Full wwPDB X-ray Structure Validation Report (i)

Jun 2, 2016 – 06:30 PM EDT

PDB ID	:	1FV3
Title	:	THE HC FRAGMENT OF TETANUS TOXIN COMPLEXED WITH AN ANALOGUE OF ITS GANGLIOSIDE RECEPTOR GT1B
Authors	:	Fotinou, C.; Emsley, P.; Black, I.; Ando, H.; Ishida, H.; Kiso, M.; Sinha, K.A.; Fairweather, N.F.; Isaacs, N.W.
Deposited on	:	2000-09-18
Resolution	:	2.30 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:

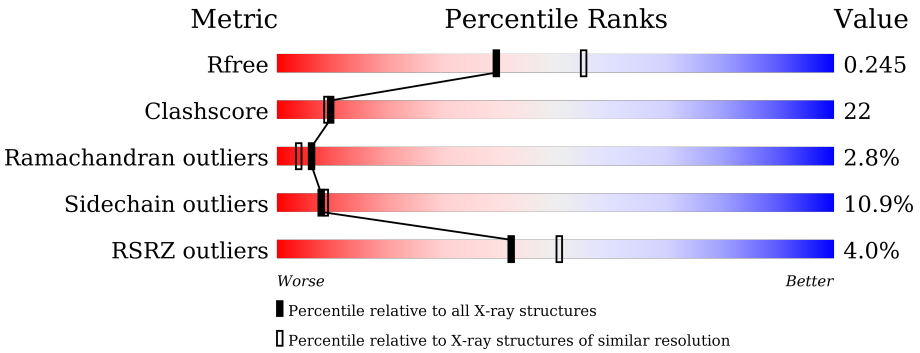
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	472	5% 49% 38% 7%
1	B	472	3% 61% 28% 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	SIA	B	5	-	-	-	X
2	SLB	B	6	-	-	-	X
2	SIA	B	7	X	-	-	X
3	PO4	B	301	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7786 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 TETANUS TOXIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	1	0
			3652	2336	612	694	10			
1	B	451	Total	C	N	O	S	0	0	0
			3648	2334	611	693	10			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	844	MET	-	SEE REMARK 999	? P04958
A	845	GLY	-	SEE REMARK 999	? P04958
A	846	SER	-	SEE REMARK 999	? P04958
A	847	SER	-	SEE REMARK 999	? P04958
A	848	HIS	-	SEE REMARK 999	? P04958
A	849	HIS	-	SEE REMARK 999	? P04958
A	850	HIS	-	SEE REMARK 999	? P04958
A	851	HIS	-	SEE REMARK 999	? P04958
A	852	HIS	-	SEE REMARK 999	? P04958
A	853	HIS	-	SEE REMARK 999	? P04958
A	854	SER	-	SEE REMARK 999	? P04958
A	855	SER	-	SEE REMARK 999	? P04958
A	856	GLY	-	SEE REMARK 999	? P04958
A	857	LEU	-	SEE REMARK 999	? P04958
A	858	VAL	-	SEE REMARK 999	? P04958
A	859	PRO	-	SEE REMARK 999	? P04958
A	860	ARG	-	SEE REMARK 999	? P04958
A	861	GLY	-	SEE REMARK 999	? P04958
A	862	SER	-	SEE REMARK 999	? P04958
A	863	HIS	-	SEE REMARK 999	? P04958
A	864	MET	-	SEE REMARK 999	? P04958
B	844	MET	-	SEE REMARK 999	? P04958
B	845	GLY	-	SEE REMARK 999	? P04958
B	846	SER	-	SEE REMARK 999	? P04958
B	847	SER	-	SEE REMARK 999	? P04958

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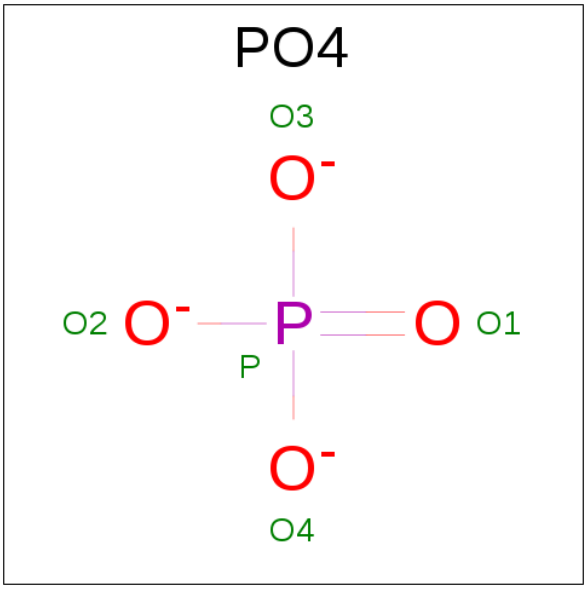
Chain	Residue	Modelled	Actual	Comment	Reference
B	848	HIS	-	SEE REMARK 999	? P04958
B	849	HIS	-	SEE REMARK 999	? P04958
B	850	HIS	-	SEE REMARK 999	? P04958
B	851	HIS	-	SEE REMARK 999	? P04958
B	852	HIS	-	SEE REMARK 999	? P04958
B	853	HIS	-	SEE REMARK 999	? P04958
B	854	SER	-	SEE REMARK 999	? P04958
B	855	SER	-	SEE REMARK 999	? P04958
B	856	GLY	-	SEE REMARK 999	? P04958
B	857	LEU	-	SEE REMARK 999	? P04958
B	858	VAL	-	SEE REMARK 999	? P04958
B	859	PRO	-	SEE REMARK 999	? P04958
B	860	ARG	-	SEE REMARK 999	? P04958
B	861	GLY	-	SEE REMARK 999	? P04958
B	862	SER	-	SEE REMARK 999	? P04958
B	863	HIS	-	SEE REMARK 999	? P04958
B	864	MET	-	SEE REMARK 999	? P04958

- Molecule 2 is a polymer of unknown type called SUGAR (7-MER).

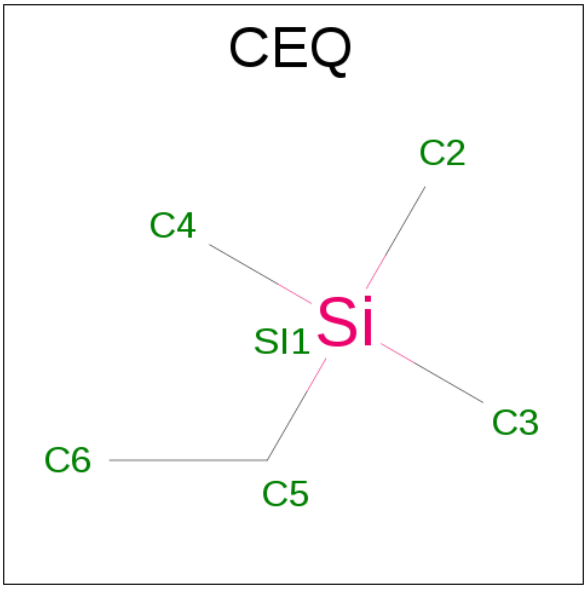
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	7	Total	C	N	O	0	0
			108	59	4	45		
2	B	7	Total	C	N	O	0	0
			108	59	4	45		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is ETHYL-TRIMETHYL-SILANE (three-letter code: CEQ) (formula: $C_5H_{14}Si$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Si 12 10 2	0	1
4	B	1	Total C Si 12 10 2	0	1

- Molecule 5 is water.

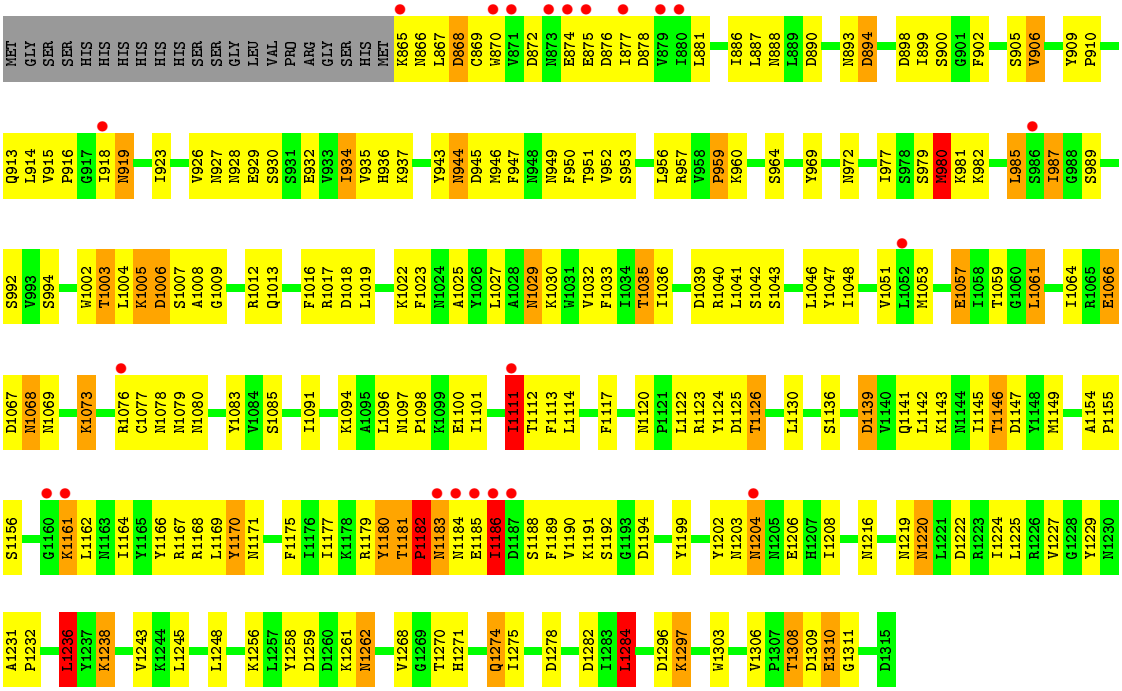
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	87	Total O 87 87	0	0
5	B	154	Total O 154 154	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

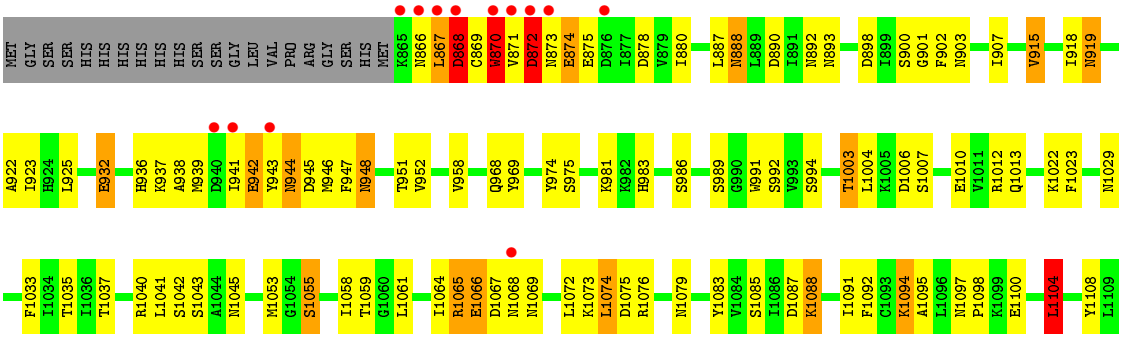
- Molecule 1: TETANUS TOXIN HEAVY CHAIN

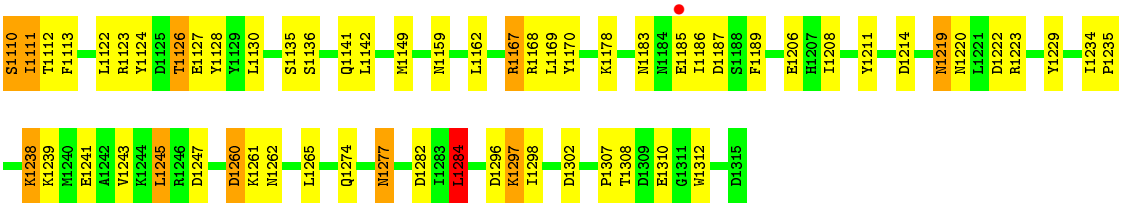
Chain A:



- Molecule 1: TETANUS TOXIN HEAVY CHAIN

Chain B:




S1110
I1111
T1112
F1113
L1122
R1123
Y1124
D1125
T1126
E1127
Y1128
Y1129
L1130
S1135
S1136
Q1141
L1142
M1149
N1159
L1162
R1167
R1168
L1169
Y1170
K1178
N1183
N1184
E1185
I1186
D1187
S1188
F1189
E1206
H1207
I1208
Y1211
D1214
N1219
N1220
L1221
D1222
R1223
Y1229
I1234
P1235
K1238
K1239
M1240
E1241
A1242
V1243
K1244
L1245
R1246
D1247
D1260
K1261
N1262
L1265
Q1274
N1277
D1282
I1283
L1284
D1296
K1297
I1298
D1302
P1307
T1308
D1309
E1310
G1311
W1312
D1315

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.31Å 53.07Å 118.28Å 90.00° 89.78° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-2.30) 96.5 (29.93-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.237 , 0.306 0.228 , 0.245	Depositor DCC
R_{free} test set	1541 reflections (3.20%)	DCC
Wilson B-factor (Å^2)	12.7	Xtriage
Anisotropy	0.846	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.29$, $< L^2 > = 0.13$	Xtriage
Estimated twinning fraction	0.225 for h,-k,-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	7786	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: BGC, NGA, PO4, SIA, GAL, CEQ, SLB

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	0/3740	1.07	20/5076 (0.4%)
1	B	0.94	1/3731 (0.0%)	1.13	19/5064 (0.4%)
All	All	0.85	1/7471 (0.0%)	1.10	39/10140 (0.4%)

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	A	0	1
2	B	1	0
All	All	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1229	TYR	CD2-CE2	-5.04	1.31	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1075	ASP	CB-CG-OD2	9.21	126.59	118.30
1	B	1222	ASP	CB-CG-OD2	8.71	126.14	118.30
1	B	1087	ASP	CB-CG-OD2	7.70	125.23	118.30
1	B	1104	LEU	CB-CG-CD1	-7.20	98.77	111.00
1	B	1282	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	945	ASP	CB-CG-OD2	6.91	124.52	118.30
1	A	1183	ASN	N-CA-C	6.88	129.57	111.00
1	A	980	MET	CB-CG-SD	-6.70	92.31	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1309	ASP	CB-CG-OD2	6.63	124.26	118.30
1	B	1260	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	872	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	1302	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	1067	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	868	ASP	CB-CG-OD2	6.24	123.91	118.30
1	A	1282	ASP	CB-CG-OD2	6.07	123.76	118.30
1	B	915	VAL	CB-CA-C	-5.99	100.03	111.40
1	B	1247	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	878	ASP	CB-CG-OD2	5.85	123.57	118.30
1	B	945	ASP	CB-CG-OD2	5.85	123.56	118.30
1	B	872	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	1222	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	1214	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	876	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	1125	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	898	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	878	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	890	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	1284	LEU	CA-CB-CG	5.57	128.11	115.30
1	B	1110	SER	N-CA-C	5.46	125.75	111.00
1	B	1104	LEU	CA-CB-CG	5.45	127.83	115.30
1	B	1296	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	1284	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	1168	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	894	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	1236	LEU	CA-CB-CG	-5.17	103.41	115.30
1	A	1186	ILE	CB-CA-C	-5.14	101.31	111.60
1	A	1216	ASN	N-CA-CB	5.10	119.79	110.60
1	A	1139	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	868	ASP	CB-CG-OD2	5.03	122.83	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	7	SIA	C2

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1182	PRO	Peptide

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	3652	0	3592	170	0
1	B	3648	0	3588	150	1
2	A	108	0	87	7	0
2	B	108	0	87	10	0
3	B	5	0	0	2	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
5	A	87	0	0	4	0
5	B	154	0	0	2	0
All	All	7786	0	7354	333	1

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 22.

All (333) 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:1145:ILE:H	1:A:1145:ILE:HD12	1.14	1.07
1:A:985:LEU:O	1:A:985:LEU:HD22	1.54	1.06
1:B:1064:ILE:O	1:B:1064:ILE:HG22	1.68	0.93
1:B:1111:ILE:HD12	1:B:1112:THR:H	1.33	0.92
1:B:1124:TYR:O	1:B:1126:THR:HG22	1.72	0.88
1:A:1297:LYS:O	1:A:1297:LYS:HE3	1.79	0.83
1:A:959:PRO:HA	1:A:1029:ASN:HB3	1.61	0.82
1:B:871:VAL:HG22	1:B:872:ASP:H	1.43	0.82
2:B:6:SLB:C8	2:B:7:SIA:O1B	2.26	0.79
1:A:1145:ILE:H	1:A:1145:ILE:CD1	1.88	0.79
1:B:871:VAL:HG23	1:B:874:GLU:HB3	1.65	0.78
1:A:932:GLU:HB3	1:A:1073:LYS:HB2	1.64	0.78
1:B:932:GLU:HB3	1:B:1073:LYS:HB2	1.66	0.78
1:B:1219:ASN:O	1:B:1220:ASN:HB3	1.84	0.78
1:B:946:MET:HE3	1:B:1065:ARG:HG2	1.65	0.76
1:B:939:MET:HA	1:B:943:TYR:HE1	1.49	0.76
1:B:1123:ARG:HB2	1:B:1126:THR:HG21	1.69	0.73
1:A:980:MET:CE	1:A:987:ILE:HG21	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:LYS:N	1:A:1161:LYS:HD3	2.04	0.72
1:B:1023:PHE:CD1	1:B:1167:ARG:HD2	2.25	0.72
1:A:926:VAL:HG12	1:A:927:ASN:H	1.53	0.71
1:B:888:ASN:HD22	1:B:888:ASN:C	1.93	0.71
1:B:936:HIS:HA	1:B:1069:ASN:HD22	1.55	0.71
1:B:874:GLU:HG3	1:B:875:GLU:N	2.05	0.71
1:A:1035:THR:HG23	1:A:1047:TYR:HB2	1.73	0.70
1:A:1261:LYS:HG3	1:A:1261:LYS:O	1.90	0.70
1:A:985:LEU:CD2	1:A:985:LEU:O	2.37	0.69
1:A:980:MET:HE2	1:A:987:ILE:HG21	1.73	0.69
1:B:1111:ILE:HD12	1:B:1112:THR:N	2.05	0.69
1:A:1124:TYR:O	1:A:1126:THR:HG22	1.93	0.69
1:A:909:TYR:HB3	1:A:910:PRO:HD2	1.75	0.69
1:B:871:VAL:HG23	1:B:874:GLU:CB	2.22	0.69
1:A:1145:ILE:N	1:A:1145:ILE:HD12	1.99	0.68
1:A:1262:ASN:O	1:A:1262:ASN:ND2	2.26	0.68
1:B:944:ASN:ND2	1:B:946:MET:HB2	2.09	0.68
1:A:1111:ILE:HD12	1:A:1111:ILE:H	1.57	0.67
1:A:1155:PRO:HB2	1:A:1168:ARG:HD3	1.76	0.67
1:B:874:GLU:HG3	1:B:875:GLU:HG2	1.76	0.67
1:B:1010:GLU:HG2	1:B:1061:LEU:HD23	1.77	0.67
1:A:1012:ARG:HD2	1:A:1057:GLU:O	1.95	0.66
1:B:915:VAL:HG23	1:B:922:ALA:HB3	1.77	0.66
1:B:936:HIS:HA	1:B:1069:ASN:ND2	2.10	0.66
1:B:1277:ASN:OD1	1:B:1277:ASN:C	2.34	0.66
1:A:1229:TYR:HB3	1:A:1236:LEU:HD13	1.77	0.65
1:A:1297:LYS:HE3	1:A:1297:LYS:HA	1.79	0.65
1:B:1260:ASP:O	1:B:1261:LYS:HD3	1.96	0.65
1:A:1270:THR:O	2:A:4:GAL:H61	1.97	0.64
1:B:1064:ILE:O	1:B:1064:ILE:CG2	2.42	0.64
1:B:871:VAL:HG23	1:B:874:GLU:HG2	1.78	0.64
1:B:918:ILE:HA	5:B:1397:HOH:O	1.95	0.64
1:A:972:ASN:ND2	1:A:1078:ASN:H	1.94	0.64
1:B:868:ASP:O	1:B:869:CYS:SG	2.56	0.64
1:A:1006:ASP:O	1:A:1006:ASP:OD1	2.16	0.63
1:A:919:ASN:O	1:A:919:ASN:ND2	2.32	0.63
1:A:869:CYS:SG	1:A:870:TRP:HE3	2.21	0.63
1:B:918:ILE:HD12	1:B:919:ASN:N	2.14	0.62
1:A:1208:ILE:HD13	1:A:1238:LYS:HG2	1.81	0.62
1:A:1142:LEU:HD13	1:A:1227:VAL:HG21	1.81	0.62
1:A:1047:TYR:CE1	1:A:1101:ILE:CD1	2.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:ASP:OD2	1:B:892:ASN:ND2	2.33	0.62
1:B:870:TRP:HE3	1:B:870:TRP:N	1.97	0.62
1:A:1112:THR:HG23	1:A:1113:PHE:HD1	1.65	0.62
1:B:1219:ASN:O	1:B:1220:ASN:CB	2.48	0.61
1:B:1310:GLU:O	1:B:1310:GLU:HG3	2.00	0.61
1:B:947:PHE:O	1:B:1040:ARG:HG3	2.00	0.61
1:B:981:LYS:HA	1:B:1067:ASP:HB2	1.83	0.61
2:A:5:SIA:H7	2:A:5:SIA:O10	2.01	0.61
1:B:900:SER:O	1:B:902:PHE:N	2.34	0.61
1:A:894:ASP:N	5:A:1390:HOH:O	2.33	0.60
1:B:871:VAL:CG2	1:B:874:GLU:HG2	2.30	0.60
1:B:925:LEU:HD13	1:B:1073:LYS:HA	1.83	0.60
1:B:938:ALA:N	1:B:942:GLU:OE2	2.34	0.60
1:A:1224:ILE:HD13	1:A:1275:ILE:HD11	1.82	0.60
1:A:1122:LEU:HD11	1:A:1177:ILE:HD12	1.83	0.60
1:A:1114:LEU:HD21	1:A:1192:SER:HB2	1.83	0.60
1:B:983:HIS:HB2	1:B:986:SER:O	2.01	0.60
1:B:871:VAL:HG22	1:B:872:ASP:N	2.15	0.60
1:B:918:ILE:HD12	1:B:918:ILE:C	2.22	0.60
1:A:1022:LYS:HZ2	1:A:1164:ILE:HB	1.67	0.59
1:A:1139:ASP:OD2	1:A:1154:ALA:HB2	2.03	0.59
1:A:1142:LEU:HD11	1:A:1227:VAL:HB	1.82	0.59
1:B:1094:LYS:HG3	1:B:1095:ALA:O	2.02	0.59
2:A:5:SIA:H7	2:A:5:SIA:C10	2.33	0.58
1:B:1239:LYS:NZ	1:B:1262:ASN:OD1	2.26	0.58
1:A:1297:LYS:HE3	1:A:1297:LYS:CA	2.33	0.58
1:A:935:VAL:O	1:A:1069:ASN:HA	2.02	0.58
1:B:968:GLN:HG3	1:B:969:TYR:CE2	2.38	0.58
1:A:1111:ILE:HD12	1:A:1111:ILE:N	2.19	0.58
1:B:991:TRP:HB3	1:B:1004:LEU:HD23	1.85	0.58
1:A:1098:PRO:HA	1:A:1101:ILE:HB	1.86	0.57
1:B:871:VAL:HG23	1:B:874:GLU:CG	2.33	0.57
1:A:1297:LYS:CE	1:A:1297:LYS:O	2.52	0.57
2:B:1:BGC:H6C1	2:B:2:GAL:H1	1.86	0.57
1:A:909:TYR:HB3	1:A:910:PRO:CD	2.34	0.57
1:B:1277:ASN:OD1	1:B:1277:ASN:O	2.23	0.57
1:B:1037:THR:OG1	1:B:1045:ASN:HB2	2.04	0.56
1:A:1259:ASP:C	1:A:1259:ASP:OD1	2.44	0.56
1:A:1018:ASP:OD2	1:A:1027:LEU:N	2.34	0.56
1:B:1169:LEU:HD12	1:B:1312:TRP:CD1	2.41	0.56
1:B:1023:PHE:CE1	1:B:1167:ARG:HD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1178:LYS:HE3	1:B:1206:GLU:OE1	2.06	0.56
1:B:1241:GLU:HG2	1:B:1243:VAL:HG13	1.86	0.56
1:A:992:SER:OG	1:A:1003:THR:HG23	2.06	0.55
1:A:1036:ILE:HD11	1:A:1046:LEU:HD13	1.88	0.55
1:A:1130:LEU:HD22	1:A:1303:TRP:CE3	2.42	0.55
1:A:1145:ILE:O	1:A:1146:THR:HB	2.05	0.55
1:A:980:MET:HE3	1:A:987:ILE:HG21	1.89	0.55
2:B:3:NGA:H1	2:B:6:SLB:C1	2.36	0.55
1:B:1310:GLU:O	1:B:1310:GLU:CG	2.55	0.55
1:B:1010:GLU:HG2	1:B:1061:LEU:CD2	2.37	0.55
1:B:887:LEU:HD12	1:B:898:ASP:OD1	2.06	0.55
1:A:1111:ILE:HG13	1:A:1248:LEU:HD11	1.88	0.55
1:B:892:ASN:O	1:B:893:ASN:HB2	2.06	0.55
1:A:1143:LYS:HB3	1:A:1147:ASP:HB3	1.89	0.54
1:A:913:GLN:C	1:A:914:LEU:HD23	2.28	0.54
1:A:1035:THR:CG2	1:A:1047:TYR:HB2	2.37	0.54
1:A:1006:ASP:C	1:A:1006:ASP:OD1	2.46	0.54
1:A:979:SER:O	1:A:1066:GLU:HB2	2.07	0.54
1:A:1164:ILE:O	1:A:1164:ILE:HG13	2.06	0.54
1:A:952:VAL:HG22	1:A:1091:ILE:HD13	1.89	0.54
1:B:974:TYR:O	1:B:994:SER:HB2	2.06	0.54
1:B:1003:THR:HB	1:B:1013:GLN:HE21	1.72	0.54
1:B:1110:SER:O	1:B:1112:THR:N	2.41	0.54
1:A:1096:LEU:HA	1:A:1100:GLU:OE1	2.08	0.54
1:A:1202:TYR:O	1:A:1203:ASN:HB2	2.08	0.54
1:B:1042:SER:OG	1:B:1043:SER:N	2.40	0.54
1:A:1122:LEU:HD12	1:A:1190:VAL:HG21	1.89	0.53
1:A:893:ASN:O	1:A:894:ASP:HB2	2.08	0.53
1:A:1208:ILE:CD1	1:A:1238:LYS:HG2	2.37	0.53
1:A:1061:LEU:N	1:A:1061:LEU:HD23	2.24	0.53
1:A:1048:ILE:HD12	1:A:1053:MET:HG3	1.91	0.53
1:A:937:LYS:NZ	1:A:1066:GLU:OE1	2.41	0.53
1:A:906:VAL:HA	1:A:934:ILE:O	2.09	0.53
1:A:1123:ARG:NH2	1:A:1189:PHE:CE2	2.77	0.53
1:B:1083:TYR:OH	1:B:1310:GLU:HG2	2.08	0.53
1:A:969:TYR:CD2	1:A:1079:ASN:HB2	2.44	0.53
1:A:980:MET:O	1:A:980:MET:HG2	2.09	0.53
1:B:1123:ARG:HB2	1:B:1126:THR:CG2	2.35	0.53
1:B:870:TRP:CE3	1:B:870:TRP:N	2.77	0.53
1:A:989:SER:O	1:A:1066:GLU:HB3	2.09	0.52
1:A:1162:LEU:O	1:A:1164:ILE:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1097:ASN:HB2	1:B:1098:PRO:HD2	1.91	0.52
1:B:1023:PHE:CE2	1:B:1136:SER:HB2	2.44	0.52
1:A:1023:PHE:CE2	1:A:1136:SER:HB2	2.44	0.52
1:A:887:LEU:HD23	1:A:1091:ILE:HG13	1.92	0.52
1:A:1155:PRO:O	1:A:1168:ARG:HG3	2.10	0.52
1:A:1180:TYR:OH	1:A:1238:LYS:NZ	2.40	0.52
1:B:1088:LYS:HG2	1:B:1108:TYR:CE1	2.44	0.52
1:B:939:MET:HA	1:B:943:TYR:CE1	2.39	0.52
1:A:1111:ILE:H	1:A:1111:ILE:CD1	2.19	0.52
2:A:1:BGC:H6C1	2:A:2:GAL:H1	1.89	0.52
1:A:1141:GLN:HG3	1:A:1142:LEU:N	2.25	0.52
1:A:1145:ILE:O	1:A:1146:THR:CB	2.58	0.51
1:B:946:MET:CE	1:B:1065:ARG:HG2	2.38	0.51
1:B:1169:LEU:HD12	1:B:1312:TRP:NE1	2.24	0.51
1:A:950:PHE:HZ	1:A:1004:LEU:HD21	1.75	0.51
1:B:952:VAL:O	1:B:1035:THR:HA	2.10	0.51
1:B:1067:ASP:C	1:B:1069:ASN:H	2.12	0.51
1:B:1169:LEU:HD12	1:B:1312:TRP:CE2	2.46	0.51
1:B:1076:ARG:HG3	1:B:1076:ARG:HH21	1.75	0.51
1:B:888:ASN:ND2	1:B:888:ASN:C	2.64	0.51
1:A:1271:HIS:HE1	2:A:3:NGA:O4	1.93	0.51
1:B:936:HIS:CD2	1:B:1069:ASN:HD21	2.29	0.51
1:A:926:VAL:HG12	1:A:927:ASN:N	2.25	0.51
1:A:906:VAL:HG13	1:A:935:VAL:HG13	1.92	0.51
2:B:6:SLB:H8	2:B:7:SIA:O1B	2.08	0.51
1:A:969:TYR:CE2	1:A:1079:ASN:HB2	2.46	0.50
1:A:1199:TYR:CD2	1:A:1206:GLU:HB3	2.45	0.50
1:B:1065:ARG:HB3	1:B:1065:ARG:CZ	2.41	0.50
1:A:1047:TYR:HA	1:A:1051:VAL:O	2.10	0.50
1:A:972:ASN:HD21	1:A:1077:CYS:HA	1.76	0.50
2:A:5:SIA:C7	2:A:5:SIA:O10	2.59	0.50
1:B:1220:ASN:ND2	1:B:1220:ASN:O	2.44	0.50
1:A:1186:ILE:H	1:A:1186:ILE:HD13	1.77	0.50
1:A:1022:LYS:NZ	1:A:1164:ILE:HB	2.27	0.50
1:B:932:GLU:HB3	1:B:1073:LYS:CD	2.42	0.50
1:A:1122:LEU:HD12	1:A:1190:VAL:CG2	2.42	0.49
1:A:1297:LYS:HE3	1:A:1297:LYS:C	2.31	0.49
1:B:869:CYS:HB2	1:B:1094:LYS:HB3	1.93	0.49
1:B:992:SER:OG	1:B:1003:THR:HG23	2.11	0.49
1:B:1169:LEU:CD1	1:B:1312:TRP:CE2	2.96	0.49
1:B:1219:ASN:ND2	2:B:3:NGA:O4	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:ASP:OD2	1:A:1039:ASP:C	2.49	0.49
1:A:972:ASN:HD21	1:A:1078:ASN:H	1.59	0.49
1:B:1074:LEU:N	1:B:1074:LEU:HD23	2.27	0.49
1:B:969:TYR:CD2	1:B:1079:ASN:HB2	2.47	0.49
1:B:1110:SER:O	1:B:1110:SER:OG	2.20	0.49
1:A:985:LEU:C	1:A:985:LEU:HD22	2.31	0.49
1:B:874:GLU:HG3	1:B:875:GLU:H	1.77	0.49
1:B:1007:SER:OG	1:B:1065:ARG:HG3	2.12	0.49
1:B:1123:ARG:CB	1:B:1126:THR:HG21	2.41	0.49
1:B:1067:ASP:OD2	1:B:1069:ASN:HB2	2.13	0.49
1:A:1047:TYR:CZ	1:A:1101:ILE:HD12	2.48	0.48
1:A:947:PHE:O	1:A:1040:ARG:HG3	2.13	0.48
1:B:1297:LYS:HG2	1:B:1298:ILE:HG13	1.94	0.48
1:A:1169:LEU:O	1:A:1170:TYR:HB2	2.14	0.48
1:B:937:LYS:HG2	1:B:942:GLU:OE1	2.13	0.48
1:B:946:MET:O	1:B:1040:ARG:NH1	2.36	0.48
1:A:1061:LEU:HD23	1:A:1061:LEU:H	1.79	0.48
1:B:872:ASP:O	1:B:873:ASN:ND2	2.47	0.48
1:B:1088:LYS:HD2	1:B:1088:LYS:N	2.29	0.48
1:B:918:ILE:O	1:B:919:ASN:HB2	2.13	0.48
1:A:1225:LEU:HD11	1:A:1268:VAL:HG13	1.96	0.47
1:B:1067:ASP:C	1:B:1069:ASN:N	2.67	0.47
1:B:1111:ILE:CD1	1:B:1112:THR:N	2.75	0.47
1:A:1179:ARG:NH1	1:A:1179:ARG:HG3	2.30	0.47
1:B:1128:TYR:HE1	1:B:1307:PRO:HG3	1.79	0.47
1:A:1139:ASP:OD2	1:A:1154:ALA:CB	2.63	0.47
1:A:1271:HIS:CE1	2:A:3:NGA:O4	2.68	0.47
1:A:1274[B]:GLN:NE2	1:A:1278:ASP:O	2.45	0.47
1:B:1128:TYR:CE1	1:B:1307:PRO:HG3	2.49	0.47
2:B:1:BGC:H6C1	2:B:2:GAL:C1	2.44	0.47
1:A:1130:LEU:HD12	1:A:1175:PHE:CZ	2.50	0.47
1:A:923:ILE:O	1:A:1085:SER:HA	2.15	0.47
1:A:1256:LYS:HD3	1:A:1258:TYR:CZ	2.49	0.47
1:A:957:ARG:NH1	1:A:1120:ASN:HD21	2.13	0.47
1:A:951:THR:HG21	1:A:1096:LEU:HD12	1.95	0.47
1:A:1175:PHE:N	1:A:1175:PHE:CD1	2.83	0.47
1:B:1141:GLN:HG3	1:B:1142:LEU:N	2.30	0.47
2:B:6:SLB:C7	2:B:7:SIA:O1B	2.63	0.47
1:B:874:GLU:CG	1:B:875:GLU:N	2.77	0.47
1:A:1130:LEU:HA	1:A:1130:LEU:HD23	1.70	0.47
1:B:1211:TYR:CE1	1:B:1223:ARG:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:989:SER:OG	1:B:1006:ASP:C	2.54	0.46
1:A:1003:THR:HB	1:A:1013:GLN:HG2	1.97	0.46
1:A:956:LEU:HD12	1:A:957:ARG:H	1.81	0.46
1:B:869:CYS:C	1:B:870:TRP:HE3	2.19	0.46
1:A:1297:LYS:CE	1:A:1297:LYS:HA	2.45	0.46
1:A:1179:ARG:HH11	1:A:1179:ARG:HG3	1.80	0.46
1:A:1170:TYR:CE1	1:A:1308:THR:HA	2.51	0.46
1:A:928:ASN:O	1:A:930:SER:N	2.49	0.46
1:B:1223:ARG:NH1	1:B:1265:LEU:O	2.49	0.46
1:B:918:ILE:CD1	1:B:918:ILE:C	2.83	0.46
1:B:941:ILE:HG22	1:B:941:ILE:O	2.15	0.46
1:A:1047:TYR:CE1	1:A:1101:ILE:HD12	2.51	0.46
1:B:868:ASP:CG	1:B:869:CYS:H	2.19	0.46
1:A:914:LEU:N	1:A:914:LEU:HD23	2.31	0.46
1:B:1012:ARG:HA	1:B:1012:ARG:HD3	1.61	0.46
1:B:1297:LYS:HE2	1:B:1298:ILE:CD1	2.46	0.46
1:A:877:ILE:O	1:A:881:LEU:HG	2.16	0.45
1:B:1243:VAL:HG21	1:B:1245:LEU:HD22	1.98	0.45
2:B:6:SLB:H7	2:B:7:SIA:O1B	2.16	0.45
1:B:981:LYS:HG2	1:B:983:HIS:CE1	2.51	0.45
1:A:951:THR:HG21	1:A:1096:LEU:CD1	2.46	0.45
1:A:1191:LYS:HB2	1:A:1194:ASP:OD1	2.17	0.45
2:B:3:NGA:H1	2:B:6:SLB:O1A	2.16	0.45
1:B:907:ILE:HG12	1:B:936:HIS:HE1	1.82	0.45
1:B:952:VAL:HG22	1:B:1091:ILE:HD13	1.98	0.45
1:B:1149:MET:HB2	1:B:1284:LEU:HG	1.99	0.45
1:B:1260:ASP:OD1	1:B:1260:ASP:N	2.49	0.45
1:B:944:ASN:HD22	1:B:946:MET:HB2	1.82	0.45
1:A:1030:LYS:HE3	1:A:1117:PHE:CZ	2.52	0.45
1:B:1110:SER:OG	1:B:1112:THR:HG22	2.16	0.45
1:B:1045:ASN:OD1	1:B:1055:SER:HB3	2.17	0.45
1:B:1211:TYR:CD1	1:B:1223:ARG:HB3	2.52	0.45
1:B:1033:PHE:CE2	1:B:1035:THR:CG2	2.99	0.45
1:B:1185:GLU:HG3	1:B:1185:GLU:O	2.16	0.45
1:A:1039:ASP:OD2	1:A:1041:LEU:N	2.45	0.44
1:A:1231:ALA:HA	1:A:1232:PRO:HD2	1.86	0.44
1:A:1149:MET:CB	1:A:1284:LEU:HG	2.47	0.44
1:B:1297:LYS:HE2	1:B:1298:ILE:HD12	2.00	0.44
1:A:1002:TRP:O	1:A:1013:GLN:HG2	2.18	0.44
1:A:1083:TYR:OH	1:A:1310:GLU:HB2	2.17	0.44
1:A:1022:LYS:HZ1	1:A:1164:ILE:CG2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1261:LYS:O	1:A:1262:ASN:OD1	2.35	0.44
1:B:1159:ASN:ND2	1:B:1162:LEU:HD12	2.32	0.44
1:A:951:THR:HA	1:A:1036:ILE:O	2.18	0.44
1:A:1036:ILE:CD1	1:A:1046:LEU:HD13	2.47	0.44
1:A:943:TYR:O	1:A:944:ASN:C	2.55	0.44
1:B:1065:ARG:HB2	3:B:301:PO4:O2	2.18	0.44
1:A:1033:PHE:HD2	5:A:1352:HOH:O	1.99	0.44
1:A:886:ILE:HA	1:A:902:PHE:HE1	1.82	0.43
1:B:869:CYS:O	1:B:871:VAL:N	2.45	0.43
1:A:1097:ASN:O	1:A:1100:GLU:HB2	2.18	0.43
1:A:953:SER:HA	1:A:1035:THR:HA	2.01	0.43
1:A:1261:LYS:O	1:A:1262:ASN:CG	2.56	0.43
1:A:915:VAL:HB	1:A:916:PRO:HD2	1.99	0.43
1:B:1012:ARG:HH21	1:B:1058:ILE:HA	1.83	0.43
1:A:1122:LEU:CD1	1:A:1190:VAL:HG21	2.49	0.43
1:A:1005:LYS:HE3	1:A:1009:GLY:HA2	2.00	0.43
1:A:1117:PHE:HB2	1:A:1306:VAL:HG22	2.01	0.43
1:B:871:VAL:CG2	1:B:872:ASP:H	2.22	0.43
1:B:939:MET:O	5:B:1417:HOH:O	2.21	0.43
1:A:886:ILE:HA	1:A:902:PHE:CE1	2.54	0.43
1:B:1065:ARG:O	1:B:1066:GLU:O	2.37	0.43
1:A:1079:ASN:C	1:A:1079:ASN:OD1	2.57	0.42
1:A:1219:ASN:O	1:A:1220:ASN:CB	2.66	0.42
1:A:1016:PHE:CE1	1:A:1053:MET:HE2	2.54	0.42
1:A:937:LYS:HE2	1:A:1068:ASN:HA	2.01	0.42
1:A:1124:TYR:CE1	1:A:1177:ILE:HG22	2.54	0.42
1:A:1149:MET:HB3	1:A:1284:LEU:HG	2.01	0.42
1:B:1110:SER:O	1:B:1112:THR:HG22	2.20	0.42
1:B:1041:LEU:HA	1:B:1041:LEU:HD23	1.80	0.42
1:B:1234:ILE:HA	1:B:1235:PRO:HD3	1.79	0.42
1:A:1181:THR:HA	1:A:1182:PRO:HD3	1.84	0.42
1:A:1017:ARG:HA	1:A:1017:ARG:HD2	1.93	0.42
1:A:1124:TYR:CZ	1:A:1179:ARG:HG2	2.55	0.42
1:B:1072:LEU:HD12	1:B:1072:LEU:N	2.34	0.42
1:B:867:LEU:O	1:B:948:ASN:ND2	2.52	0.42
1:B:923:ILE:O	1:B:1085:SER:HA	2.19	0.41
1:A:1122:LEU:HD11	1:A:1177:ILE:CD1	2.48	0.41
1:B:1208:ILE:HD11	1:B:1238:LYS:HD3	2.01	0.41
1:A:869:CYS:SG	1:A:870:TRP:CE3	3.08	0.41
1:A:1022:LYS:HZ1	1:A:1164:ILE:HG22	1.86	0.41
1:A:865:LYS:HG3	1:A:868:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:ASN:HB3	1:A:899:ILE:HG13	2.02	0.41
1:B:871:VAL:HG11	1:B:880:ILE:CG2	2.51	0.41
1:A:1169:LEU:O	1:A:1170:TYR:CB	2.68	0.41
1:A:909:TYR:CB	1:A:910:PRO:CD	2.97	0.41
1:B:969:TYR:CG	1:B:1079:ASN:HB2	2.56	0.41
1:B:1113:PHE:HE2	1:B:1189:PHE:CB	2.33	0.41
1:A:1006:ASP:O	1:A:1008:ALA:N	2.54	0.41
1:B:903:ASN:HD22	1:B:903:ASN:N	2.19	0.41
1:A:1156:SER:HB2	5:A:1319:HOH:O	2.20	0.41
1:B:1022:LYS:HD3	1:B:1022:LYS:HA	1.74	0.41
1:B:902:PHE:O	1:B:903:ASN:HB2	2.20	0.41
1:A:1097:ASN:N	1:A:1100:GLU:OE1	2.48	0.40
1:A:960:LYS:HE2	1:A:1166:TYR:CZ	2.56	0.40
1:A:899:ILE:C	1:A:900:SER:O	2.57	0.40
1:B:1033:PHE:CE2	1:B:1104:LEU:HD13	2.56	0.40
1:A:1203:ASN:O	1:A:1204:ASN:CB	2.69	0.40
1:A:867:LEU:HA	1:A:867:LEU:HD23	1.94	0.40
1:A:913:GLN:O	1:A:914:LEU:HD23	2.20	0.40
1:A:959:PRO:HB3	1:A:1311:GLY:HA2	2.03	0.40
1:B:951:THR:HB	1:B:1092:PHE:HB2	2.03	0.40
1:B:1170:TYR:CE1	1:B:1308:THR:HA	2.56	0.40
1:B:944:ASN:HA	1:B:944:ASN:HD22	1.62	0.40
1:A:868:ASP:OD1	1:A:949:ASN:ND2	2.46	0.40
1:B:1067:ASP:O	1:B:1069:ASN:N	2.55	0.40
2:B:1:BGC:C6	2:B:2:GAL:H1	2.51	0.40
1:B:1007:SER:HG	3:B:301:PO4:P	2.44	0.40
1:A:936:HIS:NE2	5:A:1387:HOH:O	2.37	0.40
1:B:1097:ASN:ND2	1:B:1100:GLU:CD	2.75	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:873:ASN:O	1:B:1127:GLU:OE1[1_565]	2.17	0.03

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	450/472 (95%)	399 (89%)	38 (8%)	13 (3%)	6	3
1	B	449/472 (95%)	396 (88%)	41 (9%)	12 (3%)	6	4
All	All	899/944 (95%)	795 (88%)	79 (9%)	25 (3%)	6	4

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	929	GLU
1	A	1025	ALA
1	A	1182	PRO
1	B	870	TRP
1	B	1066	GLU
1	B	1111	ILE
1	A	1111	ILE
1	A	1180	TYR
1	B	868	ASP
1	B	872	ASP
1	B	901	GLY
1	B	919	ASN
1	B	1187	ASP
1	A	981	LYS
1	A	1007	SER
1	B	1183	ASN
1	A	874	GLU
1	A	919	ASN
1	B	1029	ASN
1	A	866	ASN
1	A	944	ASN
1	A	1042	SER
1	A	1170	TYR
1	B	948	ASN
1	B	1219	ASN

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	408/425 (96%)	350 (86%)	58 (14%)	4 4
1	B	407/425 (96%)	375 (92%)	32 (8%)	15 19
All	All	815/850 (96%)	725 (89%)	90 (11%)	8 8

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	875	GLU
1	A	905	SER
1	A	906	VAL
1	A	918	ILE
1	A	934	ILE
1	A	946	MET
1	A	959	PRO
1	A	964	SER
1	A	977	ILE
1	A	980	MET
1	A	982	LYS
1	A	985	LEU
1	A	987	ILE
1	A	994	SER
1	A	1003	THR
1	A	1005	LYS
1	A	1006	ASP
1	A	1019	LEU
1	A	1029	ASN
1	A	1032	VAL
1	A	1035	THR
1	A	1043	SER
1	A	1057	GLU
1	A	1059	THR
1	A	1061	LEU
1	A	1064	ILE
1	A	1066	GLU

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Mol	Chain	Res	Type
1	A	1068	ASN
1	A	1073	LYS
1	A	1076	ARG
1	A	1080	ASN
1	A	1094	LYS
1	A	1111	ILE
1	A	1126	THR
1	A	1146	THR
1	A	1161	LYS
1	A	1167	ARG
1	A	1171	ASN
1	A	1181	THR
1	A	1183	ASN
1	A	1184	ASN
1	A	1185	GLU
1	A	1186	ILE
1	A	1188	SER
1	A	1204	ASN
1	A	1220	ASN
1	A	1236	LEU
1	A	1238	LYS
1	A	1243	VAL
1	A	1245	LEU
1	A	1262	ASN
1	A	1274[A]	GLN
1	A	1274[B]	GLN
1	A	1284	LEU
1	A	1296	ASP
1	A	1297	LYS
1	A	1308	THR
1	A	1310	GLU
1	B	866	ASN
1	B	867	LEU
1	B	870	TRP
1	B	874	GLU
1	B	888	ASN
1	B	932	GLU
1	B	942	GLU
1	B	944	ASN
1	B	958	VAL
1	B	975	SER
1	B	1003	THR

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Mol	Chain	Res	Type
1	B	1053	MET
1	B	1055	SER
1	B	1059	THR
1	B	1065	ARG
1	B	1068	ASN
1	B	1074	LEU
1	B	1088	LYS
1	B	1094	LYS
1	B	1104	LEU
1	B	1122	LEU
1	B	1126	THR
1	B	1130	LEU
1	B	1135	SER
1	B	1167	ARG
1	B	1186	ILE
1	B	1238	LYS
1	B	1245	LEU
1	B	1274	GLN
1	B	1277	ASN
1	B	1284	LEU
1	B	1297	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	903	ASN
1	A	972	ASN
1	A	1045	ASN
1	A	1171	ASN
1	A	1184	ASN
1	A	1220	ASN
1	B	873	ASN
1	B	892	ASN
1	B	903	ASN
1	B	928	ASN
1	B	936	HIS
1	B	944	ASN
1	B	1013	GLN
1	B	1029	ASN
1	B	1068	ASN
1	B	1069	ASN
1	B	1078	ASN

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Mol	Chain	Res	Type
1	B	1216	ASN
1	B	1220	ASN
1	B	1274	GLN
1	B	1293	HIS

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

14 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	BGC	A	1	2,4	11,11,12	1.39	2 (18%)	15,15,17	1.66	5 (33%)
2	GAL	A	2	2	10,10,12	0.98	0	12,13,17	1.52	2 (16%)
2	NGA	A	3	2	14,14,15	0.81	0	11,19,21	1.39	3 (27%)
2	GAL	A	4	2	11,11,12	0.64	0	11,15,17	0.98	0
2	SIA	A	5	2	18,21,21	1.68	2 (11%)	18,31,31	3.09	2 (11%)
2	SLB	A	6	2	18,21,21	1.04	1 (5%)	18,31,31	2.31	8 (44%)
2	SIA	A	7	2	17,20,21	0.66	0	18,28,31	1.16	2 (11%)
2	BGC	B	1	2,4	11,11,12	0.90	0	15,15,17	1.53	5 (33%)
2	GAL	B	2	2	10,10,12	1.33	1 (10%)	12,13,17	1.63	3 (25%)
2	NGA	B	3	2	14,14,15	0.64	0	11,19,21	1.49	1 (9%)
2	GAL	B	4	2	11,11,12	1.30	3 (27%)	11,15,17	0.59	0
2	SIA	B	5	2	18,21,21	1.92	2 (11%)	18,31,31	2.35	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SLB	B	6	2	18,21,21	1.09	2 (11%)	18,31,31	3.01	13 (72%)
2	SIA	B	7	-	17,20,21	1.09	2 (11%)	18,28,31	1.57	4 (22%)

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	BGC	A	1	2,4	-	0/2/18/22	0/1/1/1
2	GAL	A	2	2	-	0/2/15/22	0/1/1/1
2	NGA	A	3	2	-	0/6/22/26	0/1/1/1
2	GAL	A	4	2	-	0/2/18/22	0/1/1/1
2	SIA	A	5	2	-	0/14/38/38	0/1/1/1
2	SLB	A	6	2	-	0/14/38/38	0/1/1/1
2	SIA	A	7	2	-	0/14/34/38	0/1/1/1
2	BGC	B	1	2,4	-	0/2/18/22	0/1/1/1
2	GAL	B	2	2	-	0/2/15/22	0/1/1/1
2	NGA	B	3	2	-	0/6/22/26	0/1/1/1
2	GAL	B	4	2	-	0/2/18/22	0/1/1/1
2	SIA	B	5	2	-	0/14/38/38	0/1/1/1
2	SLB	B	6	2	-	0/14/38/38	0/1/1/1
2	SIA	B	7	-	1/1/8/9	0/14/34/38	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	GAL	C1-C2	-3.36	1.49	1.52
2	A	5	SIA	C3-C2	-3.17	1.47	1.51
2	B	5	SIA	C3-C2	-2.90	1.48	1.51
2	B	7	SIA	C3-C2	-2.50	1.48	1.52
2	A	1	BGC	O5-C5	-2.42	1.39	1.44
2	B	4	GAL	O2-C2	-2.40	1.38	1.43
2	B	4	GAL	C1-C2	-2.15	1.50	1.52
2	A	1	BGC	C3-C2	-2.11	1.49	1.52
2	B	6	SLB	O6-C6	-2.10	1.40	1.44
2	B	4	GAL	O5-C1	-2.09	1.39	1.43
2	B	7	SIA	C7-C6	-2.03	1.50	1.52
2	B	6	SLB	O2-C2	2.18	1.42	1.39
2	A	6	SLB	O2-C2	2.22	1.42	1.39
2	A	5	SIA	O2-C2	5.93	1.47	1.39
2	B	5	SIA	O2-C2	7.29	1.48	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	5	SIA	O2-C2-C3	-11.43	95.15	109.46
2	B	5	SIA	O2-C2-C3	-6.29	101.59	109.46
2	B	5	SIA	C2-C3-C4	-5.48	99.56	110.40
2	A	5	SIA	C2-C3-C4	-5.23	100.05	110.40
2	B	6	SLB	C5-N5-C10	-4.21	112.14	123.21
2	A	6	SLB	C5-N5-C10	-4.20	112.17	123.21
2	B	6	SLB	O4-C4-C3	-4.15	100.31	109.80
2	A	1	BGC	O3-C3-C2	-3.96	102.21	110.19
2	B	7	SIA	O9-C9-C8	-3.73	102.80	111.07
2	B	6	SLB	C6-C5-N5	-3.73	104.68	111.06
2	B	2	GAL	C4-C3-C2	-3.28	106.59	111.89
2	A	2	GAL	C3-C4-C5	-3.11	105.84	110.81
2	A	6	SLB	C6-C5-N5	-3.07	105.81	111.06
2	A	6	SLB	C8-C7-C6	-2.99	106.77	113.08
2	A	6	SLB	O4-C4-C3	-2.88	103.20	109.80
2	A	6	SLB	O8-C8-C9	-2.85	102.46	109.23
2	B	6	SLB	O6-C6-C7	-2.74	103.10	107.30
2	A	6	SLB	C7-C6-C5	-2.73	110.29	114.06
2	A	7	SIA	C8-C7-C6	-2.73	107.33	113.08
2	B	7	SIA	C8-C7-C6	-2.70	107.39	113.08
2	A	1	BGC	O5-C5-C4	-2.56	104.86	109.84
2	A	2	GAL	C4-C3-C2	-2.50	107.84	111.89
2	B	5	SIA	O7-C7-C6	-2.49	103.73	109.48
2	B	2	GAL	C3-C4-C5	-2.49	106.83	110.81
2	B	6	SLB	O10-C10-C11	-2.43	117.61	122.07
2	B	7	SIA	C7-C6-C5	-2.35	110.82	114.06
2	A	3	NGA	O7-C7-C8	-2.28	117.87	122.07
2	B	6	SLB	C8-C7-C6	-2.28	108.28	113.08
2	B	5	SIA	O9-C9-C8	-2.25	106.07	111.07
2	A	1	BGC	O1-C1-C2	-2.25	102.83	109.05
2	B	1	BGC	O2-C2-C3	-2.24	105.91	110.01
2	A	1	BGC	O2-C2-C3	-2.18	106.01	110.01
2	B	1	BGC	O5-C1-C2	-2.17	106.21	110.00
2	A	3	NGA	O4-C4-C3	-2.14	104.81	110.02
2	B	6	SLB	O8-C8-C7	-2.11	103.52	108.96
2	B	1	BGC	O6-C6-C5	-2.08	105.67	111.65
2	A	3	NGA	C3-C2-N2	-2.01	107.11	110.67
2	B	7	SIA	O7-C7-C8	2.06	114.08	108.73
2	A	1	BGC	O5-C5-C6	2.09	109.23	106.67
2	B	6	SLB	O9-C9-C8	2.20	115.96	111.07
2	B	1	BGC	O5-C5-C6	2.21	109.38	106.67
2	B	1	BGC	O1-C1-C2	2.23	115.22	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6	SLB	C11-C10-N5	2.44	120.77	116.10
2	A	6	SLB	C11-C10-N5	2.45	120.80	116.10
2	A	7	SIA	O6-C2-C3	2.49	114.65	109.77
2	B	5	SIA	C9-C8-C7	2.56	118.74	112.43
2	B	2	GAL	O5-C5-C6	2.68	109.96	106.67
2	B	3	NGA	C8-C7-N2	3.35	122.51	116.10
2	B	6	SLB	O7-C7-C8	3.38	117.50	108.73
2	B	6	SLB	C9-C8-C7	4.07	122.48	112.43
2	A	6	SLB	C4-C5-N5	4.30	120.08	110.31
2	B	6	SLB	O2-C2-C3	4.31	114.86	109.46
2	B	6	SLB	C4-C5-N5	5.36	122.50	110.31

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	7	SIA	C2

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	BGC	1	0
2	A	2	GAL	1	0
2	A	3	NGA	2	0
2	A	4	GAL	1	0
2	A	5	SIA	3	0
2	B	1	BGC	3	0
2	B	2	GAL	3	0
2	B	3	NGA	3	0
2	B	6	SLB	6	0
2	B	7	SIA	4	0

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	CEQ	A	8[A]	2	5,5,5	2.52	4 (80%)	6,7,7	0.81	0
4	CEQ	A	8[B]	2	5,5,5	2.48	4 (80%)	6,7,7	0.76	0
3	PO4	B	301	-	4,4,4	0.77	0	6,6,6	0.24	0
4	CEQ	B	8[A]	2	5,5,5	2.47	4 (80%)	6,7,7	0.52	0
4	CEQ	B	8[B]	2	5,5,5	2.46	4 (80%)	6,7,7	0.69	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
4	CEQ	A	8[A]	2	-	0/3/3/3	0/0/0/0
4	CEQ	A	8[B]	2	-	0/3/3/3	0/0/0/0
3	PO4	B	301	-	-	0/0/0/0	0/0/0/0
4	CEQ	B	8[A]	2	-	0/3/3/3	0/0/0/0
4	CEQ	B	8[B]	2	-	0/3/3/3	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8[A]	CEQ	SI1-C5	-3.54	1.78	1.87
4	B	8[B]	CEQ	SI1-C5	-3.42	1.79	1.87
4	A	8[B]	CEQ	SI1-C5	-3.36	1.79	1.87
4	B	8[A]	CEQ	SI1-C5	-3.31	1.79	1.87
4	A	8[A]	CEQ	SI1-C2	-2.68	1.78	1.87
4	A	8[B]	CEQ	SI1-C3	-2.66	1.78	1.87
4	B	8[A]	CEQ	SI1-C2	-2.58	1.78	1.87
4	A	8[B]	CEQ	SI1-C4	-2.58	1.78	1.87
4	B	8[A]	CEQ	SI1-C4	-2.53	1.79	1.87
4	B	8[A]	CEQ	SI1-C3	-2.53	1.79	1.87
4	B	8[B]	CEQ	SI1-C3	-2.53	1.79	1.87
4	A	8[A]	CEQ	SI1-C3	-2.48	1.79	1.87
4	B	8[B]	CEQ	SI1-C4	-2.48	1.79	1.87
4	A	8[A]	CEQ	SI1-C4	-2.44	1.79	1.87
4	B	8[B]	CEQ	SI1-C2	-2.42	1.79	1.87
4	A	8[B]	CEQ	SI1-C2	-2.39	1.79	1.87

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	PO4	2	0

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, 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	451/472 (95%)	0.13	22 (4%) 33 42	27, 37, 54, 68	0
1	B	451/472 (95%)	-0.12	14 (3%) 52 62	17, 29, 51, 71	0
All	All	902/944 (95%)	0.00	36 (3%) 42 51	17, 34, 54, 71	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	867	LEU	8.1
1	B	871	VAL	7.1
1	A	870	TRP	5.2
1	B	872	ASP	5.0
1	A	1183	ASN	4.6
1	B	943	TYR	4.5
1	B	865	LYS	4.3
1	B	866	ASN	4.0
1	A	871	VAL	3.9
1	B	876	ASP	3.7
1	B	868	ASP	3.6
1	A	1184	ASN	3.5
1	A	865	LYS	3.5
1	A	873	ASN	3.4
1	B	941	ILE	3.2
1	B	940	ASP	3.2
1	A	875	GLU	3.1
1	B	1068	ASN	3.0
1	B	870	TRP	3.0
1	A	880	ILE	2.9
1	A	1185	GLU	2.8
1	A	986	SER	2.7
1	A	1187	ASP	2.7
1	A	877	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	879	VAL	2.6
1	A	1186	ILE	2.5
1	A	874	GLU	2.5
1	A	1161	LYS	2.4
1	A	1111	ILE	2.3
1	A	1160	GLY	2.3
1	A	1052	LEU	2.2
1	B	873	ASN	2.2
1	B	1185	GLU	2.2
1	A	1204	ASN	2.1
1	A	918	ILE	2.1
1	A	1076	ARG	2.1

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)

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	SIA	B	5	21/21	0.81	0.19	6.01	46,62,68,69	0
2	SIA	B	7	20/21	0.85	0.17	3.65	44,50,60,63	0
2	SLB	B	6	21/21	0.88	0.15	2.69	42,49,54,58	0
2	SLB	A	6	21/21	0.88	0.14	1.96	47,54,60,65	0
2	GAL	A	4	11/12	0.87	0.18	1.95	46,50,51,55	0
2	NGA	A	3	14/15	0.83	0.16	1.77	50,51,53,53	0
2	SIA	A	7	20/21	0.89	0.16	1.39	44,56,65,65	0
2	NGA	B	3	14/15	0.92	0.13	0.97	36,39,42,43	0
2	GAL	B	4	11/12	0.97	0.08	-1.24	34,37,40,40	0
2	GAL	A	2	10/12	0.93	0.11	-	45,47,51,52	0
2	BGC	B	1	11/12	0.90	0.12	-	45,51,57,61	0
2	BGC	A	1	11/12	0.91	0.16	-	52,54,61,62	0
2	GAL	B	2	10/12	0.90	0.11	-	39,44,45,45	0
2	SIA	A	5	21/21	0.77	0.20	-	53,63,66,67	0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	PO4	B	301	5/5	0.97	0.09	-1.42	58,60,60,61	0
4	CEQ	A	8[A]	6/6	0.82	0.39	-	72,76,76,76	6
4	CEQ	B	8[B]	6/6	0.65	0.56	-	64,65,65,65	6
4	CEQ	A	8[B]	6/6	0.82	0.39	-	66,68,68,68	6
4	CEQ	B	8[A]	6/6	0.65	0.56	-	71,75,76,76	6

6.5 Other polymers

There are no such residues in this entry.