



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:35 AM GMT

PDB ID : 2HRR  
Title : Crystal structure of Human Liver Carboxylesterase 1 (hCE1) in covalent complex with the nerve agent Tabun (GA)  
Authors : Fleming, C.D.; Redinbo, M.R.  
Deposited on : 2006-07-20  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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

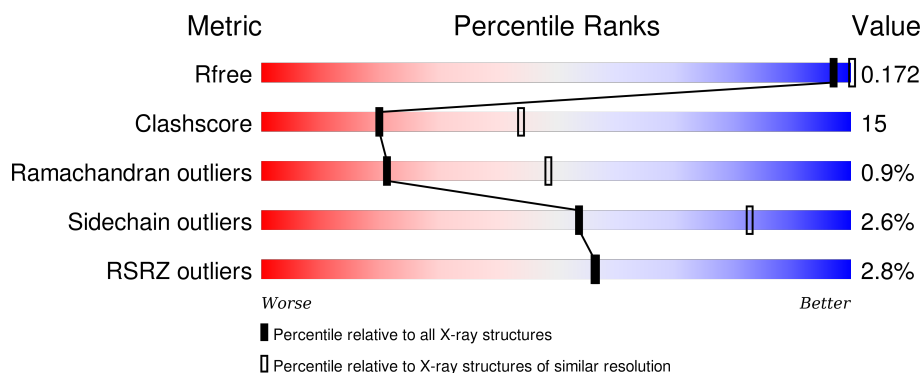
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	532	<div> <div>3%</div> <div>68%</div> <div>30%</div> <div>.</div> </div>
1	B	532	<div> <div>5%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>
1	C	532	<div> <div>%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>

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	SIA	A	182	-	-	-	X
3	SIA	B	282	-	-	-	X
3	SIA	C	382	-	-	-	X
5	SO4	A	185	-	-	X	X
5	SO4	A	285	-	-	-	X
5	SO4	B	284	-	-	-	X
5	SO4	C	184	-	-	-	X
5	SO4	C	384	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13429 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 Liver carboxylesterase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	B	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	C	531	Total	C	N	O	S	0	0	0
			4125	2659	684	762	20			

There are 3 discrepancies between the modelled and reference sequences:

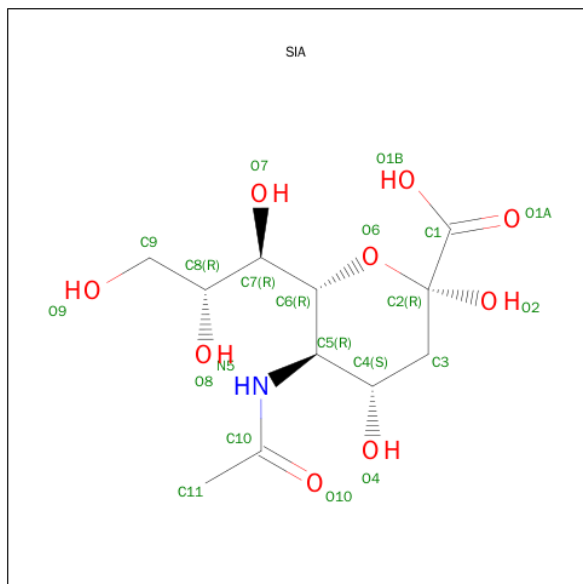
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	DELETION	UNP Q9UK77
B	?	-	GLN	DELETION	UNP Q9UK77
C	?	-	GLN	DELETION	UNP Q9UK77

- Molecule 2 is Sulfate Ion (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



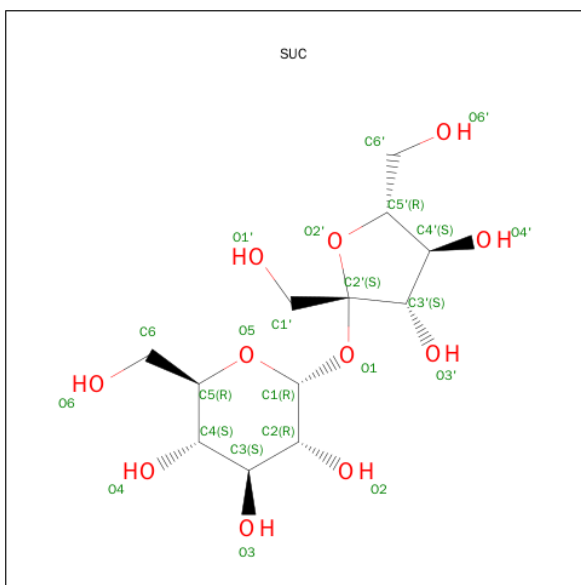
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is Sucrose (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		
3	C	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 4 is Water (three-letter code: SUC) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	12	11		
4	B	1	Total	C	O	0	0
			23	12	11		
4	C	1	Total	C	O	0	0
			23	12	11		

- Molecule 5 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



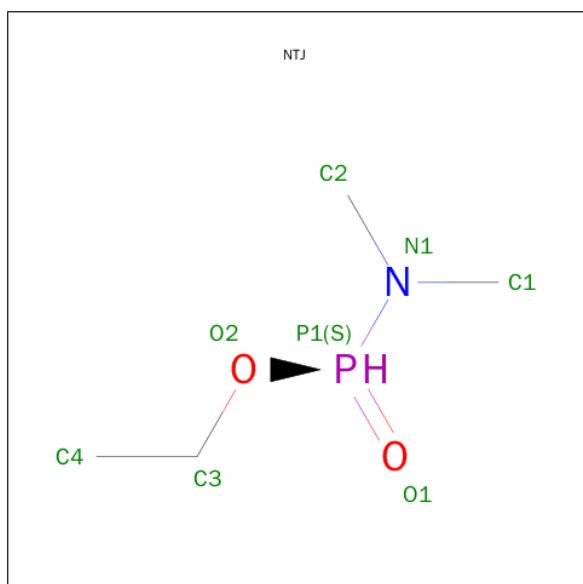
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 6 is R-ETHYL N,N-DIMETHYLPHOSPHONAMIDATE (three-letter code: NTJ) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>2</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			8	4	1	2	1		
6	B	1	Total	C	N	O	P	0	0
			8	4	1	2	1		
6	C	1	Total	C	N	O	P	0	0
			8	4	1	2	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	266	Total	O	0	0
			266	266		
7	B	241	Total	O	0	0
			241	241		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	320	Total	O	0	0
			320	320		



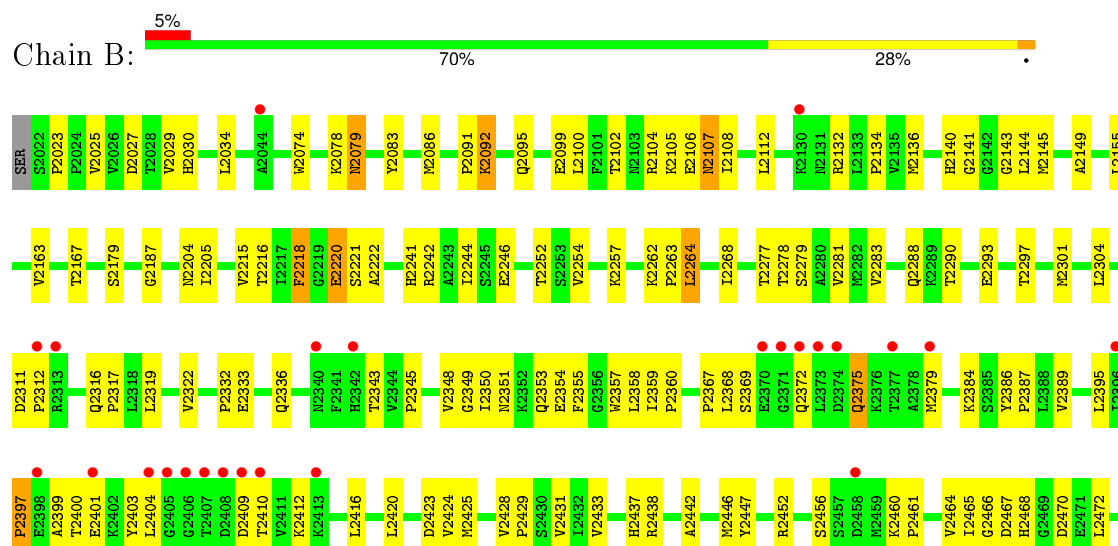
### 3 Residue-property plots

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: Liver carboxylesterase 1

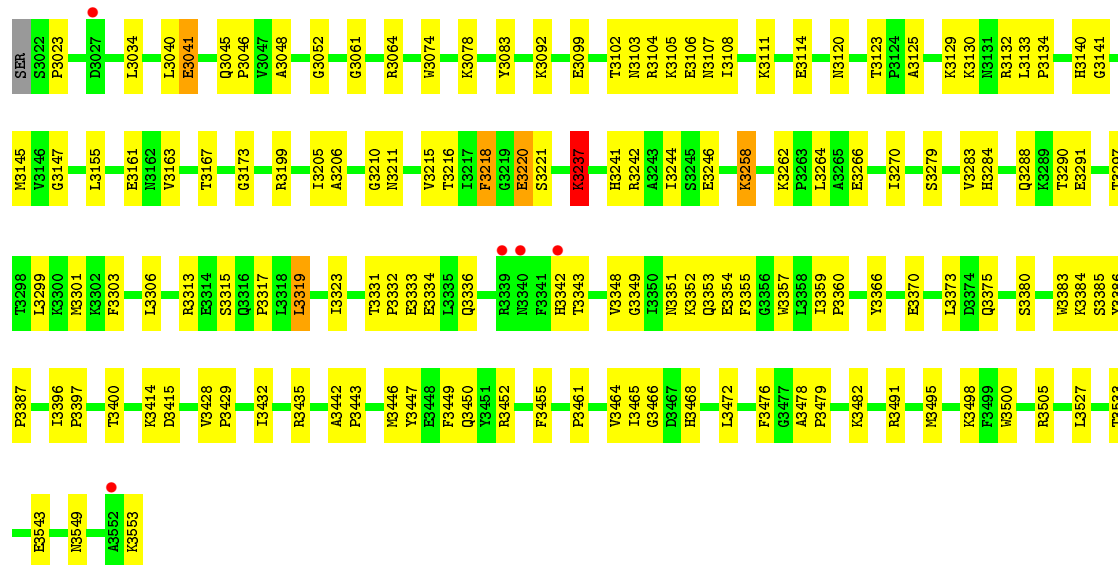
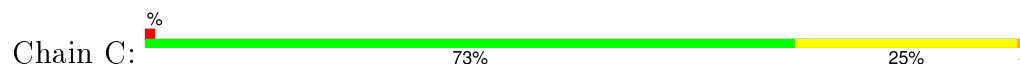


#### • Molecule 1: Liver carboxylesterase 1





• Molecule 1: Liver carboxylesterase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.57Å 181.05Å 202.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.78 – 2.70 41.78 – 2.69	Depositor EDS
% Data completeness (in resolution range)	91.0 (41.78-2.70) 91.8 (41.78-2.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.32 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.167 , 0.232 0.173 , 0.172	Depositor DCC
$R_{free}$ test set	2686 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 53086 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13429	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: SIA, NTJ, SUC, NAG, 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	0.37	1/4236 (0.0%)	0.61	3/5754 (0.1%)
1	B	0.35	1/4230 (0.0%)	0.57	1/5746 (0.0%)
1	C	0.37	1/4231 (0.0%)	0.59	1/5746 (0.0%)
All	All	0.36	3/12697 (0.0%)	0.59	5/17246 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2092	LYS	CE-NZ	-6.18	1.33	1.49
1	C	3092	LYS	CE-NZ	-6.10	1.33	1.49
1	A	1092	LYS	CE-NZ	-6.06	1.33	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1317	PRO	N-CA-C	-6.04	96.40	112.10
1	A	1092	LYS	CD-CE-NZ	5.47	124.27	111.70
1	C	3092	LYS	CD-CE-NZ	5.45	124.23	111.70
1	B	2092	LYS	CD-CE-NZ	5.32	123.94	111.70
1	A	1316	GLN	N-CA-C	5.28	125.25	111.00

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	4130	0	4129	135	0
1	B	4124	0	4125	117	0
1	C	4125	0	4124	109	0
2	A	14	0	12	1	0
2	B	14	0	13	1	0
2	C	14	0	13	0	0
3	A	21	0	18	3	0
3	B	21	0	18	6	0
3	C	21	0	18	7	0
4	A	23	0	22	2	0
4	B	23	0	22	2	0
4	C	23	0	22	1	0
5	A	10	0	0	3	0
5	B	5	0	0	0	0
5	C	10	0	0	1	0
6	A	8	0	11	1	0
6	B	8	0	11	0	0
6	C	8	0	11	0	0
7	A	266	0	0	17	0
7	B	241	0	0	8	0
7	C	320	0	0	18	0
All	All	13429	0	12569	372	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 15.

All (372) 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:C:3343:THR:HB	1:C:3442:ALA:HB2	1.31	1.11
1:B:2343:THR:HB	1:B:2442:ALA:HB2	1.46	0.98
1:B:2215:VAL:H	1:B:2241:HIS:HD2	1.12	0.95
1:A:1215:VAL:H	1:A:1241:HIS:HD2	1.17	0.92
1:C:3215:VAL:H	1:C:3241:HIS:HD2	1.07	0.90
1:C:3353:GLN:NE2	1:C:3465:ILE:H	1.71	0.88
1:A:1134:PRO:HG2	1:A:1163:VAL:HG12	1.56	0.87
1:C:3105:LYS:HG3	1:C:3106:GLU:H	1.37	0.87
1:A:1258:LYS:HD2	1:A:1258:LYS:H	1.40	0.86
1:A:1105:LYS:HG3	1:A:1106:GLU:H	1.39	0.86
1:A:1257:LYS:HE2	1:A:1318:LEU:O	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1264:LEU:HG	1:A:1317:PRO:HB2	1.59	0.84
1:C:3134:PRO:HG2	1:C:3163:VAL:HG12	1.57	0.82
1:B:2105:LYS:HG3	1:B:2106:GLU:H	1.45	0.81
1:A:1396:ILE:HB	1:A:1397:PRO:HD3	1.62	0.80
1:A:1336:GLN:HE22	1:A:1433:VAL:HA	1.44	0.80
1:B:2290:THR:OG1	1:B:2293:GLU:HG3	1.81	0.80
1:A:1102:THR:OG1	1:A:1104:ARG:HG2	1.82	0.79
1:B:2134:PRO:HG2	1:B:2163:VAL:HG12	1.66	0.78
1:A:1355:PHE:CE1	1:A:1360:PRO:HG3	2.19	0.78
1:A:1290:THR:OG1	1:A:1293:GLU:HG3	1.84	0.77
1:A:1220:GLU:HG2	1:A:1472:LEU:HD21	1.66	0.77
1:B:2220:GLU:HG2	1:B:2472:LEU:HD21	1.66	0.76
1:C:3215:VAL:H	1:C:3241:HIS:CD2	1.99	0.74
1:A:1215:VAL:H	1:A:1241:HIS:CD2	2.04	0.74
1:A:1553:LYS:HG2	7:A:8293:HOH:O	1.88	0.73
1:C:3129:LYS:HG2	1:C:3130:LYS:H	1.53	0.73
2:B:279:NAG:H83	3:B:282:SIA:H31	1.69	0.73
1:A:1105:LYS:HG3	1:A:1106:GLU:N	2.03	0.73
1:C:3216:THR:HG23	1:C:3242:ARG:HB2	1.70	0.73
1:A:1023:PRO:HB2	1:A:1034:LEU:HD21	1.71	0.73
1:B:2332:PRO:O	1:B:2336:GLN:HG3	1.89	0.72
1:A:1105:LYS:HG2	7:A:8390:HOH:O	1.90	0.72
1:A:1397:PRO:O	1:A:1401:GLU:HG3	1.92	0.70
1:A:1316:GLN:O	1:A:1317:PRO:C	2.29	0.69
1:C:3355:PHE:CE1	1:C:3360:PRO:HG3	2.27	0.69
3:C:382:SIA:H7	7:C:8026:HOH:O	1.92	0.69
1:C:3129:LYS:HG2	1:C:3130:LYS:N	2.09	0.68
1:C:3215:VAL:N	1:C:3241:HIS:HD2	1.88	0.68
1:C:3353:GLN:HE22	1:C:3465:ILE:H	1.39	0.67
1:B:2091:PRO:HB3	1:B:2112:LEU:HD11	1.77	0.67
1:C:3105:LYS:HD3	7:C:8553:HOH:O	1.95	0.66
1:B:2372:GLN:HG2	1:B:2410:THR:HB	1.77	0.66
1:A:1306:LEU:HD11	1:A:1385:SER:HA	1.77	0.66
1:C:3303:PHE:CZ	1:C:3319:LEU:HD11	2.30	0.66
1:B:2252:THR:HG22	1:B:2425:MET:O	1.96	0.65
1:C:3105:LYS:HG3	1:C:3106:GLU:N	2.09	0.64
1:C:3132:ARG:HB3	1:C:3211:ASN:HB2	1.80	0.64
1:C:3199:ARG:HG3	7:C:8461:HOH:O	1.98	0.63
1:B:2023:PRO:HB2	1:B:2034:LEU:HD21	1.78	0.63
1:B:2355:PHE:CD1	1:B:2360:PRO:HG3	2.33	0.63
1:B:2423:ASP:OD2	1:B:2543:GLU:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1262:LYS:HE3	1:A:1279:SER:OG	1.99	0.63
1:C:3386:TYR:N	1:C:3387:PRO:HD2	2.14	0.63
1:C:3083:TYR:CE2	1:C:3108:ILE:HD13	2.34	0.63
1:C:3315:SER:HB2	7:C:8703:HOH:O	1.99	0.62
1:C:3262:LYS:O	1:C:3266:GLU:HG3	1.99	0.62
3:C:382:SIA:H4	3:C:382:SIA:H113	1.82	0.62
1:A:1501:ALA:O	1:A:1505:ARG:HG2	2.00	0.62
1:B:2083:TYR:CE2	1:B:2108:ILE:HD13	2.35	0.61
1:C:3491:ARG:HD2	7:C:8051:HOH:O	1.99	0.61
1:B:2246:GLU:HG2	1:B:2447:TYR:OH	2.00	0.61
3:C:382:SIA:C7	7:C:8026:HOH:O	2.48	0.61
1:B:2278:THR:OG1	1:B:2281:VAL:HG23	2.00	0.61
1:B:2423:ASP:O	1:B:2428:VAL:HG23	2.02	0.60
1:B:2355:PHE:CE1	1:B:2360:PRO:HG3	2.37	0.60
1:B:2386:TYR:N	1:B:2387:PRO:HD2	2.16	0.60
1:A:1140:HIS:HD2	1:A:1141:GLY:O	1.85	0.60
1:C:3414:LYS:HD3	1:C:3415:ASP:N	2.17	0.60
1:A:1382:LEU:HD23	1:A:1396:ILE:HG23	1.84	0.59
1:A:1339:ARG:CD	1:A:1440:ALA:HA	2.33	0.59
1:A:1279:SER:O	1:A:1283:VAL:HG23	2.02	0.59
1:B:2461:PRO:HG2	1:B:2464:VAL:CG2	2.34	0.58
1:A:1512:GLU:HG3	7:A:8253:HOH:O	2.02	0.58
1:B:2369:SER:HA	4:B:22:SUC:H6'1	1.85	0.58
1:B:2452:ARG:HG2	1:B:2452:ARG:HH11	1.69	0.58
1:C:3396:ILE:HB	1:C:3397:PRO:HD3	1.84	0.58
1:A:1338:GLU:C	1:A:1340:ASN:H	2.06	0.57
1:A:1257:LYS:HE3	1:A:1320:GLY:H	1.69	0.57
1:A:1372:GLN:HG3	1:A:1410:THR:OG1	2.03	0.57
1:A:1161:GLU:OE2	1:A:1498:LYS:HG2	2.05	0.57
1:A:1538:LYS:HB3	1:A:1541:ASP:HB2	1.86	0.57
1:C:3332:PRO:O	1:C:3336:GLN:HG3	2.04	0.57
1:B:2351:ASN:HB3	1:B:2466:GLY:O	2.04	0.57
1:B:2079:ASN:O	3:B:282:SIA:O2	2.17	0.57
1:B:2428:VAL:HB	1:B:2429:PRO:HD3	1.87	0.57
1:B:2107:ASN:HD22	1:B:2108:ILE:H	1.52	0.57
1:A:1403:TYR:O	1:A:1416:LEU:HD13	2.06	0.56
3:A:182:SIA:O7	3:A:182:SIA:N5	2.38	0.56
1:C:3414:LYS:HE3	4:C:33:SUC:O2	2.05	0.56
1:B:2029:VAL:HG23	1:B:2204:ASN:OD1	2.05	0.56
3:B:282:SIA:H6	3:B:282:SIA:H113	1.87	0.56
1:B:2357:TRP:O	1:B:2360:PRO:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1386:TYR:N	1:A:1387:PRO:HD2	2.20	0.56
1:B:2092:LYS:HE3	7:B:8525:HOH:O	2.05	0.56
1:A:1083:TYR:CE2	1:A:1108:ILE:HD13	2.39	0.56
1:C:3246:GLU:HG2	1:C:3447:TYR:OH	2.06	0.55
1:A:1052:GLY:HA3	3:A:182:SIA:C9	2.37	0.55
1:A:1026:VAL:HG13	1:A:1207:SER:HB3	1.87	0.55
1:B:2215:VAL:H	1:B:2241:HIS:CD2	2.05	0.55
1:A:1339:ARG:HD3	1:A:1440:ALA:HA	1.88	0.55
1:A:1308:LEU:HB2	1:A:1309:GLN:HE22	1.71	0.55
1:A:1215:VAL:N	1:A:1241:HIS:HD2	1.97	0.55
1:A:1264:LEU:O	1:A:1264:LEU:HD22	2.07	0.55
1:C:3349:GLY:HA3	1:C:3447:TYR:CE1	2.41	0.55
1:A:1026:VAL:CG1	1:A:1207:SER:HB3	2.37	0.55
1:A:1308:LEU:HB2	1:A:1309:GLN:NE2	2.22	0.55
1:C:3319:LEU:N	1:C:3319:LEU:HD12	2.22	0.55
1:B:2353:GLN:NE2	1:B:2465:ILE:H	2.05	0.55
1:B:2102:THR:OG1	1:B:2104:ARG:HG2	2.06	0.54
1:B:2375:GLN:O	1:B:2379:MET:HG3	2.08	0.54
1:C:3111:LYS:HD2	7:C:8033:HOH:O	2.08	0.54
1:A:1423:ASP:OD2	1:A:1543:GLU:HG2	2.07	0.54
1:A:1241:HIS:O	1:A:1242:ARG:HD3	2.07	0.54
1:B:2220:GLU:HA	1:B:2246:GLU:O	2.08	0.54
1:B:2025:VAL:HG22	1:B:2034:LEU:HD23	1.90	0.54
1:A:1257:LYS:HE3	1:A:1320:GLY:N	2.23	0.54
1:A:1318:LEU:HB3	7:A:8171:HOH:O	2.07	0.54
1:B:2512:GLU:O	1:B:2512:GLU:HG3	2.07	0.54
1:A:1343:THR:HB	1:A:1442:ALA:HB2	1.90	0.54
1:B:2105:LYS:HG3	1:B:2106:GLU:N	2.19	0.54
3:B:282:SIA:H7	7:B:8131:HOH:O	2.07	0.54
1:B:2349:GLY:HA3	1:B:2447:TYR:CE1	2.43	0.54
1:A:1316:GLN:O	1:A:1318:LEU:HG	2.07	0.53
1:B:2359:ILE:HB	1:B:2360:PRO:HD3	1.90	0.53
1:C:3114:GLU:HG3	1:C:3291:GLU:OE1	2.09	0.53
1:B:2100:LEU:HD13	1:B:2358:LEU:HD13	1.89	0.53
1:B:2140:HIS:HD2	1:B:2141:GLY:O	1.90	0.53
1:C:3366:TYR:OH	1:C:3385:SER:HB3	2.08	0.53
1:A:1336:GLN:NE2	1:A:1433:VAL:HA	2.20	0.53
1:C:3074:TRP:CD2	1:C:3078:LYS:HE2	2.44	0.53
1:A:1478:ALA:N	1:A:1479:PRO:CD	2.71	0.53
1:A:1551:PHE:C	1:A:1553:LYS:H	2.12	0.52
1:B:2437:HIS:HE1	7:B:8034:HOH:O	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2395:LEU:HD13	1:B:2550:LEU:HG	1.91	0.52
1:A:1359:ILE:HB	1:A:1360:PRO:HD3	1.89	0.52
1:B:2221:SER:OG	1:B:2222:ALA:N	2.42	0.52
1:C:3173:GLY:HA3	7:C:8175:HOH:O	2.10	0.52
1:A:1257:LYS:HD3	7:A:8198:HOH:O	2.09	0.52
1:A:1357:TRP:O	1:A:1360:PRO:HD2	2.10	0.52
1:B:2400:THR:CG2	1:B:2404:LEU:HD12	2.39	0.52
1:B:2447:TYR:HB3	1:B:2517:TRP:CZ2	2.44	0.52
1:A:1342:HIS:HE1	7:A:8003:HOH:O	1.93	0.52
1:C:3045:GLN:NE2	1:C:3046:PRO:HD2	2.25	0.52
1:A:1089:GLN:HB2	1:A:1146:VAL:HG12	1.92	0.52
1:C:3258:LYS:HD2	1:C:3258:LYS:H	1.75	0.51
1:B:2268:ILE:HD11	1:B:2319:LEU:HD21	1.90	0.51
1:A:1338:GLU:C	1:A:1340:ASN:N	2.62	0.51
1:B:2297:THR:O	1:B:2301:MET:HG2	2.09	0.51
1:A:1499:PHE:CD2	1:A:1514:LEU:HD13	2.45	0.51
1:A:1216:THR:HG23	1:A:1242:ARG:HB2	1.93	0.51
1:C:3129:LYS:HB2	7:C:8166:HOH:O	2.10	0.51
3:C:382:SIA:C11	3:C:382:SIA:H4	2.40	0.51
1:C:3297:THR:O	1:C:3301:MET:HG2	2.10	0.51
1:B:2403:TYR:O	1:B:2416:LEU:HD13	2.09	0.51
1:A:1218:PHE:CB	1:A:1244:ILE:HB	2.39	0.51
1:A:1087:CYS:HB3	7:A:8037:HOH:O	2.10	0.51
1:B:2288:GLN:HG3	7:B:8685:HOH:O	2.10	0.51
1:B:2493:SER:O	1:B:2497:MET:HG3	2.10	0.51
1:C:3352:LYS:HG2	1:C:3450:GLN:HE21	1.76	0.51
1:A:1258:LYS:HD2	1:A:1258:LYS:N	2.18	0.51
1:C:3279:SER:O	1:C:3283:VAL:HG23	2.09	0.51
1:A:1262:LYS:HB3	1:A:1263:PRO:HD3	1.92	0.51
1:C:3354:GLU:O	1:C:3468:HIS:HB2	2.10	0.51
1:A:1111:LYS:HD3	7:A:8296:HOH:O	2.10	0.51
1:A:1368:LEU:O	4:A:11:SUC:H1	2.11	0.50
1:A:1283:VAL:HG12	1:A:1287:ARG:NH1	2.26	0.50
1:C:3343:THR:CB	1:C:3442:ALA:HB2	2.23	0.50
7:A:8343:HOH:O	3:C:382:SIA:H31	2.11	0.50
1:A:1140:HIS:HE1	7:A:8023:HOH:O	1.94	0.50
1:B:2467:ASP:N	1:B:2470:ASP:OD2	2.44	0.50
1:A:1285:CYS:HB2	7:C:8430:HOH:O	2.10	0.50
1:B:2106:GLU:HG2	7:B:8639:HOH:O	2.10	0.50
1:C:3319:LEU:H	1:C:3319:LEU:HD12	1.76	0.50
1:A:1348:VAL:O	1:A:1446:MET:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3241:HIS:O	1:C:3242:ARG:HD3	2.12	0.50
1:A:1045:GLN:NE2	1:A:1046:PRO:HD2	2.26	0.50
1:A:1338:GLU:O	1:A:1340:ASN:N	2.45	0.50
1:A:1201:VAL:O	1:A:1205:ILE:HB	2.12	0.50
1:C:3290:THR:HA	5:C:184:SO4:O3	2.12	0.50
1:B:2397:PRO:O	1:B:2401:GLU:HG3	2.11	0.50
1:A:1023:PRO:CB	1:A:1034:LEU:HD21	2.42	0.49
1:B:2216:THR:HG23	1:B:2242:ARG:HB2	1.95	0.49
1:C:3428:VAL:HB	1:C:3429:PRO:HD3	1.94	0.49
1:A:1351:ASN:ND2	1:A:1449:PHE:HB3	2.27	0.49
1:C:3218:PHE:CB	1:C:3244:ILE:HB	2.42	0.49
1:C:3359:ILE:HB	1:C:3360:PRO:HD3	1.95	0.49
1:C:3052:GLY:O	3:C:382:SIA:H92	2.13	0.49
1:A:1428:VAL:HG13	1:A:1544:VAL:HG22	1.95	0.49
1:B:2543:GLU:OE2	1:B:2543:GLU:N	2.43	0.48
1:A:1218:PHE:HB3	1:A:1244:ILE:HB	1.95	0.48
1:C:3478:ALA:N	1:C:3479:PRO:CD	2.77	0.48
1:A:1354:GLU:O	1:A:1468:HIS:HB2	2.13	0.48
1:B:2461:PRO:HG2	1:B:2464:VAL:HG21	1.95	0.48
1:A:1351:ASN:HB3	1:A:1466:GLY:O	2.13	0.48
1:C:3048:ALA:HB3	1:C:3123:THR:HG23	1.96	0.48
7:A:8682:HOH:O	1:C:3111:LYS:HE2	2.14	0.48
1:B:2461:PRO:HG2	1:B:2464:VAL:HG23	1.96	0.48
1:A:1021:SER:OG	1:A:1021:SER:O	2.32	0.48
1:B:2336:GLN:HE22	1:B:2433:VAL:HG22	1.79	0.48
1:B:2107:ASN:ND2	1:B:2108:ILE:H	2.11	0.48
1:B:2100:LEU:HD13	1:B:2358:LEU:CD1	2.44	0.48
1:C:3220:GLU:HG2	1:C:3472:LEU:HD21	1.95	0.48
1:C:3543:GLU:OE2	1:C:3543:GLU:N	2.35	0.48
1:C:3348:VAL:O	1:C:3446:MET:HA	2.14	0.48
1:A:1355:PHE:CD1	1:A:1360:PRO:HG3	2.49	0.47
1:A:1284:HIS:HA	5:A:185:SO4:O2	2.14	0.47
1:A:1342:HIS:CE1	7:A:8003:HOH:O	2.66	0.47
1:A:1236:ALA:O	1:A:1237:LYS:C	2.52	0.47
1:A:1149:ALA:HB2	1:A:1169:GLN:HG3	1.96	0.47
1:B:2456:SER:HB3	1:B:2460:LYS:HD3	1.96	0.47
7:A:8682:HOH:O	1:C:3111:LYS:HG2	2.15	0.47
1:A:1074:TRP:CD2	1:A:1078:LYS:HE2	2.49	0.47
3:B:282:SIA:H6	3:B:282:SIA:C11	2.43	0.47
1:B:2478:ALA:N	1:B:2479:PRO:CD	2.78	0.47
1:C:3323:ILE:HG12	7:C:8251:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1360:PRO:HB2	4:A:11:SUC:H61	1.96	0.47
1:A:1349:GLY:HA3	1:A:1447:TYR:CE1	2.50	0.47
1:B:2030:HIS:HD2	7:B:8134:HOH:O	1.96	0.47
1:B:2107:ASN:ND2	1:B:2108:ILE:N	2.62	0.47
1:C:3370:GLU:HG3	7:C:8176:HOH:O	2.14	0.47
1:B:2348:VAL:O	1:B:2446:MET:HA	2.15	0.46
1:C:3428:VAL:O	1:C:3432:ILE:HG13	2.16	0.46
1:C:3218:PHE:HB3	1:C:3244:ILE:HB	1.97	0.46
1:B:2354:GLU:O	1:B:2468:HIS:HB2	2.15	0.46
1:C:3288:GLN:NE2	7:C:8328:HOH:O	2.47	0.46
1:B:2074:TRP:CD2	1:B:2078:LYS:HE2	2.50	0.46
1:B:2215:VAL:N	1:B:2241:HIS:HD2	1.95	0.46
1:C:3355:PHE:CD1	1:C:3360:PRO:HG3	2.49	0.46
1:B:2409:ASP:HB3	1:B:2412:LYS:HB2	1.98	0.46
1:B:2179:SER:HB2	1:B:2187:GLY:HA3	1.98	0.46
1:B:2498:LYS:HB3	1:B:2514:LEU:HD11	1.97	0.46
1:B:2145:MET:HG3	1:B:2304:LEU:HD13	1.98	0.46
2:A:179:NAG:HO3	2:A:179:NAG:C7	2.29	0.46
1:C:3351:ASN:HB3	1:C:3466:GLY:O	2.16	0.46
1:C:3083:TYR:CZ	1:C:3108:ILE:HD13	2.51	0.45
1:C:3040:LEU:O	1:C:3041:GLU:C	2.54	0.45
1:C:3161:GLU:OE2	1:C:3498:LYS:HG2	2.16	0.45
1:B:2539:LEU:C	1:B:2541:ASP:H	2.19	0.45
3:A:182:SIA:H112	1:B:2277:THR:O	2.16	0.45
1:A:1371:GLY:HA2	1:A:1414:LYS:HE3	1.97	0.45
1:A:1389:VAL:HB	1:A:1424:VAL:HG11	1.99	0.45
1:C:3103:ASN:ND2	1:C:3476:PHE:HB3	2.30	0.45
1:A:1428:VAL:HB	1:A:1429:PRO:HD3	1.98	0.45
1:B:2262:LYS:HB3	1:B:2263:PRO:HD3	1.98	0.45
1:A:1551:PHE:C	1:A:1553:LYS:N	2.70	0.45
1:A:1284:HIS:O	1:A:1288:GLN:HG3	2.17	0.45
1:A:1291:GLU:HB2	5:A:285:SO4:O3	2.16	0.45
1:A:1451:TYR:CE2	1:A:1489:GLU:HG3	2.51	0.45
1:B:2241:HIS:O	1:B:2345:PRO:HD2	2.17	0.45
1:A:1330:LYS:HB3	1:A:1330:LYS:HE2	1.81	0.45
1:B:2149:ALA:HB1	1:B:2167:THR:HB	1.97	0.45
1:A:1246:GLU:HG2	1:A:1447:TYR:OH	2.16	0.45
1:B:2357:TRP:C	1:B:2360:PRO:HD2	2.37	0.45
1:A:1251:LEU:HB2	1:A:1429:PRO:HB3	1.99	0.45
1:A:1176:GLY:HA2	1:A:1189:TRP:HB2	1.99	0.45
1:A:1199:ARG:HH11	1:A:1199:ARG:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2343:THR:CB	1:B:2442:ALA:HB2	2.32	0.45
1:A:1287:ARG:HD2	5:A:185:SO4:O2	2.16	0.45
1:B:2539:LEU:O	1:B:2541:ASP:N	2.50	0.45
1:C:3023:PRO:HB2	1:C:3034:LEU:HD21	1.99	0.44
1:C:3505:ARG:NH1	7:C:8147:HOH:O	2.50	0.44
1:B:2333:GLU:CD	1:B:2333:GLU:H	2.20	0.44
1:C:3386:TYR:N	1:C:3387:PRO:CD	2.80	0.44
1:C:3455:PHE:CD2	1:C:3482:LYS:HD3	2.52	0.44
1:C:3140:HIS:CD2	1:C:3147:GLY:HA3	2.53	0.44
1:A:1333:GLU:H	1:A:1333:GLU:CD	2.21	0.44
1:C:3343:THR:HB	1:C:3442:ALA:CB	2.23	0.44
1:C:3317:PRO:HD3	1:C:3387:PRO:HB2	1.98	0.44
1:B:2452:ARG:HG2	1:B:2452:ARG:NH1	2.32	0.44
1:A:1199:ARG:HG2	1:A:1199:ARG:NH1	2.32	0.44
1:C:3205:ILE:HA	1:C:3205:ILE:HD12	1.84	0.44
1:B:2095:GLN:O	1:B:2099:GLU:HG3	2.18	0.44
1:B:2343:THR:HB	1:B:2442:ALA:CB	2.31	0.44
1:C:3373:LEU:HB2	1:C:3414:LYS:HB2	1.98	0.44
1:A:1197:ALA:O	1:A:1201:VAL:HG23	2.17	0.44
1:C:3140:HIS:HD2	1:C:3141:GLY:O	2.01	0.44
1:C:3064:ARG:CZ	7:C:8349:HOH:O	2.65	0.44
1:C:3333:GLU:N	1:C:3333:GLU:OE1	2.42	0.44
1:B:2438:ARG:HD2	1:B:2521:ASN:HA	2.00	0.44
1:A:1220:GLU:HA	1:A:1246:GLU:O	2.18	0.44
1:B:2395:LEU:HB3	1:B:2550:LEU:HD11	1.98	0.44
1:B:2143:GLY:O	1:B:2144:LEU:HB2	2.18	0.44
1:A:1453:PRO:HA	1:A:1489:GLU:OE1	2.18	0.44
1:A:1331:THR:HB	1:A:1333:GLU:OE1	2.18	0.44
1:C:3125:ALA:HB2	1:C:3133:LEU:CD1	2.48	0.43
1:A:1149:ALA:CB	1:A:1169:GLN:HG3	2.48	0.43
1:A:1312:PRO:HA	1:A:1315:SER:HB2	2.00	0.43
1:A:1131:ASN:HB2	7:A:8055:HOH:O	2.17	0.43
1:B:2372:GLN:HG2	1:B:2410:THR:CB	2.45	0.43
1:B:2400:THR:HG23	1:B:2404:LEU:HD12	2.01	0.43
1:A:1366:TYR:HA	1:A:1367:PRO:HD3	1.82	0.43
1:C:3357:TRP:O	1:C:3360:PRO:HD2	2.18	0.43
1:B:2107:ASN:HD22	1:B:2108:ILE:N	2.14	0.43
1:A:1392:ALA:HB3	1:A:1395:LEU:HG	2.01	0.43
1:C:3375:GLN:HE22	1:C:3400:THR:HG22	1.83	0.43
1:B:2241:HIS:C	1:B:2242:ARG:HD3	2.39	0.43
1:A:1306:LEU:HD11	1:A:1384:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3145:MET:SD	1:C:3173:GLY:HA2	2.59	0.43
1:C:3099:GLU:HG2	1:C:3107:ASN:OD1	2.19	0.43
1:B:2257:LYS:HB2	1:B:2322:VAL:HG12	2.01	0.43
1:C:3331:THR:OG1	1:C:3334:GLU:HG3	2.18	0.43
1:A:1252:THR:HG22	1:A:1254:VAL:HG12	2.00	0.43
1:B:2205:ILE:HD12	1:B:2205:ILE:HA	1.88	0.43
1:B:2218:PHE:CB	1:B:2244:ILE:HB	2.49	0.43
1:C:3220:GLU:OE2	1:C:3221:SER:HB2	2.19	0.42
1:A:1414:LYS:O	1:A:1418:LEU:HG	2.20	0.42
1:C:3306:LEU:HA	7:C:8507:HOH:O	2.18	0.42
1:B:2420:LEU:C	1:B:2420:LEU:HD23	2.39	0.42
1:B:2399:ALA:N	7:B:8203:HOH:O	2.52	0.42
1:B:2528:GLN:O	1:B:2533:THR:HA	2.19	0.42
1:A:1268:ILE:HG12	1:A:1301:MET:CE	2.48	0.42
1:C:3102:THR:OG1	1:C:3104:ARG:HG2	2.20	0.42
1:B:2312:PRO:HG3	1:B:2384:LYS:HA	2.02	0.42
1:C:3284:HIS:O	1:C:3288:GLN:HG2	2.19	0.42
1:A:1202:GLN:HG3	7:A:8014:HOH:O	2.20	0.42
1:A:1257:LYS:NZ	1:A:1319:LEU:HA	2.34	0.42
1:A:1186:ARG:HB3	1:A:1324:ASP:HB2	2.00	0.42
1:A:1152:TYR:CD1	1:A:1152:TYR:N	2.88	0.42
1:C:3452:ARG:HD2	1:C:3464:VAL:O	2.20	0.42
1:C:3549:ASN:O	1:C:3553:LYS:HG3	2.20	0.42
1:B:2025:VAL:CG2	1:B:2034:LEU:HD23	2.50	0.42
1:C:3313:ARG:HD3	1:C:3383:TRP:HH2	1.85	0.42
1:B:2553:LYS:HD3	7:B:8330:HOH:O	2.18	0.42
3:B:282:SIA:H111	1:C:3262:LYS:NZ	2.35	0.41
1:A:1372:GLN:HG3	1:A:1410:THR:CB	2.49	0.41
1:B:2538:LYS:HB3	1:B:2541:ASP:HB2	2.02	0.41
1:C:3495:MET:HE3	1:C:3533:THR:HG21	2.02	0.41
1:A:1256:VAL:O	1:A:1258:LYS:HE3	2.20	0.41
1:A:1086:MET:HG2	1:A:1111:LYS:O	2.19	0.41
1:C:3351:ASN:ND2	1:C:3449:PHE:HB3	2.34	0.41
1:B:2279:SER:O	1:B:2283:VAL:HG23	2.20	0.41
1:B:2264:LEU:HD11	1:B:2319:LEU:HD23	2.03	0.41
1:B:2312:PRO:HG3	1:B:2384:LYS:HD3	2.01	0.41
1:C:3442:ALA:HA	1:C:3443:PRO:HD3	1.90	0.41
1:A:1221:SER:HA	1:A:1247:SER:O	2.21	0.41
1:C:3380:SER:O	1:C:3384:LYS:HG2	2.20	0.41
1:B:2311:ASP:HA	1:B:2312:PRO:HD3	1.92	0.41
1:C:3237:LYS:HD3	1:C:3342:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1254:VAL:HG13	1:A:1255:LEU:HG	2.02	0.41
1:A:1418:LEU:HD12	7:A:8332:HOH:O	2.21	0.41
1:C:3125:ALA:HB2	1:C:3133:LEU:HD12	2.03	0.41
1:C:3527:LEU:HD11	1:C:3533:THR:HG22	2.02	0.41
1:B:2431:VAL:HG21	1:B:2540:LYS:HB2	2.02	0.41
1:A:1386:TYR:N	1:A:1387:PRO:CD	2.83	0.41
1:B:2349:GLY:HA3	1:B:2447:TYR:CZ	2.55	0.41
1:C:3266:GLU:O	1:C:3270:ILE:HG13	2.21	0.41
1:B:2086:MET:HG3	1:B:2112:LEU:HD23	2.02	0.41
1:B:2317:PRO:HD3	1:B:2387:PRO:HB2	2.03	0.41
1:A:1254:VAL:HG23	1:A:1387:PRO:O	2.21	0.41
1:B:2136:MET:HB3	1:B:2218:PHE:CE1	2.56	0.41
1:C:3461:PRO:HG2	1:C:3464:VAL:HG23	2.03	0.41
1:B:2367:PRO:C	1:B:2369:SER:H	2.23	0.40
1:A:1218:PHE:HA	1:A:1244:ILE:O	2.21	0.40
1:B:2495:MET:HG3	1:B:2514:LEU:HD22	2.03	0.40
1:C:3061:GLY:HA2	7:C:8349:HOH:O	2.21	0.40
1:A:1183:GLU:HG3	7:A:8431:HOH:O	2.21	0.40
1:A:1296:GLU:OE1	1:A:1296:GLU:HA	2.21	0.40
1:C:3120:ASN:HB2	1:C:3167:THR:OG1	2.21	0.40
1:B:2357:TRP:HD1	4:B:22:SUC:HO4	1.68	0.40
1:B:2350:ILE:C	1:B:2351:ASN:HD22	2.25	0.40
1:C:3435:ARG:HD2	7:C:8308:HOH:O	2.21	0.40
1:A:1498:LYS:NZ	1:A:1512:GLU:O	2.52	0.40
1:A:1468:HIS:CD2	6:A:1:NTJ:H1C2	2.55	0.40
1:C:3461:PRO:HG2	1:C:3464:VAL:CG2	2.52	0.40
1:A:1095:GLN:O	1:A:1099:GLU:HG3	2.21	0.40
1:B:2389:VAL:HB	1:B:2424:VAL:HG11	2.03	0.40
1:B:2254:VAL:O	1:B:2254:VAL:HG22	2.21	0.40
1:C:3078:LYS:HG3	3:C:382:SIA:O1A	2.21	0.40
1:C:3132:ARG:O	1:C:3211:ASN:HB2	2.22	0.40
1:C:3206:ALA:HA	1:C:3210:GLY:O	2.22	0.40
1:A:1487:GLU:O	1:A:1491:ARG:HB2	2.21	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	530/532 (100%)	493 (93%)	29 (6%)	8 (2%)	13	32
1	B	529/532 (99%)	491 (93%)	34 (6%)	4 (1%)	24	51
1	C	529/532 (99%)	505 (96%)	22 (4%)	2 (0%)	39	69
All	All	1588/1596 (100%)	1489 (94%)	85 (5%)	14 (1%)	21	49

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1237	LYS
1	A	1315	SER
1	B	2540	LYS
1	A	1310	GLY
1	A	1406	GLY
1	B	2368	LEU
1	B	2375	GLN
1	A	1185	SER
1	A	1253	SER
1	A	1339	ARG
1	C	3237	LYS
1	A	1375	GLN
1	C	3041	GLU
1	B	2397	PRO

### 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	448/448 (100%)	434 (97%)	14 (3%)	47	78
1	B	447/448 (100%)	435 (97%)	12 (3%)	52	82
1	C	447/448 (100%)	438 (98%)	9 (2%)	63	87
All	All	1342/1344 (100%)	1307 (97%)	35 (3%)	54	83

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1021	SER
1	A	1155	LEU
1	A	1162	ASN
1	A	1218	PHE
1	A	1258	LYS
1	A	1264	LEU
1	A	1299	LEU
1	A	1317	PRO
1	A	1366	TYR
1	A	1370	GLU
1	A	1450	GLN
1	A	1458	ASP
1	A	1465	ILE
1	A	1499	PHE
1	B	2027	ASP
1	B	2079	ASN
1	B	2107	ASN
1	B	2132	ARG
1	B	2155	LEU
1	B	2218	PHE
1	B	2220	GLU
1	B	2264	LEU
1	B	2316	GLN
1	B	2500	TRP
1	B	2505	ARG
1	B	2532	ASN
1	C	3155	LEU
1	C	3218	PHE
1	C	3220	GLU
1	C	3237	LYS
1	C	3258	LYS
1	C	3264	LEU
1	C	3299	LEU
1	C	3319	LEU

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Mol	Chain	Res	Type
1	C	3500	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1045	GLN
1	A	1131	ASN
1	A	1140	HIS
1	A	1162	ASN
1	A	1202	GLN
1	A	1241	HIS
1	A	1288	GLN
1	A	1309	GLN
1	A	1336	GLN
1	A	1351	ASN
1	A	1353	GLN
1	A	1375	GLN
1	A	1436	ASN
1	A	1450	GLN
1	A	1528	GLN
1	A	1532	ASN
1	A	1534	GLN
1	A	1537	GLN
1	B	2030	HIS
1	B	2045	GLN
1	B	2140	HIS
1	B	2202	GLN
1	B	2241	HIS
1	B	2351	ASN
1	B	2353	GLN
1	B	2372	GLN
1	B	2436	ASN
1	B	2450	GLN
1	B	2532	ASN
1	B	2534	GLN
1	B	2537	GLN
1	C	3045	GLN
1	C	3140	HIS
1	C	3241	HIS
1	C	3288	GLN
1	C	3353	GLN
1	C	3436	ASN

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Mol	Chain	Res	Type
1	C	3450	GLN
1	C	3506	ASN
1	C	3537	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 ⓘ

17 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
6	NTJ	A	1	1	3,7,7	1.37	0	4,8,8	2.27	3 (75%)
4	SUC	A	11	-	24,24,24	0.92	1 (4%)	36,36,36	0.87	1 (2%)
2	NAG	A	179	1	14,14,15	0.62	0	15,19,21	0.84	1 (6%)
3	SIA	A	182	-	17,21,21	1.07	1 (5%)	19,31,31	0.80	0
5	SO4	A	185	-	4,4,4	0.21	0	6,6,6	0.09	0
5	SO4	A	285	-	4,4,4	0.19	0	6,6,6	0.10	0
6	NTJ	B	2	1	3,7,7	1.30	0	4,8,8	2.32	3 (75%)
4	SUC	B	22	-	24,24,24	0.98	1 (4%)	36,36,36	0.73	0
2	NAG	B	279	1	14,14,15	0.53	0	15,19,21	0.73	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SIA	B	282	-	17,21,21	1.01	1 (5%)	19,31,31	1.00	1 (5%)
5	SO4	B	284	-	4,4,4	0.21	0	6,6,6	0.09	0
5	SO4	C	184	-	4,4,4	0.23	0	6,6,6	0.07	0
6	NTJ	C	3	1	3,7,7	1.41	0	4,8,8	2.27	3 (75%)
4	SUC	C	33	-	24,24,24	0.85	1 (4%)	36,36,36	0.71	0
2	NAG	C	379	1	14,14,15	0.69	0	15,19,21	0.73	0
3	SIA	C	382	-	17,21,21	0.87	1 (5%)	19,31,31	0.96	1 (5%)
5	SO4	C	384	-	4,4,4	0.19	0	6,6,6	0.08	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
6	NTJ	A	1	1	-	0/1/7/7	0/0/0/0
4	SUC	A	11	-	-	0/12/51/51	0/2/2/2
2	NAG	A	179	1	-	0/6/23/26	0/1/1/1
3	SIA	A	182	-	-	0/14/38/38	0/1/1/1
5	SO4	A	185	-	-	0/0/0/0	0/0/0/0
5	SO4	A	285	-	-	0/0/0/0	0/0/0/0
6	NTJ	B	2	1	-	0/1/7/7	0/0/0/0
4	SUC	B	22	-	-	0/12/51/51	0/2/2/2
2	NAG	B	279	1	-	1/6/23/26	0/1/1/1
3	SIA	B	282	-	-	1/14/38/38	0/1/1/1
5	SO4	B	284	-	-	0/0/0/0	0/0/0/0
5	SO4	C	184	-	-	0/0/0/0	0/0/0/0
6	NTJ	C	3	1	-	0/1/7/7	0/0/0/0
4	SUC	C	33	-	-	0/12/51/51	0/2/2/2
2	NAG	C	379	1	-	0/6/23/26	0/1/1/1
3	SIA	C	382	-	-	1/14/38/38	0/1/1/1
5	SO4	C	384	-	-	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	B	282	SIA	C7-C6	2.09	1.55	1.52
3	C	382	SIA	O6-C2	2.10	1.44	1.42
3	A	182	SIA	O6-C2	2.48	1.45	1.42
4	A	11	SUC	O5-C1	2.73	1.48	1.41
4	C	33	SUC	O5-C1	2.94	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	22	SUC	O5-C1	3.14	1.49	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2	NTJ	C1-N1-C2	-2.78	108.88	113.50
6	A	1	NTJ	P1-N1-C2	-2.72	108.97	121.74
6	C	3	NTJ	C1-N1-C2	-2.69	109.03	113.50
6	A	1	NTJ	C1-N1-C2	-2.64	109.12	113.50
6	B	2	NTJ	P1-N1-C2	-2.62	109.41	121.74
6	B	2	NTJ	P1-N1-C1	-2.62	109.41	121.74
6	C	3	NTJ	P1-N1-C2	-2.60	109.51	121.74
6	C	3	NTJ	P1-N1-C1	-2.55	109.76	121.74
6	A	1	NTJ	P1-N1-C1	-2.50	109.97	121.74
2	B	279	NAG	C2-N2-C7	-2.24	120.16	123.04
2	A	179	NAG	C3-C4-C5	2.03	113.73	110.20
4	A	11	SUC	C2'-O1-C1	2.26	123.49	117.53
3	C	382	SIA	O6-C6-C7	2.57	111.15	107.26
3	B	282	SIA	O6-C6-C7	2.79	111.49	107.26

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	279	NAG	O7-C7-N2-C2
3	C	382	SIA	O10-C10-N5-C5
3	B	282	SIA	O10-C10-N5-C5

There are no ring outliers.

12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1	NTJ	1	0
4	A	11	SUC	2	0
2	A	179	NAG	1	0
3	A	182	SIA	3	0
5	A	185	SO4	2	0
5	A	285	SO4	1	0
4	B	22	SUC	2	0
2	B	279	NAG	1	0
3	B	282	SIA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	184	SO4	1	0
4	C	33	SUC	1	0
3	C	382	SIA	7	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	532/532 (100%)	-0.38	15 (2%) 56 57	6, 23, 67, 86	0
1	B	531/532 (99%)	-0.16	25 (4%) 35 34	6, 28, 69, 83	0
1	C	531/532 (99%)	-0.46	5 (0%) 85 86	3, 21, 45, 79	0
All	All	1594/1596 (99%)	-0.33	45 (2%) 56 57	3, 24, 64, 86	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1370	GLU	5.9
1	B	2409	ASP	4.8
1	B	2404	LEU	4.3
1	B	2406	GLY	4.3
1	A	1340	ASN	3.9
1	B	2371	GLY	3.6
1	B	2405	GLY	3.5
1	A	1371	GLY	3.4
1	B	2410	THR	3.2
1	B	2407	THR	3.1
1	C	3342	HIS	3.0
1	B	2408	ASP	3.0
1	A	1021	SER	2.9
1	B	2370	GLU	2.8
1	B	2396	ILE	2.8
1	B	2342	HIS	2.7
1	B	2044	ALA	2.7
1	A	1341	PHE	2.6
1	B	2340	ASN	2.6
1	A	1307	ASP	2.6
1	A	1410	THR	2.5
1	B	2398	GLU	2.5
1	C	3027	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1376	LYS	2.3
1	C	3552	ALA	2.3
1	B	2401	GLU	2.3
1	A	1372	GLN	2.2
1	B	2374	ASP	2.2
1	B	2130	LYS	2.2
1	C	3340	ASN	2.2
1	B	2379	MET	2.2
1	A	1041	GLU	2.2
1	B	2312	PRO	2.2
1	C	3339	ARG	2.1
1	B	2377	THR	2.1
1	B	2373	LEU	2.1
1	A	1407	THR	2.1
1	A	1401	GLU	2.1
1	A	1378	ALA	2.1
1	A	1459	MET	2.0
1	B	2372	GLN	2.0
1	B	2313	ARG	2.0
1	B	2458	ASP	2.0
1	A	1342	HIS	2.0
1	B	2413	LYS	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	185	5/5	0.92	0.49	28.84	147,147,147,148	0
5	SO4	B	284	5/5	0.91	0.49	23.17	149,149,149,149	0
5	SO4	C	384	5/5	0.83	0.47	22.58	140,140,141,141	0
5	SO4	A	285	5/5	0.92	0.46	10.11	144,144,144,144	0
5	SO4	C	184	5/5	0.71	0.50	7.89	165,166,166,166	0
3	SIA	A	182	21/21	0.76	0.35	6.41	72,83,88,89	0
3	SIA	B	282	21/21	0.77	0.33	4.89	42,61,65,66	0
3	SIA	C	382	21/21	0.77	0.32	3.73	75,79,83,85	0
4	SUC	C	33	23/23	0.95	0.14	0.54	26,31,35,38	0
6	NTJ	C	3	8/8	0.96	0.18	0.53	36,40,42,45	0
4	SUC	A	11	23/23	0.87	0.23	0.35	47,54,67,70	0
6	NTJ	B	2	8/8	0.97	0.18	0.31	39,39,41,42	0
4	SUC	B	22	23/23	0.92	0.19	-0.13	58,61,63,64	0
6	NTJ	A	1	8/8	0.98	0.12	-0.82	38,39,42,43	0
2	NAG	A	179	14/15	0.61	0.37	-	55,59,62,62	0
2	NAG	B	279	14/15	0.83	0.49	-	64,69,71,71	0
2	NAG	C	379	14/15	0.72	0.45	-	61,66,69,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.