
1:A:150:LEU:HD21	1:A:175:LEU:HD23	1.92	0.52
1:A:17:LYS:HE3	1:A:75:GLU:HA	1.91	0.52
1:A:11:ILE:HG21	7:A:610:0SF:H9	1.92	0.52
1:A:136:VAL:H	1:A:199:GLN:NE2	2.06	0.51
1:A:43:ILE:HG21	1:A:171:ILE:HG23	1.93	0.50
1:A:67:LEU:HD12	1:A:91:VAL:HG13	1.94	0.49
1:A:293:LYS:HE3	1:A:303:THR:HG21	1.95	0.49
1:A:136:VAL:HB	1:A:217:LEU:HD11	1.96	0.48
1:A:54:GLN:HB2	1:A:103:THR:HG23	1.96	0.48
1:A:287:LEU:HB2	1:A:321:VAL:HG12	1.96	0.48
1:A:193:ILE:HG21	1:A:475:LEU:HD21	1.95	0.48
1:A:251:SER:HB3	1:A:254:LEU:HD13	1.97	0.47
1:A:20:LEU:HB3	1:A:74:VAL:HG11	1.96	0.47
1:A:301:PHE:HB3	1:A:308:PHE:CZ	2.50	0.47
1:A:125:ILE:HG12	1:A:187:ILE:HD13	1.97	0.47
1:A:19:ALA:HB2	1:A:260:MET:HB3	1.97	0.46
1:A:198:VAL:HG21	3:A:605:2OB:H112	1.97	0.46
1:A:186:GLU:O	1:A:190:ILE:HG13	2.16	0.46
1:A:214:ASP:HB2	1:A:237:ILE:HD11	1.98	0.44
1:A:430:THR:HA	1:A:433:MET:HG3	1.99	0.44
1:A:413:ILE:O	1:A:417:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ALA:HB1	7:A:610:0SF:C4	2.47	0.44
1:A:142:ASP:HB3	1:A:144:TYR:OH	2.18	0.44
1:A:274:ALA:HB1	1:A:329:PRO:HD2	2.00	0.44
1:A:175:LEU:HG	1:A:179:LEU:HD12	1.99	0.43
1:A:365:GLU:HB3	1:A:391:PRO:HA	2.00	0.43
1:A:418:ILE:HB	1:A:419:PRO:HD3	1.99	0.43
1:A:375:TYR:HB3	1:A:446:PRO:HG2	2.00	0.43
1:A:84:VAL:HG21	3:A:605:2OB:H262	2.00	0.43
1:A:16:THR:HG21	1:A:257:ASP:HA	2.01	0.43
1:A:447:GLU:HB3	1:A:449:ILE:HD11	2.02	0.42
1:A:232:HIS:CD2	1:A:232:HIS:N	2.88	0.42
1:A:336:LYS:HD2	1:A:370:THR:HG21	2.02	0.41
1:A:15:ILE:HD13	3:A:605:2OB:H6	2.03	0.41
1:A:197:PHE:CE1	1:A:201:ARG:HD3	2.55	0.41
1:A:15:ILE:HG12	3:A:605:2OB:H71	2.01	0.41
1:A:275:LYS:HA	1:A:328:MET:HG3	2.02	0.41
1:A:136:VAL:N	1:A:199:GLN:HE22	2.14	0.41
1:A:354:ASP:HB3	1:A:357:HIS:CD2	2.55	0.41
1:A:15:ILE:HG23	1:A:228:LEU:HG	2.03	0.41
1:A:189:VAL:CG2	1:A:190:ILE:N	2.84	0.41
1:A:125:ILE:HG21	1:A:187:ILE:HG21	2.02	0.41
1:A:378:LYS:HD3	1:A:439:SER:HA	2.03	0.41
1:A:15:ILE:HD11	1:A:20:LEU:HD13	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	470/476 (99%)	426 (91%)	39 (8%)	5 (1%)	17 56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	ILE
1	A	289	GLY
1	A	206	LEU
1	A	310	GLU
1	A	465	GLU

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	422/424 (100%)	354 (84%)	68 (16%)	3 13

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	15	ILE
1	A	20	LEU
1	A	21	LEU
1	A	22	VAL
1	A	32	GLN
1	A	39	SER
1	A	50	MET
1	A	62	ILE
1	A	63	GLN
1	A	67	LEU
1	A	73	GLN
1	A	75	GLU
1	A	80	LYS
1	A	82	ILE
1	A	123	LEU
1	A	127	THR
1	A	133	SER
1	A	135	ARG
1	A	137	ARG
1	A	150	LEU
1	A	151	LEU

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Mol	Chain	Res	Type
1	A	152	LEU
1	A	154	LEU
1	A	155	GLN
1	A	170	PHE
1	A	179	LEU
1	A	180	LYS
1	A	189	VAL
1	A	213	VAL
1	A	224	THR
1	A	228	LEU
1	A	232	HIS
1	A	243	GLU
1	A	244	ASP
1	A	249	THR
1	A	271	HIS
1	A	279	GLN
1	A	290	ASP
1	A	296	LEU
1	A	297	GLU
1	A	306	GLU
1	A	310	GLU
1	A	317	SER
1	A	331	ILE
1	A	334	GLN
1	A	342	SER
1	A	344	VAL
1	A	349	LEU
1	A	374	SER
1	A	376	SER
1	A	380	LEU
1	A	385	LEU
1	A	386	ASP
1	A	388	GLN
1	A	393	THR
1	A	400	SER
1	A	407	SER
1	A	409	LEU
1	A	416	VAL
1	A	425	LEU
1	A	433	MET
1	A	435	SER
1	A	441	PHE

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Mol	Chain	Res	Type
1	A	443	ILE
1	A	455	LEU
1	A	465	GLU
1	A	471	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	126	ASN
1	A	199	GLN
1	A	231	HIS
1	A	279	GLN
1	A	302	ASN
1	A	357	HIS
1	A	372	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)

4 carbohydrates 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	NAG	A	601	1,2	14,14,15	0.28	0	15,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	602	2	14,14,15	0.28	0	15,19,21	0.73	1 (6%)
2	MAN	A	603	2	11,11,12	0.43	0	14,15,17	1.32	1 (7%)
2	FUC	A	604	2	10,10,11	0.40	0	14,14,16	1.39	1 (7%)

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	NAG	A	601	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	602	2	-	0/6/23/26	0/1/1/1
2	MAN	A	603	2	-	0/2/19/22	1/1/1/1
2	FUC	A	604	2	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	602	NAG	C1-O5-C5	2.55	115.49	112.25
2	A	603	MAN	C1-O5-C5	4.48	117.93	112.25
2	A	604	FUC	C1-O5-C5	4.76	119.73	112.38

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	603	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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	2OB	A	605	-	38,38,50	0.45	0	56,56,68	0.78	1 (1%)
3	2OB	A	606	-	50,50,50	0.76	1 (2%)	68,68,68	1.35	7 (10%)
4	PCW	A	607	-	53,53,53	1.29	4 (7%)	57,61,61	1.09	6 (10%)
5	PGE	A	608	-	9,9,9	0.76	0	8,8,8	0.59	0
7	0SF	A	610	-	39,40,40	0.98	3 (7%)	51,58,58	1.00	3 (5%)

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	2OB	A	605	-	-	0/19/77/89	0/4/4/4
3	2OB	A	606	-	-	0/31/89/89	0/4/4/4
4	PCW	A	607	-	-	0/57/57/57	0/0/0/0
5	PGE	A	608	-	-	0/7/7/7	0/0/0/0
7	0SF	A	610	-	-	0/30/35/35	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	610	0SF	O3-C23	-2.77	1.38	1.43
7	A	610	0SF	C12-N2	2.31	1.38	1.34
7	A	610	0SF	C12-N1	2.42	1.39	1.34
4	A	607	PCW	P-O2P	2.53	1.60	1.51
3	A	606	2OB	O1-C48	4.11	1.46	1.34
4	A	607	PCW	O2-C31	4.12	1.46	1.34
4	A	607	PCW	O3-C11	4.27	1.46	1.33
4	A	607	PCW	P-O1P	5.95	1.80	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	606	2OB	C21-C20-C22	-4.02	103.64	110.35
7	A	610	0SF	F3-C20-O2	-3.15	103.57	111.19
4	A	607	PCW	O3-C11-O11	-2.49	117.06	123.49
3	A	605	2OB	O1-C3-C4	-2.49	102.75	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	606	2OB	C4-C5-C6	-2.04	117.10	120.57
7	A	610	0SF	C22-N3-C12	-2.02	118.64	120.86
3	A	606	2OB	C13-C17-C20	2.04	123.01	119.46
7	A	610	0SF	F5-C24-C23	2.50	114.54	112.12
4	A	607	PCW	C2-O2-C31	2.51	123.91	117.89
3	A	606	2OB	C4-C5-C10	2.56	120.15	116.43
4	A	607	PCW	O2-C31-C32	2.60	117.17	111.53
3	A	606	2OB	C11-C9-C8	2.67	115.62	111.74
4	A	607	PCW	O2-C2-C1	2.70	117.86	108.36
3	A	606	2OB	O1-C48-C47	3.30	118.70	111.53
4	A	607	PCW	C3-O3-C11	3.33	126.16	116.85
4	A	607	PCW	O3-C11-C12	3.70	123.16	111.90
3	A	606	2OB	C15-C14-C13	3.72	108.66	103.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	2OB	5	0
3	A	606	2OB	1	0
4	A	607	PCW	4	0
7	A	610	0SF	2	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	472/476 (99%)	-0.34	8 (1%) 73 53	66, 95, 161, 190	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	ASP	2.9
1	A	357	HIS	2.5
1	A	355	GLN	2.3
1	A	318	GLN	2.1
1	A	359	VAL	2.0
1	A	315	PHE	2.0
1	A	356	GLN	2.0
1	A	397	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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
2	FUC	A	604	10/11	0.94	0.26	0.44	159,160,161,161	0
2	NAG	A	601	14/15	0.89	0.32	-	157,159,164,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MAN	A	603	11/12	0.69	0.41	-	179,181,181,182	0
2	NAG	A	602	14/15	0.90	0.45	-	166,170,176,178	0

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	PCW	A	607	54/54	0.89	0.41	4.80	89,102,153,154	0
3	2OB	A	605	35/47	0.89	0.33	4.46	66,93,101,104	0
3	2OB	A	606	47/47	0.97	0.30	2.17	55,69,106,111	0
7	0SF	A	610	38/38	0.94	0.27	1.62	92,103,139,144	21
5	PGE	A	608	10/10	0.92	0.22	0.81	75,82,87,87	0
6	CL	A	609	1/1	0.94	0.19	-0.18	108,108,108,108	0

6.5 Other polymers (i)

There are no such residues in this entry.