WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:30 pm GMT

PDB ID : 2JCL
Title : CRYSTAL STRUCTURE OF ALPHA-1,3 GALACTOSYLTRANSFERASE
(R365K) IN THE ABSENCE OF LIGANDS
Authors : Jamaluddin, H.; Tumbale, P.; Withers, S.G.; Acharya, K.R.; Brew, K.
Deposited on : 2006-12-26
Resolution : 3.29 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

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 3.29 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	Percentile Ranks	Value
Rfree		0.266
Clashscore		23
Ramachandran outliers		2.9%
Sidechain outliers		11.7%
RSRZ outliers		2.2%

Worse — *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
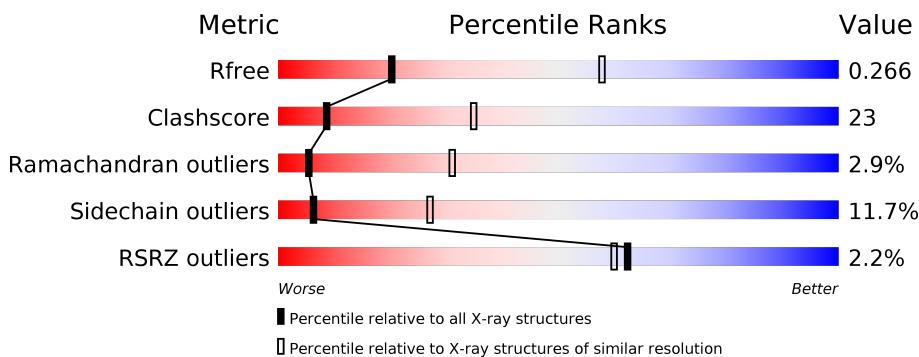
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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	289	2% · 52% 38% 6% ·
1	B	289	2% · 51% 38% 6% · ·
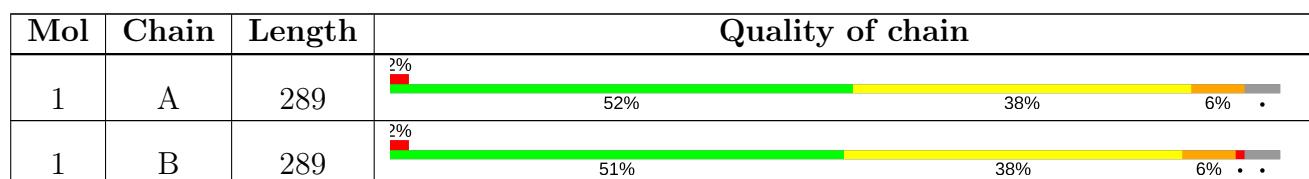
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	3360	-	-	-	X
2	SO4	B	3361	-	-	-	X
2	SO4	B	3362	-	-	-	X
2	SO4	B	3364	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4698 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 N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYL TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2306	1511	378	405	12			
1	B	277	Total	C	N	O	S	0	0	0
			2306	1511	378	405	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1365	LYS	ARG	ENGINEERED MUTATION	UNP P14769
B	2365	LYS	ARG	ENGINEERED MUTATION	UNP P14769

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	33	Total 33	O 33	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 the various outlier classes 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: N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYLTRANSFERAS E
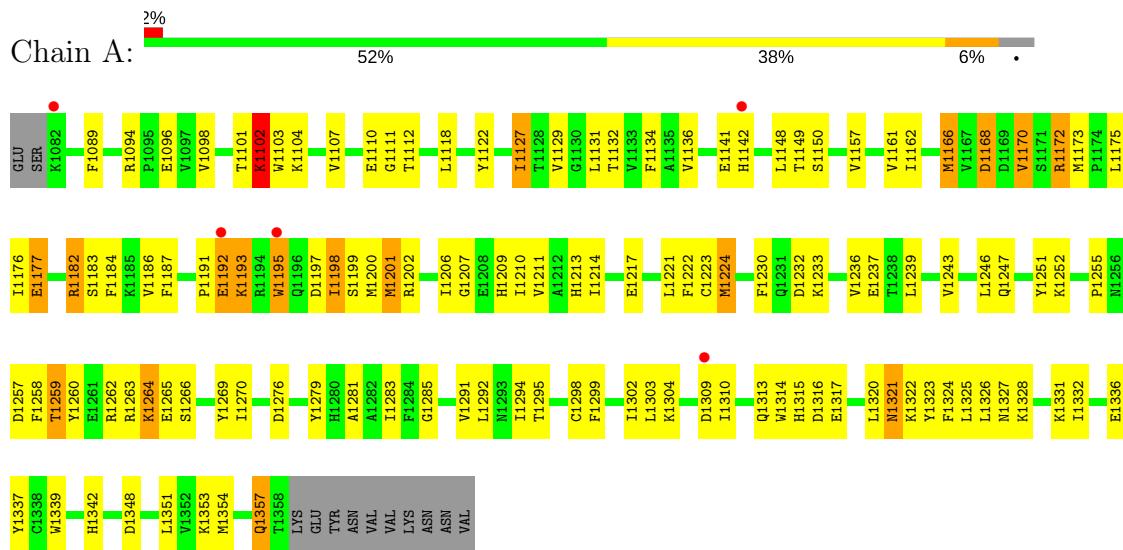
• Molecule 1: N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYLTRANSFERAS E
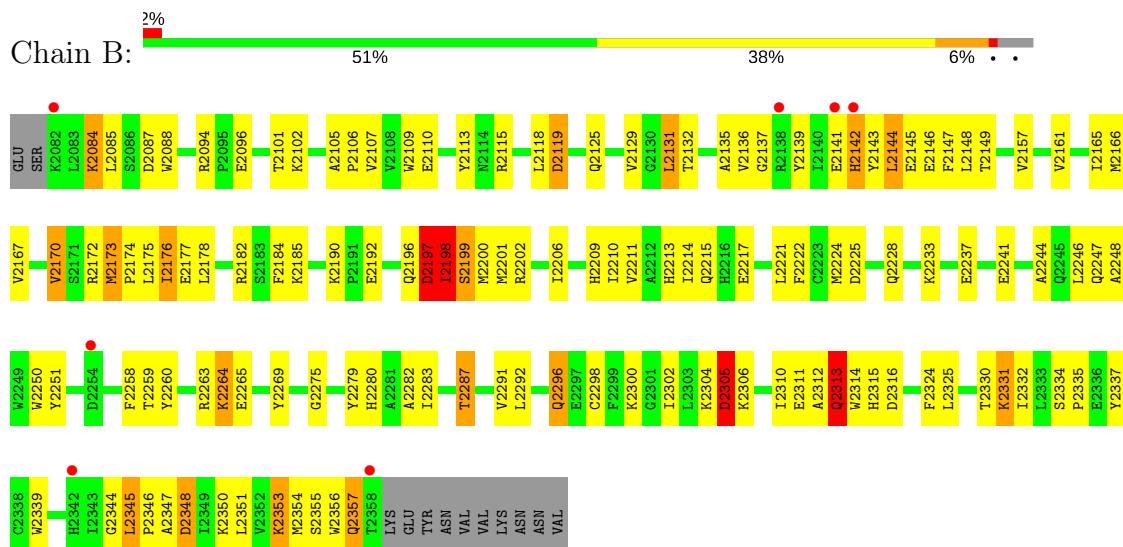
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.93Å　　103.26Å　　121.49Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	25.81　–　3.29 25.82　–　3.29	Depositor EDS
% Data completeness (in resolution range)	99.1 (25.81-3.29) 99.1 (25.82-3.29)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205　,　0.280 0.200　,　0.266	Depositor DCC
R_{free} test set	960 reflections (5.42%)	DCC
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 56.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4698	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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, 0.333 respectively for untwinned datasets, and 0.375, 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

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	0.76	1/2378 (0.0%)	0.75	0/3222
1	B	0.74	1/2378 (0.0%)	0.87	4/3222 (0.1%)
All	All	0.75	2/4756 (0.0%)	0.81	4/6444 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2197	ASP	C-N	7.26	1.50	1.34
1	A	1339	TRP	CB-CG	-6.31	1.38	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2198	ILE	O-C-N	-17.13	95.30	122.70
1	B	2198	ILE	C-N-CA	11.95	151.56	121.70
1	B	2198	ILE	CA-C-N	9.94	139.06	117.20
1	B	2197	ASP	O-C-N	-6.60	112.14	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2197	ASP	Mainchain,Peptide
1	B	2198	ILE	Mainchain

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	2306	0	2266	100	0
1	B	2306	0	2266	112	0
2	B	25	0	0	0	0
3	A	28	0	0	2	0
3	B	33	0	0	3	0
All	All	4698	0	4532	209	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 23.

All (209) 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:B:2283:ILE:HD11	1:B:2354:MET:HE1	1.28	1.14
1:B:2357:GLN:HA	1:B:2357:GLN:HE21	1.16	1.04
1:B:2283:ILE:HD11	1:B:2354:MET:CE	1.88	1.02
1:B:2144:LEU:HD23	1:B:2174:PRO:HD2	1.46	0.97
1:A:1192:GLU:HB2	1:A:1193:LYS:HA	1.48	0.94
1:B:2197:ASP:HB3	1:B:2200:MET:HG3	1.48	0.93
1:A:1192:GLU:CB	1:A:1193:LYS:HA	2.04	0.86
1:B:2144:LEU:HD23	1:B:2174:PRO:CD	2.09	0.82
1:B:2357:GLN:HA	1:B:2357:GLN:NE2	1.96	0.81
1:B:2198:ILE:O	1:B:2201:MET:N	2.12	0.81
1:B:2210:ILE:HA	1:B:2214:ILE:HB	1.63	0.80
1:A:1237:GLU:O	1:A:1331:LYS:HE2	1.82	0.79
1:B:2197:ASP:CB	1:B:2200:MET:HG3	2.12	0.79
1:A:1110:GLU:HA	1:A:1110:GLU:OE1	1.83	0.78
1:A:1170:VAL:O	1:A:1173:MET:HB3	1.84	0.77
1:A:1122:TYR:HB3	1:A:1127:ILE:HD12	1.65	0.77
1:A:1192:GLU:HB3	1:A:1198:ILE:HG13	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2211:VAL:HA	1:B:2215:GLN:HE21	1.50	0.76
1:B:2283:ILE:CD1	1:B:2354:MET:HE1	2.14	0.74
1:B:2339:TRP:O	1:B:2355:SER:HA	1.88	0.74
1:A:1102:LYS:HD3	1:A:1102:LYS:H	1.52	0.73
1:B:2197:ASP:HB3	1:B:2200:MET:CG	2.18	0.73
1:B:2141:GLU:OE2	1:B:2172:ARG:HD2	1.88	0.73
1:A:1281:ALA:HA	1:A:1320:LEU:CD2	2.19	0.72
1:A:1111:GLY:HA2	3:A:2002:HOH:O	1.89	0.71
1:A:1291:VAL:O	1:A:1295:THR:HG23	1.90	0.71
1:A:1129:VAL:O	1:A:1161:VAL:HA	1.91	0.71
1:A:1210:ILE:HA	1:A:1214:ILE:HB	1.72	0.70
1:A:1107:VAL:HG22	1:A:1332:ILE:HB	1.73	0.69
1:B:2357:GLN:HE21	1:B:2357:GLN:CA	1.96	0.67
1:A:1320:LEU:HD11	1:A:1324:PHE:CE1	2.29	0.67
1:B:2275:GLY:HA2	1:B:2325:LEU:HD13	1.76	0.67
1:B:2084:LYS:O	1:B:2087:ASP:HB2	1.93	0.67
1:A:1094:ARG:HD3	1:A:1110:GLU:O	1.96	0.66
1:B:2145:GLU:O	1:B:2146:GLU:C	2.30	0.66
1:A:1200:MET:HG2	1:A:1299:PHE:CE1	2.29	0.66
1:B:2135:ALA:HB3	1:B:2167:VAL:HG12	1.77	0.65
1:A:1351:LEU:HD23	1:A:1353:LYS:HZ1	1.61	0.65
1:B:2196:GLN:O	1:B:2198:ILE:N	2.30	0.65
1:B:2283:ILE:CD1	1:B:2354:MET:CE	2.73	0.64
1:B:2144:LEU:O	1:B:2147:PHE:HB3	1.98	0.64
1:B:2144:LEU:CD2	1:B:2174:PRO:HD2	2.25	0.64
1:B:2143:TYR:O	1:B:2145:GLU:N	2.30	0.63
1:B:2214:ILE:HG21	1:B:2221:LEU:HD13	1.80	0.63
1:B:2259:THR:HB	1:B:2314:TRP:HE1	1.63	0.63
1:A:1102:LYS:CD	1:A:1102:LYS:H	2.10	0.63
1:B:2246:LEU:HD12	1:B:2335:PRO:HD3	1.80	0.63
1:A:1132:THR:HG23	1:A:1221:LEU:HD11	1.79	0.63
1:A:1207:GLY:O	1:A:1211:VAL:HG23	1.99	0.62
1:B:2280:HIS:CD2	1:B:2282:ALA:H	2.17	0.62
1:B:2144:LEU:O	1:B:2147:PHE:N	2.32	0.62
1:A:1299:PHE:HA	1:A:1302:ILE:HD12	1.80	0.62
1:B:2118:LEU:HD12	1:B:2237:GLU:HA	1.81	0.62
1:B:2298:CYS:O	1:B:2302:ILE:HG13	2.00	0.61
1:A:1246:LEU:HG	1:A:1332:ILE:CG2	2.31	0.61
1:B:2305:ASP:O	1:B:2310:ILE:HG22	2.01	0.61
1:A:1264:LYS:HA	1:A:1269:TYR:CG	2.35	0.61
1:B:2137:GLY:HA2	1:B:2172:ARG:NH1	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1337:TYR:CE2	1:A:1353:LYS:HG2	2.37	0.60
1:A:1118:LEU:CD1	1:A:1237:GLU:HA	2.31	0.60
1:B:2213:HIS:O	1:B:2217:GLU:HG3	2.02	0.59
1:B:2143:TYR:O	1:B:2144:LEU:C	2.40	0.59
1:A:1141:GLU:OE1	1:A:1172:ARG:HG2	2.03	0.58
1:A:1281:ALA:HA	1:A:1320:LEU:HD22	1.84	0.58
1:B:2251:TYR:CD2	1:B:2335:PRO:HG2	2.37	0.58
1:B:2135:ALA:O	1:B:2167:VAL:HA	2.03	0.58
1:A:1177:GLU:HB3	3:B:2004:HOH:O	2.03	0.58
1:B:2197:ASP:OD1	1:B:2306:LYS:NZ	2.35	0.58
1:B:2221:LEU:HD23	1:B:2291:VAL:HG11	1.85	0.58
1:B:2311:GLU:OE1	1:B:2311:GLU:HA	2.04	0.57
1:B:2107:VAL:HG22	1:B:2332:ILE:HB	1.87	0.57
1:A:1351:LEU:HD23	1:A:1353:LYS:NZ	2.20	0.56
1:B:2237:GLU:HG3	1:B:2337:TYR:OH	2.06	0.56
1:B:2197:ASP:OD1	1:B:2306:LYS:CE	2.54	0.56
1:A:1175:LEU:HD11	1:B:2175:LEU:HD11	1.88	0.55
1:B:2165:ILE:HD11	1:B:2184:PHE:CD2	2.41	0.55
1:A:1263:ARG:NH1	1:A:1310:ILE:HD11	2.22	0.55
1:A:1298:CYS:O	1:A:1302:ILE:HG13	2.05	0.55
1:B:2337:TYR:HA	1:B:2353:LYS:HB2	1.89	0.55
1:A:1131:LEU:HA	1:A:1222:PHE:O	2.06	0.55
1:A:1101:THR:C	1:A:1103:TRP:H	2.10	0.55
1:A:1209:HIS:O	1:A:1210:ILE:C	2.45	0.55
1:A:1213:HIS:ND1	1:A:1214:ILE:N	2.54	0.55
1:A:1279:TYR:N	1:A:1321:ASN:HD21	2.06	0.54
1:A:1259:THR:HB	1:A:1314:TRP:CD1	2.42	0.54
1:A:1283:ILE:HD11	1:A:1354:MET:CE	2.38	0.54
1:A:1281:ALA:HA	1:A:1320:LEU:HD23	1.88	0.54
1:B:2197:ASP:OD1	1:B:2306:LYS:HE3	2.07	0.54
1:A:1236:VAL:HA	1:A:1239:LEU:HG	1.89	0.54
1:A:1313:GLN:HG2	3:A:2020:HOH:O	2.07	0.53
1:A:1357:GLN:HA	1:A:1357:GLN:HE21	1.74	0.53
1:A:1224:MET:HB3	1:A:1283:ILE:HG12	1.89	0.53
1:A:1213:HIS:O	1:A:1217:GLU:HG3	2.08	0.53
1:B:2211:VAL:HA	1:B:2215:GLN:NE2	2.21	0.53
1:B:2088:TRP:CD1	1:B:2118:LEU:HD21	2.44	0.53
1:B:2209:HIS:ND1	1:B:2213:HIS:NE2	2.53	0.53
1:B:2279:TYR:CE1	1:B:2324:PHE:HB3	2.44	0.53
1:A:1243:VAL:N	1:A:1285:GLY:O	2.33	0.53
1:A:1157:VAL:HG21	1:A:1233:LYS:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2157:VAL:HG21	1:B:2233:LYS:HE3	1.92	0.52
1:B:2283:ILE:HD11	1:B:2354:MET:HE2	1.82	0.52
1:B:2199:SER:OG	1:B:2316:ASP:HB3	2.09	0.52
1:A:1255:PRO:HA	1:A:1258:PHE:CD1	2.45	0.52
1:A:1201:MET:O	1:A:1202:ARG:C	2.48	0.52
1:A:1243:VAL:HG22	1:A:1331:LYS:HB3	1.91	0.52
1:B:2196:GLN:HG2	1:B:2201:MET:HB2	1.91	0.51
1:A:1281:ALA:HB2	1:A:1317:GLU:HA	1.91	0.51
1:A:1148:LEU:O	1:A:1149:THR:C	2.49	0.51
1:B:2237:GLU:O	1:B:2331:LYS:HE2	2.11	0.51
1:A:1186:VAL:HG12	1:A:1187:PHE:N	2.26	0.51
1:A:1251:TYR:OH	1:A:1348:ASP:HB2	2.10	0.51
1:A:1264:LYS:HA	1:A:1269:TYR:CD1	2.46	0.50
1:A:1177:GLU:HG2	3:B:2004:HOH:O	2.11	0.50
1:A:1270:ILE:HD11	1:A:1322:LYS:HA	1.93	0.50
1:B:2144:LEU:O	1:B:2145:GLU:C	2.48	0.50
1:A:1184:PHE:C	1:A:1184:PHE:CD1	2.84	0.50
1:A:1337:TYR:HA	1:A:1353:LYS:HB2	1.94	0.50
1:B:2202:ARG:O	1:B:2206:ILE:HG13	2.12	0.50
1:A:1255:PRO:HA	1:A:1258:PHE:CE1	2.47	0.50
1:B:2141:GLU:O	1:B:2142:HIS:C	2.50	0.50
1:B:2264:LYS:HA	1:B:2269:TYR:CG	2.46	0.50
1:A:1192:GLU:HB3	1:A:1198:ILE:CG1	2.41	0.50
1:B:2344:GLY:O	1:B:2346:PRO:HD3	2.12	0.50
1:A:1279:TYR:H	1:A:1321:ASN:HD21	1.60	0.49
1:B:2137:GLY:HA2	1:B:2172:ARG:HH11	1.77	0.49
1:A:1322:LYS:HE2	1:A:1326:LEU:HD11	1.94	0.49
1:A:1103:TRP:CE2	1:A:1328:LYS:HB3	2.47	0.49
1:A:1089:PHE:CE1	1:A:1112:THR:HB	2.48	0.49
1:B:2106:PRO:HD2	1:B:2330:THR:O	2.11	0.49
1:B:2198:ILE:HA	1:B:2201:MET:HB3	1.94	0.49
1:A:1134:PHE:CD2	1:A:1166:MET:HB3	2.49	0.48
1:B:2315:HIS:O	1:B:2316:ASP:C	2.52	0.48
1:B:2275:GLY:HA2	1:B:2325:LEU:CD1	2.40	0.48
1:A:1192:GLU:CB	1:A:1193:LYS:CA	2.86	0.48
1:B:2300:LYS:O	1:B:2304:LYS:HG3	2.13	0.48
1:A:1213:HIS:CE1	1:A:1214:ILE:HG13	2.48	0.48
1:A:1264:LYS:HG2	1:A:1265:GLU:OE2	2.14	0.48
1:B:2176:ILE:HD12	1:B:2178:LEU:HD21	1.96	0.47
1:B:2247:GLN:OE1	1:B:2250:TRP:HD1	1.96	0.47
1:A:1314:TRP:O	1:A:1317:GLU:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2176:ILE:HD12	1:B:2178:LEU:CD2	2.45	0.47
1:A:1262:ARG:O	1:A:1269:TYR:HE1	1.97	0.47
1:A:1199:SER:HB3	1:A:1316:ASP:CG	2.34	0.47
1:A:1232:ASP:OD2	1:A:1351:LEU:HD11	2.15	0.47
1:B:2224:MET:HA	1:B:2282:ALA:O	2.15	0.47
1:B:2088:TRP:CG	1:B:2118:LEU:HD21	2.50	0.47
1:B:2136:VAL:O	1:B:2139:TYR:HB2	2.15	0.47
1:B:2248:ALA:HA	1:B:2335:PRO:HB3	1.97	0.47
1:B:2347:ALA:O	1:B:2350:LYS:HE3	2.15	0.46
1:B:2241:GLU:HA	1:B:2287:THR:HG23	1.98	0.46
1:A:1107:VAL:HA	1:A:1332:ILE:O	2.16	0.46
1:B:2101:THR:HG23	1:B:2105:ALA:O	2.15	0.46
1:B:2197:ASP:HB3	1:B:2200:MET:CB	2.46	0.46
1:B:2165:ILE:HG22	1:B:2167:VAL:HG13	1.97	0.46
1:B:2196:GLN:HG3	1:B:2197:ASP:H	1.79	0.46
1:A:1200:MET:HG2	1:A:1299:PHE:HE1	1.77	0.46
1:A:1182:ARG:O	1:B:2185:LYS:HD2	2.15	0.46
1:A:1197:ASP:O	1:A:1198:ILE:C	2.54	0.45
1:A:1210:ILE:HG21	1:A:1292:LEU:HB2	1.98	0.45
1:B:2348:ASP:OD1	1:B:2348:ASP:N	2.50	0.45
1:B:2131:LEU:HA	1:B:2222:PHE:O	2.16	0.45
1:B:2178:LEU:HD23	1:B:2178:LEU:HA	1.44	0.45
1:B:2258:PHE:HD1	1:B:2260:TYR:CZ	2.35	0.45
1:B:2264:LYS:HD3	1:B:2264:LYS:H	1.81	0.44
1:A:1258:PHE:C	1:A:1260:TYR:H	2.20	0.44
1:B:2115:ARG:O	1:B:2119:ASP:HB2	2.17	0.44
1:B:2109:TRP:CD2	1:B:2334:SER:HB2	2.53	0.44
1:A:1198:ILE:HG22	1:A:1199:SER:N	2.33	0.44
1:A:1246:LEU:HG	1:A:1332:ILE:HG21	1.98	0.44
1:B:2250:TRP:O	1:B:2251:TYR:C	2.55	0.44
1:A:1177:GLU:CG	3:B:2004:HOH:O	2.63	0.44
1:B:2197:ASP:CB	1:B:2200:MET:CG	2.86	0.44
1:B:2292:LEU:O	1:B:2296:GLN:HB2	2.17	0.44
1:A:1258:PHE:HD1	1:A:1260:TYR:CZ	2.36	0.43
1:B:2145:GLU:O	1:B:2147:PHE:N	2.51	0.43
1:B:2129:VAL:O	1:B:2161:VAL:HA	2.19	0.43
1:B:2131:LEU:HD11	1:B:2147:PHE:HZ	1.84	0.43
1:B:2165:ILE:HD11	1:B:2184:PHE:CE2	2.54	0.43
1:A:1101:THR:C	1:A:1103:TRP:N	2.72	0.43
1:A:1283:ILE:HD11	1:A:1354:MET:HE3	1.99	0.43
1:B:2170:VAL:O	1:B:2173:MET:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1315:HIS:N	1:A:1315:HIS:CD2	2.86	0.42
1:B:2085:LEU:C	1:B:2087:ASP:H	2.22	0.42
1:B:2339:TRP:CZ2	1:B:2346:PRO:CD	3.02	0.42
1:A:1150:SER:HB2	1:A:1230:PHE:HB2	2.00	0.42
1:A:1320:LEU:HD11	1:A:1324:PHE:HE1	1.78	0.42
1:A:1136:VAL:HG13	1:A:1168:ASP:HB3	2.01	0.42
1:B:2210:ILE:HG21	1:B:2292:LEU:HB2	2.01	0.42
1:A:1258:PHE:O	1:A:1260:TYR:N	2.46	0.42
1:B:2115:ARG:O	1:B:2115:ARG:HG2	2.20	0.42
1:A:1110:GLU:N	1:A:1336:GLU:OE1	2.46	0.41
1:A:1251:TYR:CE1	1:A:1252:LYS:HG3	2.56	0.41
1:B:2246:LEU:HD12	1:B:2334:SER:HA	2.01	0.41
1:B:2110:GLU:HA	1:B:2113:TYR:HE2	1.85	0.41
1:A:1110:GLU:CA	1:A:1110:GLU:OE1	2.57	0.41
1:A:1323:TYR:C	1:A:1323:TYR:CD1	2.93	0.41
1:B:2131:LEU:HD12	1:B:2132:THR:N	2.36	0.41
1:B:2244:ALA:HB1	1:B:2279:TYR:CD2	2.55	0.41
1:A:1291:VAL:HA	1:A:1294:ILE:HD12	2.03	0.41
1:B:2148:LEU:HD21	1:B:2165:ILE:HG12	2.03	0.41
1:A:1175:LEU:HD21	1:B:2175:LEU:HD21	2.03	0.41
1:B:2225:ASP:O	1:B:2228:GLN:HG2	2.20	0.41
1:B:2312:ALA:O	1:B:2313:GLN:C	2.59	0.41
1:A:1221:LEU:HD23	1:A:1291:VAL:HG11	2.03	0.40
1:A:1162:ILE:HA	1:A:1183:SER:O	2.22	0.40
1:B:2263:ARG:HB3	1:B:2265:GLU:OE2	2.20	0.40
1:B:2094:ARG:NH2	1:B:2348:ASP:O	2.54	0.40
1:A:1166:MET:HB2	1:A:1166:MET:HE3	1.96	0.40
1:B:2196:GLN:CG	1:B:2197:ASP:N	2.83	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	275/289 (95%)	242 (88%)	26 (10%)	7 (2%)	6	34
1	B	275/289 (95%)	234 (85%)	32 (12%)	9 (3%)	4	28
All	All	550/578 (95%)	476 (86%)	58 (10%)	16 (3%)	5	31

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1192	GLU
1	A	1198	ILE
1	B	2144	LEU
1	B	2198	ILE
1	B	2313	GLN
1	A	1096	GLU
1	A	1102	LYS
1	B	2142	HIS
1	B	2197	ASP
1	B	2305	ASP
1	B	2356	TRP
1	B	2096	GLU
1	B	2345	LEU
1	A	1195	TRP
1	A	1259	THR
1	A	1191	PRO

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	248/260 (95%)	217 (88%)	31 (12%)	5	24
1	B	248/260 (95%)	221 (89%)	27 (11%)	7	30
All	All	496/520 (95%)	438 (88%)	58 (12%)	6	27

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1098	VAL
1	A	1102	LYS
1	A	1104	LYS
1	A	1127	ILE
1	A	1142	HIS
1	A	1166	MET
1	A	1168	ASP
1	A	1170	VAL
1	A	1172	ARG
1	A	1176	ILE
1	A	1177	GLU
1	A	1182	ARG
1	A	1193	LYS
1	A	1195	TRP
1	A	1201	MET
1	A	1206	ILE
1	A	1223	CYS
1	A	1224	MET
1	A	1247	GLN
1	A	1257	ASP
1	A	1264	LYS
1	A	1266	SER
1	A	1276	ASP
1	A	1303	LEU
1	A	1304	LYS
1	A	1309	ASP
1	A	1321	ASN
1	A	1325	LEU
1	A	1327	ASN
1	A	1342	HIS
1	A	1357	GLN
1	B	2084	LYS
1	B	2102	LYS
1	B	2119	ASP
1	B	2125	GLN
1	B	2131	LEU
1	B	2149	THR
1	B	2166	MET
1	B	2170	VAL
1	B	2173	MET
1	B	2176	ILE
1	B	2177	GLU
1	B	2182	ARG

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Mol	Chain	Res	Type
1	B	2190	LYS
1	B	2192	GLU
1	B	2198	ILE
1	B	2199	SER
1	B	2264	LYS
1	B	2287	THR
1	B	2296	GLN
1	B	2305	ASP
1	B	2313	GLN
1	B	2331	LYS
1	B	2345	LEU
1	B	2348	ASP
1	B	2351	LEU
1	B	2353	LYS
1	B	2357	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1196	GLN
1	A	1280	HIS
1	A	1296	GLN
1	A	1315	HIS
1	A	1321	ASN
1	A	1357	GLN
1	B	2125	GLN
1	B	2196	GLN
1	B	2215	GLN
1	B	2280	HIS
1	B	2296	GLN
1	B	2313	GLN
1	B	2357	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 ⓘ

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	SO4	B	3360	-	4,4,4	0.25	0	6,6,6	0.28	0
2	SO4	B	3361	-	4,4,4	0.35	0	6,6,6	0.39	0
2	SO4	B	3362	-	4,4,4	0.46	0	6,6,6	0.53	0
2	SO4	B	3363	-	4,4,4	0.31	0	6,6,6	0.31	0
2	SO4	B	3364	-	4,4,4	0.14	0	6,6,6	0.25	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
2	SO4	B	3360	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3361	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3362	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3363	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3364	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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, 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	277/289 (95%)	-0.15	5 (1%)	69	66	16, 32, 67, 94	1 (0%)
1	B	277/289 (95%)	-0.18	7 (2%)	58	54	16, 32, 54, 62	2 (0%)
All	All	554/578 (95%)	-0.16	12 (2%)	62	60	16, 32, 58, 94	3 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1195	TRP	4.1
1	A	1082	LYS	3.5
1	B	2358	THR	3.1
1	B	2082	LYS	3.0
1	B	2138	ARG	2.7
1	B	2142	HIS	2.6
1	A	1142	HIS	2.4
1	A	1192	GLU	2.4
1	B	2254	ASP	2.1
1	A	1309	ASP	2.1
1	B	2342	HIS	2.1
1	B	2141	GLU	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
2	SO4	B	3362	5/5	0.83	0.35	5.50	124,125,125,125	0
2	SO4	B	3364	5/5	0.97	0.29	3.51	75,75,75,77	0
2	SO4	B	3360	5/5	0.87	0.30	3.26	95,96,96,96	0
2	SO4	B	3361	5/5	0.90	0.41	2.97	111,111,111,112	0
2	SO4	B	3363	5/5	0.92	0.63	-	101,101,101,102	0

6.5 Other polymers ⓘ

There are no such residues in this entry.