



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:50 AM GMT

PDB ID : 2IWG
Title : COMPLEX BETWEEN THE PRYSPRY DOMAIN OF TRIM21 AND IGG
FC
Authors : James, L.C.; Keeble, A.H.; Rhodes, D.A.; Trowsdale, J.
Deposited on : 2006-06-30
Resolution : 2.35 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 ⓘ symbol.

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

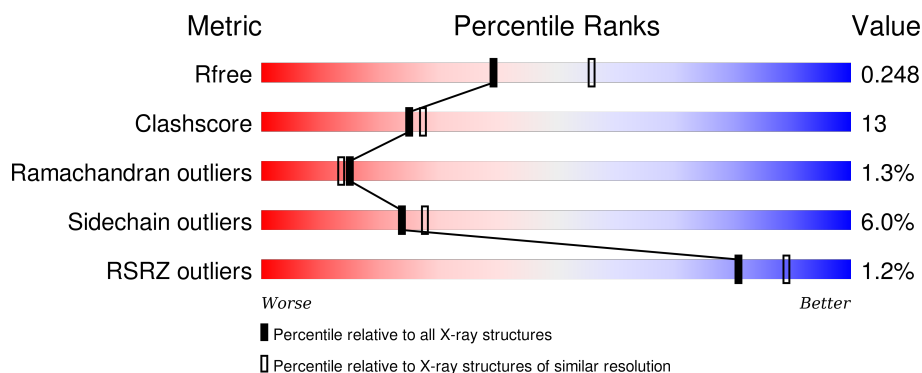
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	207	 2% 65% 29% 6%
1	D	207	 % 62% 33% 5%
2	B	181	 58% 35% 6%
2	E	181	 % 64% 31% 5%

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	MAN	A	1446	X	-	-	-
3	MAN	D	1446	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6590 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 IG GAMMA-1 CHAIN C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1658	1056	279	317	6			
1	D	207	Total	C	N	O	S	0	0	0
			1658	1056	279	317	6			

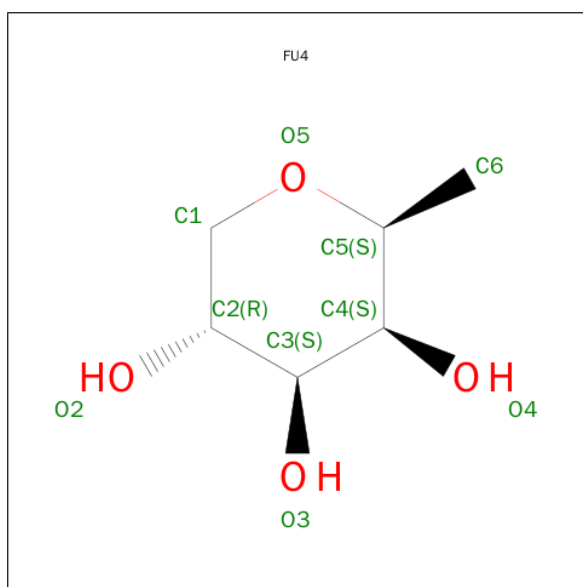
- Molecule 2 is a protein called 52 KDA RO PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1455	936	248	264	7			
2	E	181	Total	C	N	O	S	0	0	0
			1455	936	248	264	7			

- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	7	Total	C	N	O	0	0
			86	48	3	35		
3	D	7	Total	C	N	O	0	0
			86	48	3	35		

- Molecule 4 is SUGAR (2,6-ANHYDRO-1-DEOXY-D-GALACTITOL) (three-letter code: FU4) (formula: C₆H₁₂O₄).



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

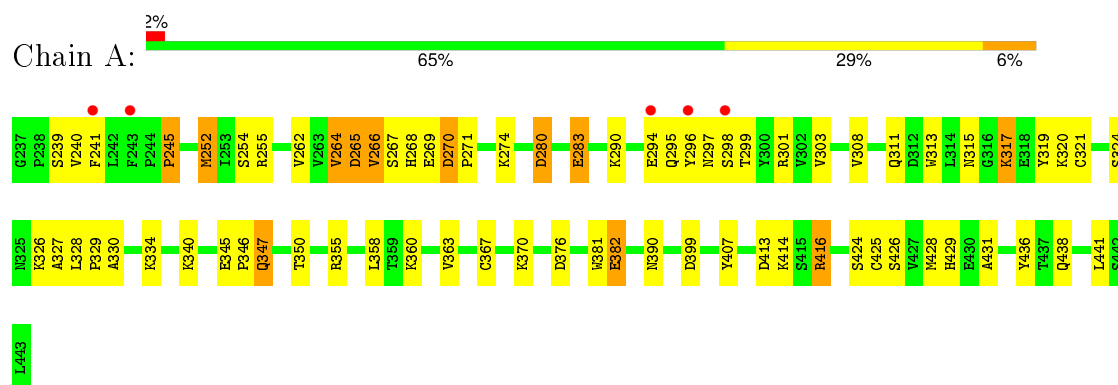
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		
5	B	31	Total	O	0	0
			31	31		
5	D	42	Total	O	0	0
			42	42		
5	E	51	Total	O	0	0
			51	51		

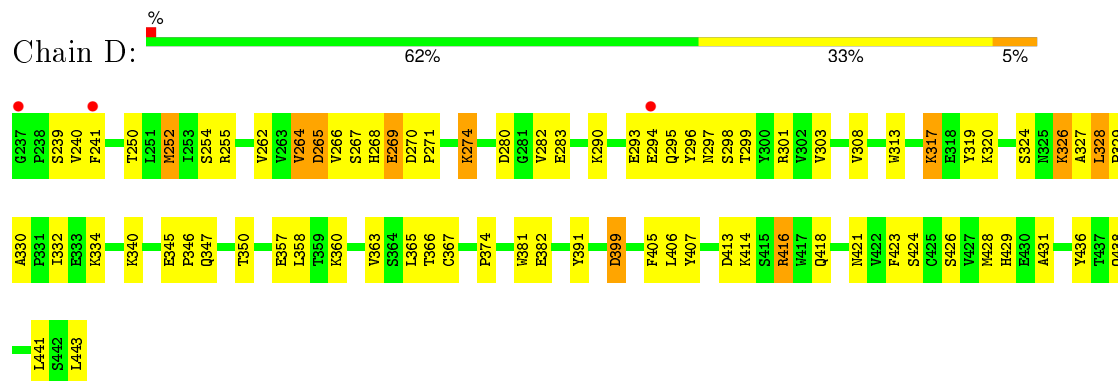
3 Residue-property plots

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.

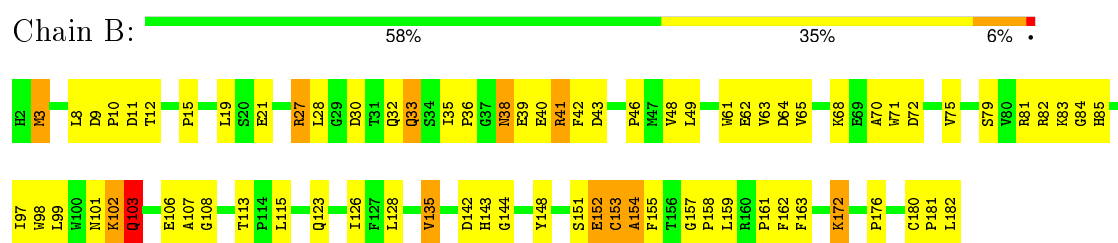
• Molecule 1: IG GAMMA-1 CHAIN C



• Molecule 1: IG GAMMA-1 CHAIN C

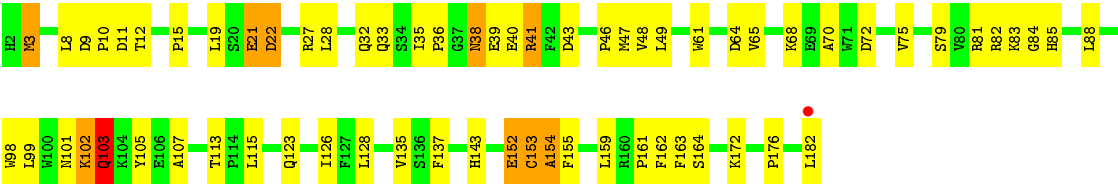


• Molecule 2: 52 KDA RO PROTEIN



• Molecule 2: 52 KDA RO PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	112.49Å 112.49Å 194.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.59 – 2.35 97.42 – 2.35	Depositor EDS
% Data completeness (in resolution range)	86.1 (97.59-2.35) 86.1 (97.42-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.253 0.213 , 0.248	Depositor DCC
R_{free} test set	2533 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 49869 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6590	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: FU4, GAL, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.63	16/1704 (0.9%)	1.16	7/2322 (0.3%)
1	D	1.65	22/1704 (1.3%)	1.20	10/2322 (0.4%)
2	B	1.74	28/1505 (1.9%)	1.44	17/2050 (0.8%)
2	E	1.69	23/1505 (1.5%)	1.47	17/2050 (0.8%)
All	All	1.68	89/6418 (1.4%)	1.31	51/8744 (0.6%)

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
1	D	0	1
3	A	1	0
3	D	1	0
All	All	2	2

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	135	VAL	CB-CG1	-9.28	1.33	1.52
2	B	135	VAL	CB-CG1	-8.98	1.33	1.52
2	E	163	PHE	CG-CD2	8.63	1.51	1.38
1	D	407	TYR	CG-CD1	8.62	1.50	1.39
1	A	296	TYR	CE2-CZ	8.24	1.49	1.38
2	B	98	TRP	CG-CD1	7.83	1.47	1.36
2	E	163	PHE	CE1-CZ	7.81	1.52	1.37
1	D	294	GLU	CD-OE2	7.77	1.34	1.25
2	B	152	GLU	CG-CD	7.72	1.63	1.51
1	A	294	GLU	CD-OE2	7.69	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	153	CYS	CB-SG	7.60	1.95	1.82
1	D	296	TYR	CE2-CZ	7.53	1.48	1.38
1	A	407	TYR	CD2-CE2	7.51	1.50	1.39
2	B	3	MET	CG-SD	7.51	2.00	1.81
1	D	347	GLN	CG-CD	7.50	1.68	1.51
2	E	137	PHE	CD1-CE1	7.42	1.54	1.39
1	A	425	CYS	CB-SG	-7.37	1.69	1.82
2	B	153	CYS	CB-SG	7.32	1.94	1.82
1	A	407	TYR	CD1-CE1	7.17	1.50	1.39
1	A	296	TYR	CE1-CZ	7.07	1.47	1.38
2	E	40	GLU	CG-CD	7.03	1.62	1.51
2	B	40	GLU	CG-CD	6.72	1.62	1.51
2	E	65	VAL	CB-CG1	6.71	1.67	1.52
2	E	68	LYS	CE-NZ	-6.66	1.32	1.49
2	B	162	PHE	CE1-CZ	6.63	1.50	1.37
1	D	405	PHE	CE2-CZ	6.61	1.50	1.37
2	E	3	MET	CG-SD	6.50	1.98	1.81
1	D	294	GLU	CG-CD	6.45	1.61	1.51
1	D	391	TYR	CD1-CE1	-6.44	1.29	1.39
1	A	296	TYR	CD1-CE1	6.43	1.49	1.39
2	B	108	GLY	N-CA	6.42	1.55	1.46
1	A	321	CYS	CB-SG	-6.38	1.71	1.82
1	A	296	TYR	CG-CD2	6.32	1.47	1.39
2	B	68	LYS	CE-NZ	-6.26	1.33	1.49
2	B	98	TRP	N-CA	-6.26	1.33	1.46
1	D	296	TYR	CD1-CE1	6.24	1.48	1.39
2	E	48	VAL	CB-CG2	6.22	1.66	1.52
2	B	148	TYR	CE2-CZ	6.19	1.46	1.38
2	E	162	PHE	CE1-CZ	6.16	1.49	1.37
1	D	294	GLU	CD-OE1	6.15	1.32	1.25
1	D	296	TYR	CG-CD2	6.12	1.47	1.39
1	D	282	VAL	CB-CG2	6.09	1.65	1.52
1	A	347	GLN	CG-CD	6.07	1.65	1.51
1	D	407	TYR	CD1-CE1	6.07	1.48	1.39
1	D	407	TYR	CE2-CZ	5.98	1.46	1.38
2	B	98	TRP	CE3-CZ3	-5.98	1.28	1.38
1	A	283	GLU	CD-OE2	5.92	1.32	1.25
2	B	103	GLN	N-CA	5.88	1.58	1.46
1	A	252	MET	N-CA	5.84	1.58	1.46
1	D	326	LYS	CD-CE	5.84	1.65	1.51
2	B	106	GLU	CD-OE2	5.81	1.32	1.25
2	B	152	GLU	CD-OE1	5.78	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	126	ILE	CA-CB	5.75	1.68	1.54
1	D	423	PHE	CE1-CZ	5.71	1.48	1.37
2	B	48	VAL	CB-CG1	5.70	1.64	1.52
2	B	48	VAL	CB-CG2	5.64	1.64	1.52
1	D	357	GLU	CD-OE1	5.64	1.31	1.25
2	B	75	VAL	CB-CG1	-5.61	1.41	1.52
1	D	293	GLU	CD-OE1	5.58	1.31	1.25
2	E	98	TRP	N-CA	-5.57	1.35	1.46
1	A	294	GLU	CG-CD	5.57	1.60	1.51
1	D	296	TYR	CE1-CZ	5.51	1.45	1.38
2	B	65	VAL	CB-CG2	5.51	1.64	1.52
2	E	152	GLU	CB-CG	5.49	1.62	1.52
2	B	152	GLU	CD-OE2	5.42	1.31	1.25
1	A	407	TYR	CG-CD1	5.41	1.46	1.39
1	D	407	TYR	CD2-CE2	5.41	1.47	1.39
2	E	39	GLU	CD-OE1	5.40	1.31	1.25
2	E	126	ILE	CA-CB	5.37	1.67	1.54
1	D	330	ALA	CA-CB	5.34	1.63	1.52
2	B	106	GLU	CD-OE1	5.34	1.31	1.25
2	E	64	ASP	CB-CG	5.33	1.62	1.51
2	B	41	ARG	CZ-NH2	-5.32	1.26	1.33
2	B	163	PHE	CG-CD2	5.27	1.46	1.38
2	E	105	TYR	CB-CG	-5.27	1.43	1.51
2	E	41	ARG	CZ-NH2	-5.27	1.26	1.33
2	E	22	ASP	CB-CG	5.22	1.62	1.51
2	E	39	GLU	CG-CD	5.21	1.59	1.51
1	A	382	GLU	CB-CG	5.18	1.61	1.52
2	B	71	TRP	CG-CD1	5.18	1.44	1.36
1	A	330	ALA	CA-CB	5.17	1.63	1.52
1	D	269	GLU	CG-CD	5.15	1.59	1.51
2	B	172	LYS	C-O	5.15	1.33	1.23
2	E	75	VAL	CB-CG1	-5.13	1.42	1.52
1	D	274	LYS	CD-CE	5.11	1.64	1.51
2	B	33	GLN	CG-CD	5.07	1.62	1.51
2	E	152	GLU	CG-CD	5.06	1.59	1.51
2	B	39	GLU	CD-OE1	5.05	1.31	1.25
2	E	21	GLU	CG-CD	5.03	1.59	1.51

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	41	ARG	NE-CZ-NH2	-12.66	113.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	41	ARG	NE-CZ-NH1	12.62	126.61	120.30
2	E	64	ASP	CB-CG-OD2	12.30	129.37	118.30
2	B	41	ARG	NE-CZ-NH2	-12.27	114.17	120.30
2	E	41	ARG	NE-CZ-NH1	11.73	126.16	120.30
2	B	72	ASP	CB-CG-OD2	10.96	128.16	118.30
2	E	72	ASP	CB-CG-OD2	10.64	127.87	118.30
2	B	64	ASP	CB-CG-OD2	10.24	127.52	118.30
2	E	43	ASP	CB-CG-OD1	9.74	127.06	118.30
2	E	72	ASP	OD1-CG-OD2	-9.40	105.45	123.30
2	E	72	ASP	CB-CG-OD1	9.00	126.40	118.30
2	B	72	ASP	OD1-CG-OD2	-8.94	106.32	123.30
2	E	43	ASP	CB-CG-OD2	-8.77	110.41	118.30
2	B	43	ASP	CB-CG-OD1	8.36	125.82	118.30
2	B	72	ASP	CB-CG-OD1	7.94	125.45	118.30
2	E	9	ASP	CB-CG-OD2	-7.72	111.35	118.30
2	B	68	LYS	CD-CE-NZ	-7.31	94.88	111.70
2	B	11	ASP	CB-CG-OD2	7.17	124.75	118.30
2	B	27	ARG	NE-CZ-NH1	7.06	123.83	120.30
2	B	43	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	D	365	LEU	CB-CG-CD2	6.86	122.65	111.00
1	A	301	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	416	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	E	11	ASP	CB-CG-OD2	6.43	124.09	118.30
1	D	399	ASP	CB-CG-OD1	-6.33	112.61	118.30
2	E	82	ARG	NE-CZ-NH2	6.01	123.31	120.30
2	B	9	ASP	CB-CG-OD2	-5.85	113.03	118.30
2	E	48	VAL	CA-CB-CG1	5.84	119.67	110.90
1	A	355	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	328	LEU	CA-CB-CG	5.70	128.42	115.30
2	B	79	SER	CB-CA-C	-5.69	99.29	110.10
2	E	103	GLN	N-CA-C	5.67	126.30	111.00
1	A	266	VAL	N-CA-C	-5.67	95.70	111.00
2	B	103	GLN	N-CA-C	5.57	126.05	111.00
1	D	265	ASP	CB-CA-C	5.47	121.35	110.40
1	D	406	LEU	CB-CG-CD2	-5.47	101.70	111.00
2	E	79	SER	CB-CA-C	-5.46	99.73	110.10
1	A	280	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	416	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	D	265	ASP	N-CA-C	5.34	125.42	111.00
2	B	84	GLY	N-CA-C	5.32	126.39	113.10
1	D	301	ARG	NE-CZ-NH2	-5.31	117.65	120.30
2	E	64	ASP	OD1-CG-OD2	-5.24	113.35	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	88	LEU	CB-CG-CD1	-5.20	102.15	111.00
1	A	265	ASP	N-CA-C	5.19	125.01	111.00
1	A	270	ASP	CB-CG-OD1	5.13	122.92	118.30
2	B	3	MET	CA-CB-CG	-5.10	104.63	113.30
2	B	48	VAL	CA-CB-CG1	5.08	118.53	110.90
1	D	365	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	D	252	MET	CG-SD-CE	5.04	108.26	100.20
2	E	84	GLY	N-CA-C	5.00	125.61	113.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1446	MAN	C1
3	D	1446	MAN	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	VAL	Peptide
1	D	264	VAL	Peptide

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	1658	0	1625	38	0
1	D	1658	0	1625	39	0
2	B	1455	0	1381	37	0
2	E	1455	0	1381	36	0
3	A	86	0	73	7	0
3	D	86	0	73	7	0
4	A	10	0	12	3	0
4	D	10	0	12	4	0
5	A	48	0	0	2	0
5	B	31	0	0	3	0
5	D	42	0	0	2	0
5	E	51	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6590	0	6182	160	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1445:NAG:HN2	4:A:1451:FU4:H1C1	1.11	1.08
3:D:1445:NAG:HN2	4:D:1451:FU4:H1C1	1.12	1.07
1:A:265:ASP:HB3	1:A:299:THR:HB	1.30	1.06
1:D:265:ASP:HB3	1:D:299:THR:HB	1.39	1.00
3:D:1444:NAG:O6	4:D:1451:FU4:H2	1.71	0.88
1:A:265:ASP:HB3	1:A:299:THR:CB	2.06	0.85
2:B:101:ASN:O	2:B:102:LYS:O	1.96	0.83
3:A:1444:NAG:O6	4:A:1451:FU4:H2	1.78	0.83
2:E:38:ASN:HD21	2:E:41:ARG:NH1	1.82	0.78
2:E:101:ASN:O	2:E:102:LYS:O	2.00	0.78
1:D:265:ASP:HB3	1:D:299:THR:CB	2.15	0.77
1:A:239:SER:HB2	1:A:264:VAL:HG23	1.66	0.77
2:E:3:MET:CB	2:E:182:LEU:HD13	2.16	0.76
2:B:3:MET:CB	2:B:182:LEU:HD13	2.15	0.76
2:B:3:MET:HB2	2:B:182:LEU:HD13	1.67	0.75
1:D:239:SER:HB2	1:D:264:VAL:HG23	1.68	0.75
3:A:1445:NAG:H83	3:A:1447:MAN:O4	1.88	0.74
3:D:1445:NAG:N2	4:D:1451:FU4:H1C1	1.97	0.71
1:D:290:LYS:HB2	1:D:303:VAL:HG23	1.72	0.71
2:E:3:MET:HB2	2:E:182:LEU:HD13	1.72	0.71
2:B:153:CYS:O	2:B:154:ALA:HB3	1.89	0.71
3:D:1445:NAG:H83	3:D:1447:MAN:O4	1.90	0.71
2:E:153:CYS:O	2:E:154:ALA:HB3	1.92	0.69
1:D:252:MET:HA	1:D:428:MET:HE1	1.75	0.68
3:A:1445:NAG:N2	4:A:1451:FU4:H1C1	1.97	0.68
1:D:252:MET:HG2	1:D:428:MET:HE1	1.77	0.67
1:D:421:ASN:O	5:D:2032:HOH:O	2.11	0.67
1:A:252:MET:HA	1:A:428:MET:HE1	1.77	0.67
2:E:12:THR:HG21	2:E:49:LEU:HB2	1.77	0.66
2:E:19:LEU:HD12	2:E:19:LEU:N	2.10	0.66
1:A:252:MET:HG2	1:A:428:MET:HE1	1.78	0.66
1:A:290:LYS:HB2	1:A:303:VAL:HG23	1.75	0.65
2:B:38:ASN:HD21	2:B:41:ARG:NH1	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:LYS:C	1:D:328:LEU:H	1.99	0.65
1:D:382:GLU:HG2	1:D:424:SER:HB2	1.76	0.65
1:A:382:GLU:HG2	1:A:424:SER:HB2	1.78	0.64
2:B:81:ARG:NH2	2:B:85:HIS:O	2.31	0.64
1:A:347:GLN:HG2	5:A:2024:HOH:O	1.97	0.64
2:B:35:ILE:HB	2:B:36:PRO:HD2	1.80	0.64
2:E:154:ALA:HB3	5:E:2035:HOH:O	1.98	0.64
1:A:350:THR:HB	1:A:441:LEU:HD22	1.81	0.63
1:D:350:THR:HB	1:D:441:LEU:HD22	1.79	0.63
1:A:241:PHE:CE1	3:A:1446:MAN:H2	2.34	0.63
1:A:326:LYS:C	1:A:328:LEU:H	2.03	0.62
1:D:241:PHE:CE1	3:D:1446:MAN:H2	2.33	0.62
2:B:12:THR:HG21	2:B:49:LEU:HB2	1.80	0.62
2:E:35:ILE:HB	2:E:36:PRO:HD2	1.80	0.62
2:E:38:ASN:H	2:E:38:ASN:ND2	1.98	0.62
1:D:274:LYS:HB3	1:D:324:SER:HB2	1.82	0.61
1:A:274:LYS:HB3	1:A:324:SER:HB2	1.83	0.61
1:A:358:LEU:HD23	1:A:363:VAL:HG11	1.81	0.60
2:B:62:GLU:HB3	5:B:2013:HOH:O	2.00	0.60
2:B:19:LEU:N	2:B:19:LEU:HD12	2.16	0.60
2:B:101:ASN:C	2:B:102:LYS:O	2.38	0.59
2:E:3:MET:HB3	2:E:182:LEU:HD13	1.85	0.59
2:B:38:ASN:H	2:B:38:ASN:HD22	1.50	0.59
2:E:154:ALA:CB	5:E:2035:HOH:O	2.51	0.58
2:B:38:ASN:ND2	2:B:38:ASN:H	2.00	0.58
2:E:19:LEU:N	2:E:19:LEU:CD1	2.66	0.58
2:B:153:CYS:O	2:B:154:ALA:CB	2.52	0.57
1:A:252:MET:HG2	1:A:428:MET:CE	2.33	0.57
2:E:38:ASN:H	2:E:38:ASN:HD22	1.51	0.57
1:D:254:SER:OG	1:D:255:ARG:NH1	2.38	0.56
2:B:154:ALA:O	2:B:155:PHE:HB2	2.05	0.56
1:A:347:GLN:CG	5:A:2024:HOH:O	2.51	0.56
1:A:241:PHE:CE2	3:A:1445:NAG:H4	2.41	0.56
2:E:154:ALA:O	2:E:155:PHE:HB2	2.05	0.56
2:E:38:ASN:HD21	2:E:41:ARG:HH11	1.52	0.56
1:D:358:LEU:HD23	1:D:363:VAL:HG11	1.88	0.56
1:A:266:VAL:HG12	1:A:271:PRO:HA	1.88	0.56
1:D:280:ASP:OD2	1:D:317:LYS:HD2	2.06	0.55
1:A:320:LYS:HG3	1:A:334:LYS:O	2.06	0.55
1:D:429:HIS:HD2	1:D:431:ALA:H	1.55	0.55
1:D:429:HIS:CD2	1:D:431:ALA:H	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:CYS:HB2	1:D:381:TRP:CZ2	2.42	0.54
1:D:436:TYR:OH	1:D:438:GLN:NE2	2.37	0.54
2:E:81:ARG:NH2	2:E:85:HIS:O	2.40	0.54
2:E:61:TRP:CZ2	2:E:161:PRO:HB3	2.43	0.54
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.42	0.54
2:E:22:ASP:N	5:E:2004:HOH:O	2.40	0.54
2:E:107:ALA:HB3	2:E:113:THR:HB	1.89	0.53
1:D:266:VAL:HG12	1:D:271:PRO:HA	1.90	0.53
2:B:28:LEU:HD13	2:B:46:PRO:HB3	1.90	0.53
1:A:254:SER:OG	1:A:255:ARG:NH1	2.41	0.53
2:B:63:VAL:N	5:B:2013:HOH:O	2.42	0.52
2:E:101:ASN:C	2:E:102:LYS:O	2.46	0.52
1:A:436:TYR:OH	1:A:438:GLN:NE2	2.37	0.52
2:E:153:CYS:O	2:E:154:ALA:CB	2.56	0.52
1:A:429:HIS:CD2	1:A:431:ALA:H	2.28	0.52
1:D:240:VAL:HB	1:D:332:ILE:HD11	1.92	0.52
1:D:326:LYS:C	1:D:328:LEU:N	2.64	0.51
1:D:252:MET:HG2	1:D:428:MET:CE	2.40	0.51
1:A:280:ASP:OD2	1:A:317:LYS:HD2	2.11	0.51
2:B:3:MET:HB3	2:B:182:LEU:HD13	1.91	0.50
2:B:35:ILE:HD12	2:B:41:ARG:CZ	2.42	0.50
1:A:413:ASP:HB2	1:A:416:ARG:HG3	1.94	0.50
2:B:19:LEU:N	2:B:19:LEU:CD1	2.74	0.50
1:A:240:VAL:HG13	1:A:262:VAL:O	2.12	0.50
1:D:241:PHE:CE2	3:D:1445:NAG:H4	2.47	0.49
2:B:128:LEU:HD21	2:B:159:LEU:HD12	1.94	0.49
1:A:429:HIS:HD2	1:A:431:ALA:H	1.61	0.49
1:A:308:VAL:HG12	1:A:319:TYR:CE2	2.48	0.49
2:E:28:LEU:HD13	2:E:46:PRO:HB3	1.93	0.49
2:B:3:MET:HB2	2:B:182:LEU:CD1	2.39	0.49
1:A:245:PRO:HD2	1:A:313:TRP:CH2	2.48	0.48
2:B:27:ARG:HB3	2:B:176:PRO:HB3	1.95	0.48
1:A:326:LYS:C	1:A:328:LEU:N	2.66	0.48
1:D:414:LYS:O	1:D:418:GLN:HB2	2.13	0.48
1:D:413:ASP:HB2	1:D:416:ARG:HG3	1.96	0.48
1:D:308:VAL:HG12	1:D:319:TYR:CE2	2.48	0.48
2:B:99:LEU:HD11	2:B:103:GLN:N	2.29	0.48
2:E:38:ASN:ND2	2:E:41:ARG:HH11	2.12	0.47
2:E:35:ILE:HD12	2:E:41:ARG:CZ	2.44	0.47
2:B:107:ALA:HB3	2:B:113:THR:HB	1.95	0.47
1:D:320:LYS:HG3	1:D:334:LYS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.64	0.47
1:A:252:MET:HA	1:A:428:MET:CE	2.45	0.46
1:D:252:MET:HA	1:D:428:MET:CE	2.44	0.46
1:D:252:MET:CG	1:D:428:MET:HE1	2.44	0.46
2:E:38:ASN:ND2	2:E:41:ARG:NH1	2.58	0.46
2:B:61:TRP:CZ2	2:B:161:PRO:HB3	2.49	0.46
2:E:3:MET:HB2	2:E:182:LEU:CD1	2.44	0.46
3:D:1444:NAG:C6	4:D:1451:FU4:H2	2.46	0.45
2:E:27:ARG:HB3	2:E:176:PRO:HB3	1.98	0.45
1:A:265:ASP:CB	1:A:299:THR:CB	2.90	0.45
2:B:70:ALA:HA	2:B:99:LEU:O	2.16	0.45
1:D:443:LEU:HB2	5:D:2040:HOH:O	2.15	0.45
2:E:15:PRO:HB2	2:E:32:GLN:HG3	1.99	0.45
2:E:10:PRO:O	2:E:41:ARG:NH2	2.51	0.44
1:D:250:THR:HG21	1:D:313:TRP:CD1	2.52	0.44
2:B:180:CYS:HA	2:B:181:PRO:HD3	1.78	0.44
1:D:240:VAL:HG13	1:D:262:VAL:O	2.18	0.44
1:D:295:GLN:O	1:D:298:SER:N	2.51	0.44
1:A:360:LYS:O	1:A:414:LYS:HD3	2.17	0.43
2:E:19:LEU:CD1	2:E:19:LEU:H	2.32	0.43
1:A:345:GLU:HA	1:A:346:PRO:HD2	1.86	0.43
1:D:374:PRO:O	1:D:429:HIS:HE1	2.02	0.43
1:D:345:GLU:HA	1:D:346:PRO:HD2	1.81	0.43
1:A:267:SER:C	1:A:269:GLU:N	2.71	0.43
2:E:99:LEU:HD11	2:E:103:GLN:N	2.34	0.43
2:B:42:PHE:CE2	2:B:82:ARG:HD3	2.54	0.43
1:D:267:SER:C	1:D:269:GLU:N	2.72	0.43
2:E:70:ALA:HA	2:E:99:LEU:O	2.18	0.43
2:B:15:PRO:HB2	2:B:32:GLN:HG3	2.01	0.42
2:E:35:ILE:HB	2:E:36:PRO:CD	2.48	0.42
2:B:142:ASP:O	2:B:144:GLY:N	2.52	0.42
2:B:35:ILE:HB	2:B:36:PRO:CD	2.49	0.42
2:B:10:PRO:O	2:B:41:ARG:NH2	2.52	0.42
1:A:295:GLN:O	1:A:298:SER:N	2.53	0.42
1:D:350:THR:HA	1:D:366:THR:O	2.19	0.42
2:B:157:GLY:HA3	2:B:158:PRO:HD2	1.86	0.42
2:E:128:LEU:HD21	2:E:159:LEU:HD12	2.02	0.42
2:E:47:MET:HG2	2:E:164:SER:HB2	2.01	0.41
2:B:101:ASN:ND2	5:B:2018:HOH:O	2.54	0.41
1:A:311:GLN:HG3	1:A:315:ASN:ND2	2.36	0.41
2:B:181:PRO:O	2:B:182:LEU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:H	1:A:317:LYS:HG2	1.70	0.40
1:D:360:LYS:O	1:D:414:LYS:HD3	2.21	0.40
2:B:97:ILE:HG22	2:B:107:ALA:HA	2.03	0.40
3:A:1445:NAG:C8	3:A:1447:MAN:O4	2.65	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	205/207 (99%)	192 (94%)	11 (5%)	2 (1%)	19	20
1	D	205/207 (99%)	194 (95%)	9 (4%)	2 (1%)	19	20
2	B	179/181 (99%)	163 (91%)	13 (7%)	3 (2%)	11	9
2	E	179/181 (99%)	164 (92%)	12 (7%)	3 (2%)	11	9
All	All	768/776 (99%)	713 (93%)	45 (6%)	10 (1%)	15	13

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	102	LYS
2	B	143	HIS
2	E	102	LYS
2	E	143	HIS
2	B	154	ALA
2	E	154	ALA
1	A	327	ALA
1	D	327	ALA
1	D	329	PRO
1	A	329	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	193/193 (100%)	182 (94%)	11 (6%)	25	30
1	D	193/193 (100%)	185 (96%)	8 (4%)	37	48
2	B	158/158 (100%)	145 (92%)	13 (8%)	14	15
2	E	158/158 (100%)	148 (94%)	10 (6%)	22	25
All	All	702/702 (100%)	660 (94%)	42 (6%)	24	28

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	PRO
1	A	268	HIS
1	A	270	ASP
1	A	283	GLU
1	A	297	ASN
1	A	317	LYS
1	A	340	LYS
1	A	376	ASP
1	A	390	ASN
1	A	399	ASP
1	A	426	SER
2	B	8	LEU
2	B	21	GLU
2	B	30	ASP
2	B	33	GLN
2	B	38	ASN
2	B	83	LYS
2	B	103	GLN
2	B	115	LEU
2	B	123	GLN
2	B	135	VAL
2	B	151	SER
2	B	152	GLU
2	B	172	LYS

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Mol	Chain	Res	Type
1	D	268	HIS
1	D	270	ASP
1	D	283	GLU
1	D	297	ASN
1	D	317	LYS
1	D	340	LYS
1	D	399	ASP
1	D	426	SER
2	E	8	LEU
2	E	21	GLU
2	E	33	GLN
2	E	38	ASN
2	E	83	LYS
2	E	103	GLN
2	E	115	LEU
2	E	123	GLN
2	E	152	GLU
2	E	172	LYS

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	390	ASN
1	A	429	HIS
1	A	434	ASN
2	B	25	GLN
2	B	33	GLN
2	B	38	ASN
1	D	390	ASN
1	D	429	HIS
1	D	434	ASN
1	D	438	GLN
2	E	25	GLN
2	E	33	GLN
2	E	38	ASN

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$
3	NAG	A	1444	1,3	14,14,15	1.28	2 (14%)	15,19,21	2.02	3 (20%)
3	NAG	A	1445	3	14,14,15	0.87	0	15,19,21	1.58	4 (26%)
3	MAN	A	1446	3	11,11,12	0.88	1 (9%)	14,15,17	2.09	5 (35%)
3	MAN	A	1447	3	11,11,12	0.81	0	14,15,17	2.43	6 (42%)
3	NAG	A	1448	3	14,14,15	0.71	0	15,19,21	1.62	1 (6%)
3	MAN	A	1449	3	11,11,12	1.78	4 (36%)	14,15,17	2.39	6 (42%)
3	GAL	A	1450	3	11,11,12	0.84	1 (9%)	14,15,17	2.06	4 (28%)
3	NAG	D	1444	1,3	14,14,15	1.06	1 (7%)	15,19,21	2.03	4 (26%)
3	NAG	D	1445	3	14,14,15	0.79	0	15,19,21	1.49	3 (20%)
3	MAN	D	1446	3	11,11,12	0.91	1 (9%)	14,15,17	1.87	5 (35%)
3	MAN	D	1447	3	11,11,12	0.86	0	14,15,17	2.24	4 (28%)
3	NAG	D	1448	3	14,14,15	0.67	0	15,19,21	1.73	1 (6%)
3	MAN	D	1449	3	11,11,12	1.45	2 (18%)	14,15,17	2.52	5 (35%)
3	GAL	D	1450	3	11,11,12	1.06	0	14,15,17	2.29	6 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1444	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1445	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	A	1446	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	1447	3	-	0/2/19/22	0/1/1/1
3	NAG	A	1448	3	-	0/6/23/26	0/1/1/1
3	MAN	A	1449	3	-	0/2/19/22	0/1/1/1
3	GAL	A	1450	3	-	0/2/19/22	0/1/1/1
3	NAG	D	1444	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1445	3	-	0/6/23/26	0/1/1/1
3	MAN	D	1446	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	D	1447	3	-	0/2/19/22	0/1/1/1
3	NAG	D	1448	3	-	0/6/23/26	0/1/1/1
3	MAN	D	1449	3	-	0/2/19/22	0/1/1/1
3	GAL	D	1450	3	-	0/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1444	NAG	C1-C2	2.01	1.55	1.52
3	D	1446	MAN	O5-C1	2.01	1.47	1.43
3	A	1449	MAN	C1-C2	2.07	1.57	1.52
3	A	1444	NAG	C8-C7	2.19	1.54	1.50
3	A	1446	MAN	O5-C1	2.20	1.47	1.43
3	D	1449	MAN	C4-C3	2.25	1.58	1.52
3	A	1450	GAL	C1-C2	2.25	1.57	1.52
3	A	1449	MAN	C4-C3	2.27	1.58	1.52
3	A	1444	NAG	C1-C2	2.49	1.55	1.52
3	A	1449	MAN	C4-C5	2.72	1.58	1.53
3	D	1449	MAN	C2-C3	2.84	1.56	1.52
3	A	1449	MAN	C2-C3	3.36	1.57	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1449	MAN	C1-C2-C3	-5.27	103.30	109.54
3	A	1449	MAN	C1-C2-C3	-4.89	103.76	109.54
3	A	1446	MAN	O3-C3-C4	-4.63	99.91	110.34
3	A	1444	NAG	O4-C4-C5	-4.36	97.69	109.24
3	D	1444	NAG	O4-C4-C5	-4.32	97.79	109.24
3	A	1447	MAN	O3-C3-C4	-3.99	101.36	110.34
3	D	1446	MAN	O3-C3-C4	-3.74	101.91	110.34
3	A	1447	MAN	O5-C1-C2	-3.60	105.02	110.86
3	D	1447	MAN	O5-C1-C2	-3.46	105.24	110.86
3	D	1445	NAG	O7-C7-C8	-3.27	116.07	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1447	MAN	O3-C3-C4	-2.93	103.75	110.34
3	A	1445	NAG	O7-C7-C8	-2.91	116.71	122.06
3	A	1446	MAN	O6-C6-C5	-2.88	101.81	111.33
3	D	1450	GAL	O6-C6-C5	-2.84	101.95	111.33
3	A	1447	MAN	O6-C6-C5	-2.60	102.76	111.33
3	D	1446	MAN	O6-C6-C5	-2.54	102.93	111.33
3	D	1450	GAL	C1-O5-C5	-2.51	109.06	112.25
3	A	1450	GAL	O6-C6-C5	-2.49	103.09	111.33
3	A	1445	NAG	C2-N2-C7	-2.30	120.08	123.04
3	D	1444	NAG	C1-O5-C5	-2.02	109.69	112.25
3	A	1449	MAN	C2-C3-C4	2.05	114.53	111.04
3	D	1449	MAN	C2-C3-C4	2.19	114.76	111.04
3	A	1449	MAN	O3-C3-C4	2.20	115.30	110.34
3	D	1449	MAN	O2-C2-C1	2.23	113.68	109.21
3	D	1446	MAN	C3-C4-C5	2.29	114.18	110.20
3	A	1450	GAL	C2-C3-C4	2.32	114.98	111.04
3	A	1450	GAL	O5-C5-C6	2.41	112.58	107.35
3	D	1446	MAN	O5-C5-C6	2.55	112.88	107.35
3	A	1446	MAN	C3-C4-C5	2.61	114.75	110.20
3	A	1445	NAG	C4-C3-C2	2.64	115.33	111.23
3	A	1449	MAN	O2-C2-C1	2.76	114.73	109.21
3	D	1445	NAG	C4-C3-C2	2.77	115.54	111.23
3	D	1450	GAL	O4-C4-C3	2.82	116.70	110.34
3	A	1446	MAN	O5-C5-C6	2.87	113.55	107.35
3	D	1445	NAG	C8-C7-N2	2.88	121.61	116.11
3	A	1446	MAN	C1-C2-C3	2.93	113.00	109.54
3	D	1449	MAN	O2-C2-C3	2.94	116.03	110.12
3	A	1449	MAN	O2-C2-C3	2.98	116.10	110.12
3	A	1444	NAG	O3-C3-C4	3.07	117.24	110.34
3	D	1444	NAG	O3-C3-C4	3.17	117.47	110.34
3	D	1450	GAL	O5-C5-C6	3.21	114.29	107.35
3	A	1445	NAG	C8-C7-N2	3.22	122.27	116.11
3	D	1450	GAL	C2-C3-C4	3.27	116.60	111.04
3	A	1447	MAN	C1-O5-C5	3.28	116.41	112.25
3	A	1447	MAN	C1-C2-C3	3.31	113.46	109.54
3	D	1447	MAN	C1-C2-C3	3.35	113.50	109.54
3	D	1446	MAN	C1-C2-C3	3.42	113.58	109.54
3	A	1447	MAN	C2-C3-C4	3.72	117.36	111.04
3	D	1447	MAN	C2-C3-C4	4.15	118.09	111.04
3	D	1444	NAG	O5-C5-C6	4.17	116.38	107.35
3	A	1444	NAG	O5-C5-C6	4.33	116.71	107.35
3	A	1449	MAN	C1-O5-C5	4.86	118.42	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1450	GAL	O2-C2-C1	5.19	119.61	109.21
3	A	1448	NAG	C1-O5-C5	5.27	118.94	112.25
3	A	1450	GAL	O2-C2-C1	5.44	120.11	109.21
3	D	1448	NAG	C1-O5-C5	5.64	119.41	112.25
3	D	1449	MAN	C1-O5-C5	5.72	119.51	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	1446	MAN	C1
3	A	1446	MAN	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1444	NAG	1	0
3	A	1445	NAG	5	0
3	A	1446	MAN	1	0
3	A	1447	MAN	2	0
3	D	1444	NAG	2	0
3	D	1445	NAG	4	0
3	D	1446	MAN	1	0
3	D	1447	MAN	1	0

5.6 Ligand geometry [i](#)

2 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	FU4	A	1451	-	10,10,10	1.66	3 (30%)	14,14,14	2.95	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FU4	D	1451	-	10,10,10	1.42	2 (20%)	14,14,14	2.88	6 (42%)

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	FU4	A	1451	-	-	0/0/17/17	0/1/1/1
4	FU4	D	1451	-	-	0/0/17/17	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1451	FU4	C6-C5	2.11	1.56	1.51
4	D	1451	FU4	C2-C3	2.39	1.55	1.52
4	A	1451	FU4	C6-C5	2.40	1.57	1.51
4	A	1451	FU4	C1-C2	2.58	1.58	1.52
4	A	1451	FU4	C2-C3	2.79	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1451	FU4	O3-C3-C2	-2.47	105.53	110.00
4	D	1451	FU4	O2-C2-C3	-2.21	105.67	110.12
4	A	1451	FU4	O3-C3-C2	-2.17	106.08	110.00
4	D	1451	FU4	C6-C5-C4	2.04	117.10	113.08
4	D	1451	FU4	O4-C4-C5	2.06	114.68	109.84
4	A	1451	FU4	C6-C5-C4	2.28	117.56	113.08
4	D	1451	FU4	O5-C5-C6	4.94	114.30	106.13
4	A	1451	FU4	O5-C5-C6	5.86	115.83	106.13
4	D	1451	FU4	C1-C2-C3	7.94	118.93	109.54
4	A	1451	FU4	C1-C2-C3	8.05	119.07	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1451	FU4	3	0
4	D	1451	FU4	4	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, 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(Å ²)	Q<0.9
1	A	207/207 (100%)	0.30	5 (2%) 62 74	48, 78, 90, 90	0
1	D	207/207 (100%)	0.38	3 (1%) 78 87	48, 78, 90, 90	0
2	B	181/181 (100%)	0.29	0 100 100	48, 64, 82, 89	0
2	E	181/181 (100%)	0.26	1 (0%) 90 95	49, 64, 82, 89	0
All	All	776/776 (100%)	0.31	9 (1%) 81 89	48, 70, 90, 90	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	TYR	3.7
1	D	241	PHE	2.9
1	A	243	PHE	2.4
1	A	298	SER	2.3
1	D	237	GLY	2.2
1	A	241	PHE	2.2
1	A	294	GLU	2.2
2	E	182	LEU	2.1
1	D	294	GLU	2.1

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

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
3	GAL	D	1450	11/12	0.94	0.22	1.89	83,85,90,90	0
3	GAL	A	1450	11/12	0.98	0.13	-0.98	83,85,90,90	0
3	NAG	A	1448	14/15	0.96	0.14	-	76,87,90,90	0
3	MAN	A	1447	11/12	0.93	0.13	-	89,90,90,90	0
3	MAN	A	1449	11/12	0.85	0.13	-	89,90,90,90	0
3	MAN	D	1446	11/12	0.95	0.07	-	88,89,90,90	0
3	MAN	D	1449	11/12	0.84	0.18	-	89,90,90,90	0
3	MAN	A	1446	11/12	0.88	0.10	-	88,89,90,90	0
3	NAG	A	1445	14/15	0.96	0.10	-	88,89,90,90	0
3	NAG	A	1444	14/15	0.90	0.12	-	87,90,90,90	0
3	NAG	D	1448	14/15	0.97	0.18	-	76,88,90,90	0
3	MAN	D	1447	11/12	0.92	0.17	-	89,90,90,90	0
3	NAG	D	1445	14/15	0.94	0.13	-	88,89,90,90	0
3	NAG	D	1444	14/15	0.87	0.14	-	87,90,90,90	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, 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(\AA^2)	Q<0.9
4	FU4	D	1451	10/10	0.91	0.16	-	89,90,90,90	0
4	FU4	A	1451	10/10	0.92	0.16	-	89,90,90,90	0

6.5 Other polymers

There are no such residues in this entry.