



wwPDB X-ray Structure Validation Summary Report

Oct 7, 2014 – 11:46 AM EDT

PDB ID : 4R2G
Title : Crystal Structure of PGT124 Fab bound to HIV-1 JRCSF gp120 core and to CD4
Authors : Garces, F.; Wilson, I.A.
Deposited on : 2014-08-11
Resolution : 3.28 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

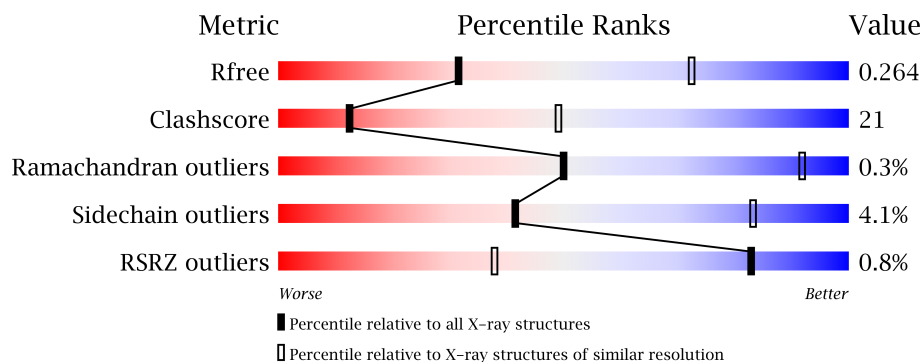
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23828
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23828

1 Overall quality at a glance

The reported resolution of this entry is 3.28 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}	66092	1151 (3.36-3.20)
Clashscore	79885	1464 (3.36-3.20)
Ramachandran outliers	78287	1435 (3.36-3.20)
Sidechain outliers	78261	1433 (3.36-3.20)
RSRZ outliers	66119	1152 (3.36-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	309	
1	E	309	
1	K	309	
1	O	309	
2	B	184	
2	F	184	
2	H	184	
2	L	184	
3	C	214	
3	I	214	
3	M	214	
3	P	214	
4	D	236	
4	J	236	

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Mol	Chain	Length	Quality of chain
4	N	236	
4	Q	236	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 29158 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Surface protein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	303	Total	C	N	O	S	0	0	0
			2383	1491	422	451	19			
1	O	303	Total	C	N	O	S	0	0	0
			2383	1491	422	451	19			
1	A	302	Total	C	N	O	S	0	0	0
			2375	1485	421	450	19			
1	K	303	Total	C	N	O	S	0	0	0
			2383	1491	422	451	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	317	THR	-	LINKER	UNP P20871
E	318	ARG	-	LINKER	UNP P20871
E	319	PRO	-	LINKER	UNP P20871
O	317	THR	-	LINKER	UNP P20871
O	318	ARG	-	LINKER	UNP P20871
O	319	PRO	-	LINKER	UNP P20871
A	317	THR	-	LINKER	UNP P20871
A	318	ARG	-	LINKER	UNP P20871
A	319	PRO	-	LINKER	UNP P20871
K	317	THR	-	LINKER	UNP P20871
K	318	ARG	-	LINKER	UNP P20871
K	319	PRO	-	LINKER	UNP P20871

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	175	Total	C	N	O	S	0	0	0
			1363	851	239	269	4			
2	B	175	Total	C	N	O	S	0	0	0
			1363	851	239	269	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	176	Total	C	N	O	S	0	0	0
			1368	854	240	270	4			
2	L	173	Total	C	N	O	S	0	0	0
			1345	839	235	267	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	MET	-	EXPRESSION TAG	UNP P01730
B	0	MET	-	EXPRESSION TAG	UNP P01730
H	0	MET	-	EXPRESSION TAG	UNP P01730
L	0	MET	-	EXPRESSION TAG	UNP P01730

- Molecule 3 is a protein called PGT124 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			
3	C	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			
3	I	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			
3	M	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			

- Molecule 4 is a protein called PGT124 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Q	228	Total	C	N	O	S	0	0	0
			1732	1099	289	339	5			
4	D	225	Total	C	N	O	S	0	0	0
			1716	1091	286	334	5			
4	J	226	Total	C	N	O	S	0	0	0
			1720	1093	287	335	5			
4	N	228	Total	C	N	O	S	0	0	0
			1735	1101	290	339	5			

- Molecule 5 is a polymer of unknown type called SUGAR (10-MER).

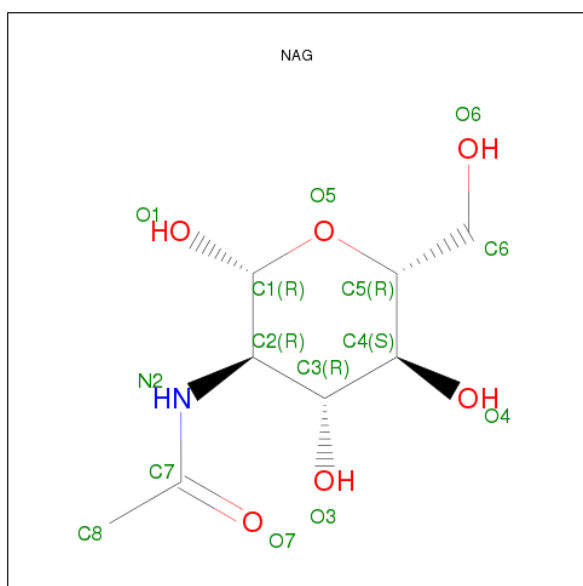
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	10	Total	C	N	O	0	0
			116	64	2	50		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	O	10	Total	C	N	O	0	0
			116	64	2	50		
5	A	10	Total	C	N	O	0	0
			116	64	2	50		
5	K	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

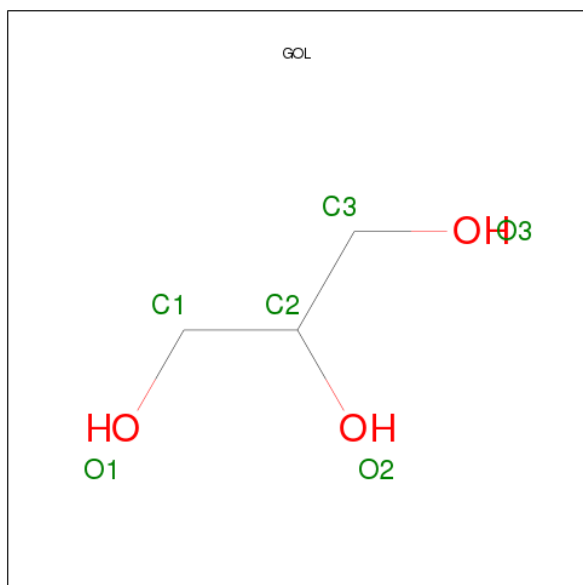
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	O	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	K	1	Total	Cl	0	0
			1	1		
7	E	1	Total	Cl	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	Q	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	J	1	Total	C	O	0	0
			6	3	3		
8	N	1	Total	C	O	0	0
			6	3	3		

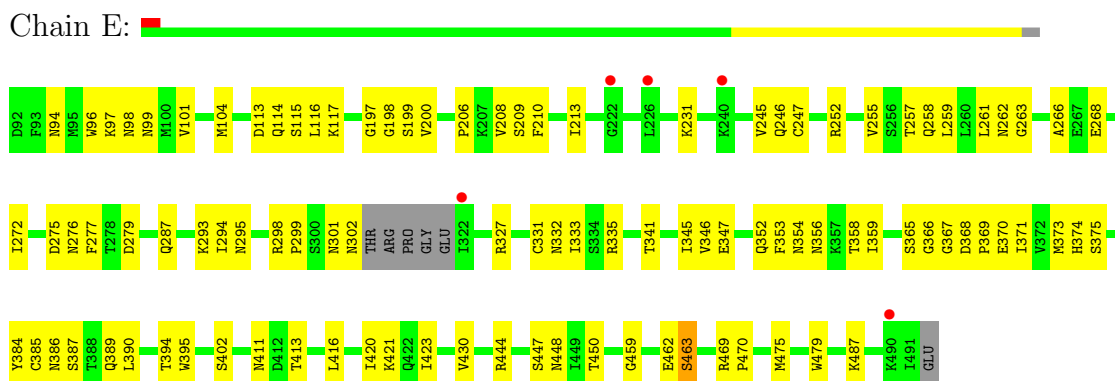
- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	2	Total	C	N	O	0	0
			28	16	2	10		
9	A	2	Total	C	N	O	0	0
			28	16	2	10		

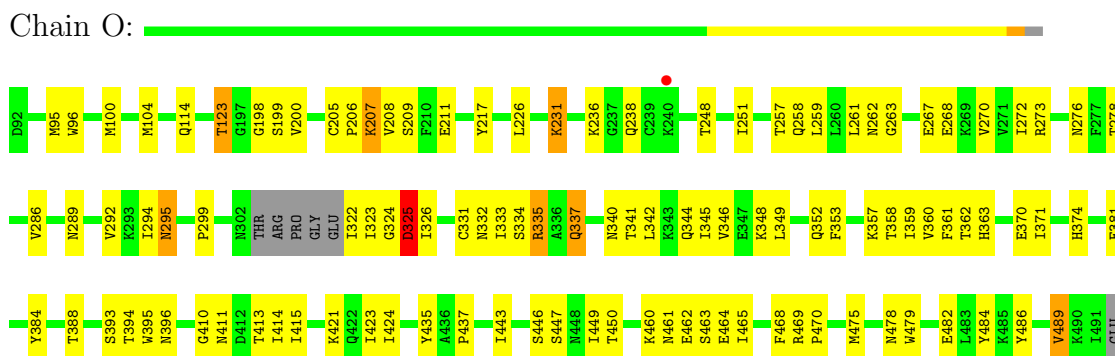
3 Residue-property plots

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.

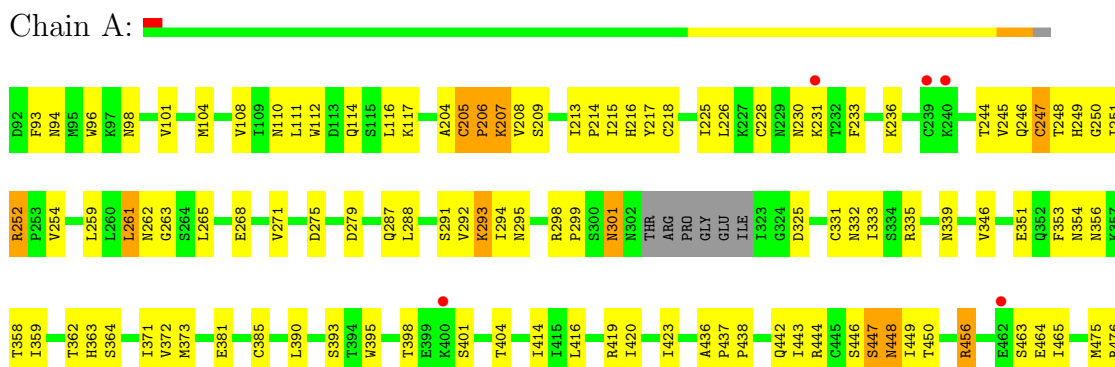
- Molecule 1: Surface protein gp160

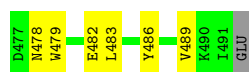


- Molecule 1: Surface protein gp160



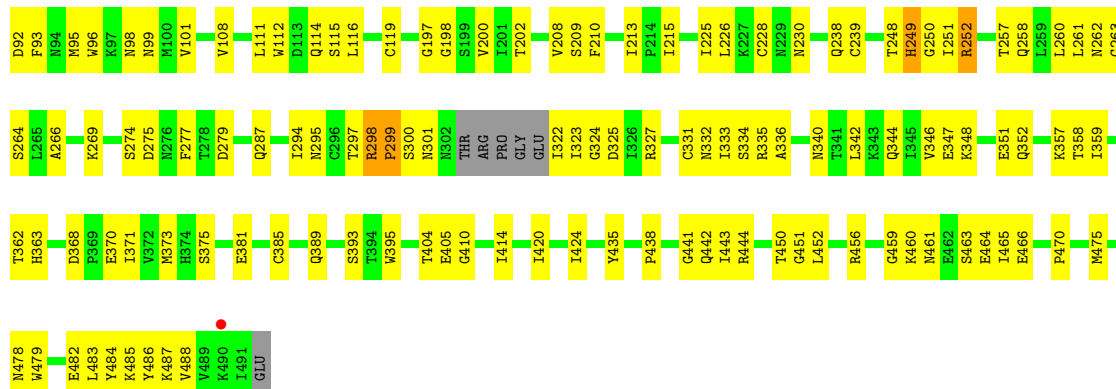
- Molecule 1: Surface protein gp160





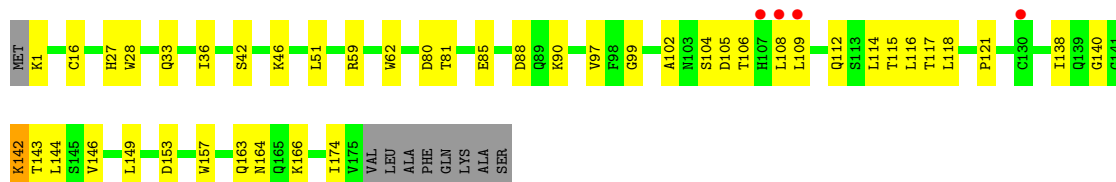
- Molecule 1: Surface protein gp160

Chain K:



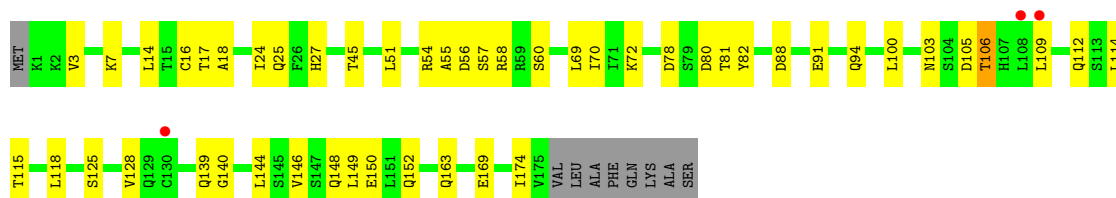
- Molecule 2: T-cell surface glycoprotein CD4

Chain F:



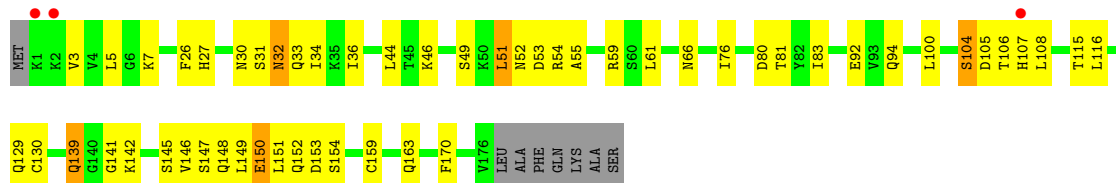
- Molecule 2: T-cell surface glycoprotein CD4

Chain B:



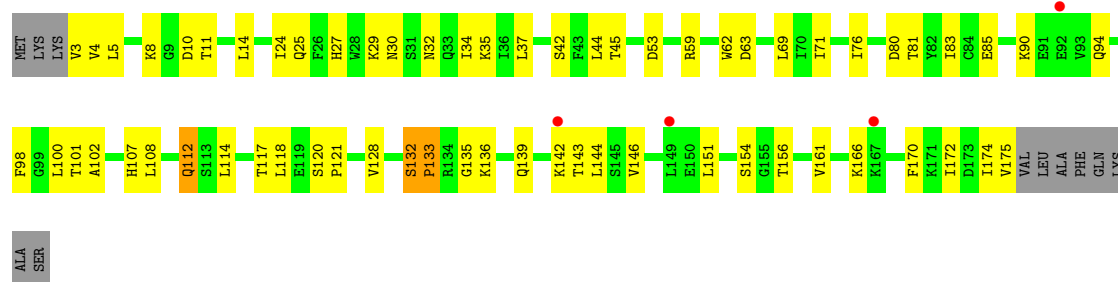
- Molecule 2: T-cell surface glycoprotein CD4

Chain H:



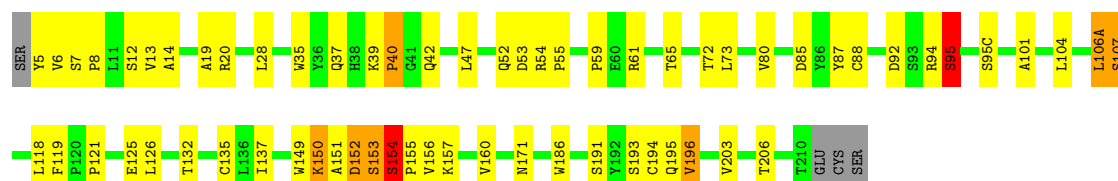
- Molecule 2: T-cell surface glycoprotein CD4

Chain L:



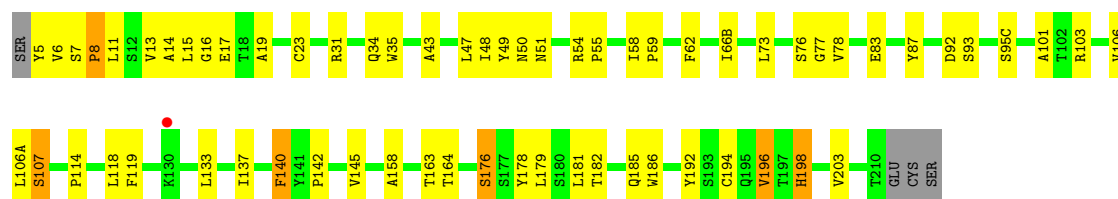
• Molecule 3: PGT124 Light Chain

Chain P:



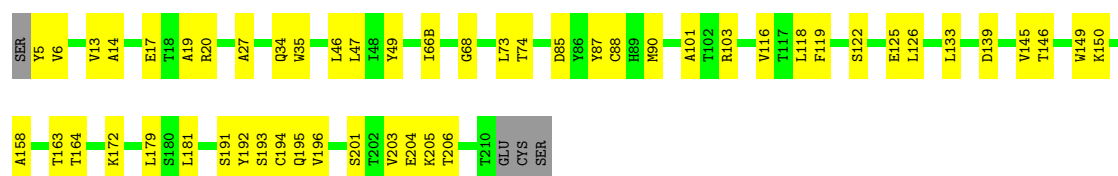
• Molecule 3: PGT124 Light Chain

Chain C:



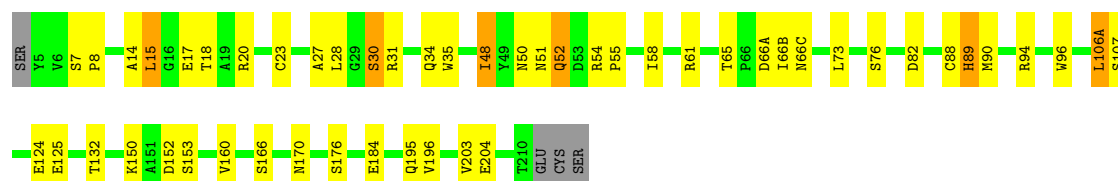
• Molecule 3: PGT124 Light Chain

Chain I:



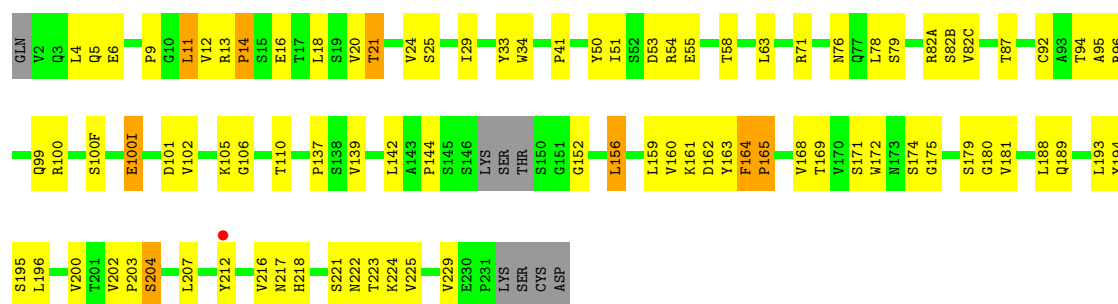
• Molecule 3: PGT124 Light Chain

Chain M:



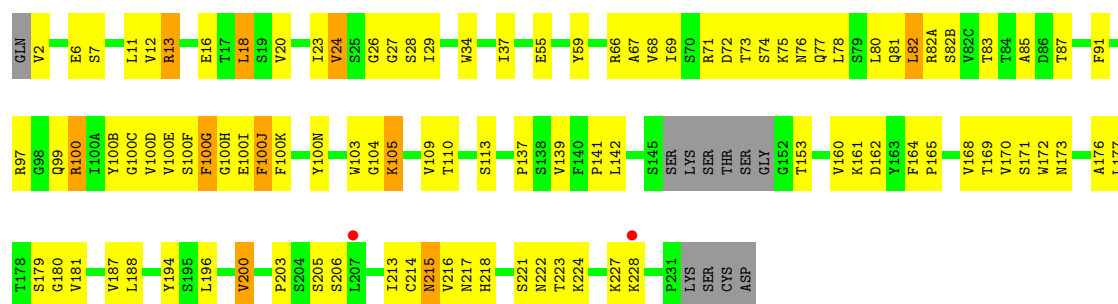
• Molecule 4: PGT124 Heavy Chain

Chain Q:



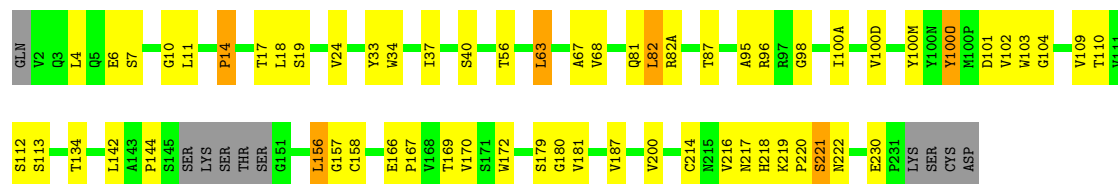
• Molecule 4: PGT124 Heavy Chain

Chain D:



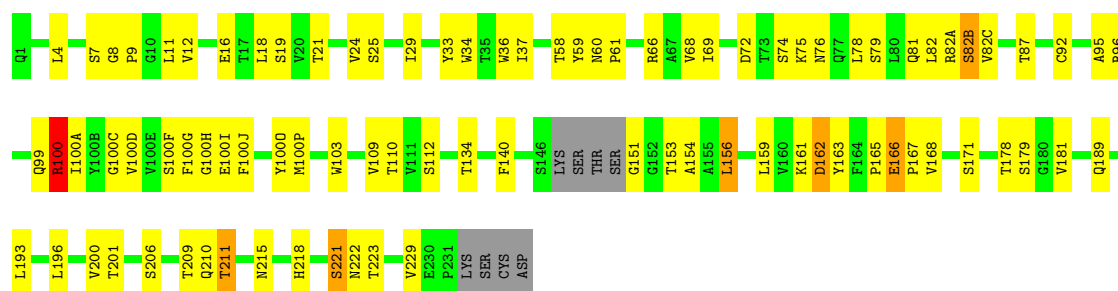
• Molecule 4: PGT124 Heavy Chain

Chain J:



• Molecule 4: PGT124 Heavy Chain

Chain N:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	164.41Å 165.44Å 229.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.65 – 3.28 39.65 – 3.28	Depositor EDS
% Data completeness (in resolution range)	98.4 (39.65-3.28) 98.5 (39.65-3.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.207 , 0.263 0.209 , 0.264	Depositor DCC
R_{free} test set	4719 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	94.1	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 19.1	EDS
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 94615 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	29158	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, BMA, 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	0.38	1/2419 (0.0%)	0.60	2/3268 (0.1%)
1	E	0.40	1/2427 (0.0%)	0.61	1/3279 (0.0%)
1	K	0.35	1/2427 (0.0%)	0.60	2/3279 (0.1%)
1	O	0.36	0/2427	0.56	0/3279
2	B	0.32	0/1382	0.54	0/1863
2	F	0.34	0/1382	0.59	0/1863
2	H	0.33	1/1387 (0.1%)	0.59	3/1870 (0.2%)
2	L	0.31	1/1364 (0.1%)	0.53	1/1841 (0.1%)
3	C	0.37	1/1638 (0.1%)	0.61	1/2238 (0.0%)
3	I	0.38	0/1638	0.61	0/2238
3	M	0.43	0/1638	0.67	1/2238 (0.0%)
3	P	0.53	2/1638 (0.1%)	0.71	4/2238 (0.2%)
4	D	0.39	0/1759	0.66	3/2402 (0.1%)
4	J	0.41	1/1763 (0.1%)	0.66	2/2407 (0.1%)
4	N	0.51	2/1778 (0.1%)	0.74	4/2427 (0.2%)
4	Q	0.46	1/1775 (0.1%)	0.68	2/2423 (0.1%)
All	All	0.40	12/28842 (0.0%)	0.63	26/39153 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	M	0	1
3	P	0	2
All	All	0	3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	40	PRO	N-CD	11.64	1.64	1.47
4	N	100	ARG	CA-C	-8.85	1.29	1.52
3	C	8	PRO	N-CD	-5.79	1.39	1.47
1	A	206	PRO	N-CD	5.63	1.55	1.47
1	K	299	PRO	N-CD	5.29	1.55	1.47

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	14	PRO	N-CA-C	8.06	133.06	112.10
3	P	107	SER	N-CA-C	-6.74	92.79	111.00
4	N	100	ARG	C-N-CA	-6.55	105.33	121.70
4	D	74	SER	N-CA-CB	6.48	120.22	110.50
3	P	40	PRO	CA-N-CD	-6.45	102.47	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	106(A)	LEU	Peptide
3	P	106(A)	LEU	Peptide
3	P	95	SER	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2375	0	2335	136	0
1	E	2383	0	2342	96	0
1	K	2383	0	2350	180	0
1	O	2383	0	2342	119	0
2	B	1363	0	1389	41	0
2	F	1363	0	1389	40	0
2	H	1368	0	1391	64	0
2	L	1345	0	1360	47	0
3	C	1595	0	1541	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1595	0	1543	37	0
3	M	1595	0	1541	39	0
3	P	1595	0	1540	64	0
4	D	1716	0	1683	94	0
4	J	1720	0	1686	45	0
4	N	1735	0	1702	62	0
4	Q	1732	0	1696	81	0
5	A	116	0	96	13	0
5	E	116	0	96	11	0
5	K	116	0	96	28	0
5	O	116	0	96	17	0
6	A	84	0	78	7	0
6	E	112	0	104	3	0
6	K	70	0	65	4	0
6	O	98	0	91	6	0
7	A	1	0	0	0	0
7	E	1	0	0	1	0
7	K	1	0	0	1	0
7	O	1	0	0	0	0
8	D	6	0	8	5	0
8	J	6	0	8	14	0
8	N	6	0	8	3	0
8	Q	6	0	8	0	0
9	A	56	0	50	6	0
All	All	29158	0	28634	1214	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

The worst 5 of 1214 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:332:ASN:ND2	5:K:501:NAG:H82	1.26	1.44
3:P:150:LYS:CB	3:P:193:SER:OG	1.64	1.41
6:O:515:NAG:H62	6:O:516:NAG:C8	1.51	1.38
8:J:301:GOL:H32	5:K:504:MAN:C2	1.60	1.32
1:K:335:ARG:NE	1:K:410:GLY:HA3	1.48	1.29

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/309 (96%)	276 (93%)	20 (7%)	2 (1%)	30	80
1	E	299/309 (97%)	272 (91%)	27 (9%)	0	100	100
1	K	299/309 (97%)	275 (92%)	23 (8%)	1 (0%)	50	92
1	O	299/309 (97%)	279 (93%)	17 (6%)	3 (1%)	22	75
2	B	173/184 (94%)	164 (95%)	8 (5%)	1 (1%)	33	83
2	F	173/184 (94%)	164 (95%)	9 (5%)	0	100	100
2	H	174/184 (95%)	157 (90%)	16 (9%)	1 (1%)	33	83
2	L	171/184 (93%)	160 (94%)	11 (6%)	0	100	100
3	C	208/214 (97%)	191 (92%)	17 (8%)	0	100	100
3	I	208/214 (97%)	186 (89%)	22 (11%)	0	100	100
3	M	208/214 (97%)	198 (95%)	10 (5%)	0	100	100
3	P	208/214 (97%)	194 (93%)	12 (6%)	2 (1%)	22	75
4	D	221/236 (94%)	197 (89%)	23 (10%)	1 (0%)	38	85
4	J	222/236 (94%)	209 (94%)	12 (5%)	1 (0%)	38	85
4	N	224/236 (95%)	206 (92%)	18 (8%)	0	100	100
4	Q	224/236 (95%)	204 (91%)	20 (9%)	0	100	100
All	All	3609/3772 (96%)	3332 (92%)	265 (7%)	12 (0%)	50	92

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	100(J)	PHE
1	A	205	CYS
1	O	231	LYS
2	B	106	THR
2	H	150	GLU

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	270/276 (98%)	260 (96%)	10 (4%)	45	85
1	E	271/276 (98%)	264 (97%)	7 (3%)	59	90
1	K	271/276 (98%)	263 (97%)	8 (3%)	53	88
1	O	271/276 (98%)	263 (97%)	8 (3%)	53	88
2	B	159/166 (96%)	157 (99%)	2 (1%)	80	95
2	F	159/166 (96%)	154 (97%)	5 (3%)	52	88
2	H	159/166 (96%)	155 (98%)	4 (2%)	60	90
2	L	157/166 (95%)	151 (96%)	6 (4%)	44	85
3	C	176/180 (98%)	169 (96%)	7 (4%)	42	84
3	I	176/180 (98%)	173 (98%)	3 (2%)	73	94
3	M	176/180 (98%)	164 (93%)	12 (7%)	22	67
3	P	176/180 (98%)	166 (94%)	10 (6%)	29	74
4	D	194/204 (95%)	180 (93%)	14 (7%)	21	64
4	J	194/204 (95%)	183 (94%)	11 (6%)	29	74
4	N	196/204 (96%)	182 (93%)	14 (7%)	21	64
4	Q	196/204 (96%)	185 (94%)	11 (6%)	30	75
All	All	3201/3304 (97%)	3069 (96%)	132 (4%)	41	83

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	147	SER
4	J	230	GLU
1	A	447	SER
3	I	181	LEU
4	J	63	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	198	HIS
4	D	76	ASN
3	M	52	GLN
2	B	33	GLN
2	B	103	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

44 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	$\# Z > 2$
5	NAG	A	501	1,5	12,14,15	0.58	0	15,19,21	0.79	0
5	NAG	A	502	5	12,14,15	0.63	0	15,19,21	1.31	2 (13%)
5	BMA	A	503	5	10,11,12	1.17	1 (10%)	11,15,17	5.12	4 (36%)
5	MAN	A	504	5	10,11,12	0.64	0	11,15,17	0.79	0
5	MAN	A	505	5	10,11,12	0.65	0	11,15,17	1.14	2 (18%)
5	MAN	A	506	5	10,11,12	0.62	0	11,15,17	0.92	1 (9%)
5	MAN	A	507	5	10,11,12	0.62	0	11,15,17	0.92	1 (9%)
5	MAN	A	508	5	10,11,12	0.63	0	11,15,17	1.11	1 (9%)
5	MAN	A	509	5	10,11,12	0.69	0	11,15,17	0.87	0
5	MAN	A	510	5	10,11,12	0.68	0	11,15,17	0.70	0
9	NAG	A	511	1,9	12,14,15	0.63	0	15,19,21	0.94	2 (13%)
9	NAG	A	512	9	12,14,15	0.60	0	15,19,21	0.91	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	A	513	1,9	12,14,15	0.59	0	15,19,21	0.87	1 (6%)
9	NAG	A	514	9	12,14,15	0.57	0	15,19,21	0.86	1 (6%)
5	NAG	E	501	1,5	12,14,15	0.58	0	15,19,21	0.78	0
5	NAG	E	502	5	12,14,15	0.65	0	15,19,21	1.32	2 (13%)
5	BMA	E	503	5	10,11,12	1.18	1 (10%)	11,15,17	5.14	4 (36%)
5	MAN	E	504	5	10,11,12	0.65	0	11,15,17	0.78	0
5	MAN	E	505	5	10,11,12	0.65	0	11,15,17	1.13	2 (18%)
5	MAN	E	506	5	10,11,12	0.61	0	11,15,17	0.92	1 (9%)
5	MAN	E	507	5	10,11,12	0.63	0	11,15,17	0.92	1 (9%)
5	MAN	E	508	5	10,11,12	0.63	0	11,15,17	0.76	0
5	MAN	E	509	5	10,11,12	0.72	1 (10%)	11,15,17	0.83	0
5	MAN	E	510	5	10,11,12	0.65	0	11,15,17	0.80	0
5	NAG	K	501	1,5	12,14,15	0.58	0	15,19,21	0.78	0
5	NAG	K	502	5	12,14,15	0.64	0	15,19,21	1.31	2 (13%)
5	BMA	K	503	5	10,11,12	1.18	1 (10%)	11,15,17	5.12	4 (36%)
5	MAN	K	504	5	10,11,12	0.63	0	11,15,17	0.78	0
5	MAN	K	505	5	10,11,12	0.66	0	11,15,17	1.15	2 (18%)
5	MAN	K	506	5	10,11,12	0.60	0	11,15,17	0.92	1 (9%)
5	MAN	K	507	5	10,11,12	0.61	0	11,15,17	0.90	1 (9%)
5	MAN	K	508	5	10,11,12	0.60	0	11,15,17	0.86	1 (9%)
5	MAN	K	509	5	10,11,12	0.69	0	11,15,17	0.86	0
5	MAN	K	510	5	10,11,12	0.68	0	11,15,17	0.70	0
5	NAG	O	501	1,5	12,14,15	0.57	0	15,19,21	0.78	0
5	NAG	O	502	5	12,14,15	0.64	0	15,19,21	1.31	2 (13%)
5	BMA	O	503	5	10,11,12	1.18	1 (10%)	11,15,17	5.12	4 (36%)
5	MAN	O	504	5	10,11,12	0.64	0	11,15,17	0.78	0
5	MAN	O	505	5	10,11,12	0.65	0	11,15,17	1.13	2 (18%)
5	MAN	O	506	5	10,11,12	0.61	0	11,15,17	0.92	1 (9%)
5	MAN	O	507	5	10,11,12	0.62	0	11,15,17	0.91	1 (9%)
5	MAN	O	508	5	10,11,12	0.59	0	11,15,17	0.85	1 (9%)
5	MAN	O	509	5	10,11,12	0.69	0	11,15,17	0.86	0
5	MAN	O	510	5	10,11,12	0.69	0	11,15,17	0.70	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
5	NAG	A	501	1,5	-	1/6/23/26	0/1/1/1
5	NAG	A	502	5	-	0/6/23/26	0/1/1/1
5	BMA	A	503	5	-	0/2/19/22	0/1/1/1
5	MAN	A	504	5	-	0/2/19/22	0/1/1/1
5	MAN	A	505	5	-	0/2/19/22	0/1/1/1
5	MAN	A	506	5	-	0/2/19/22	0/1/1/1
5	MAN	A	507	5	-	0/2/19/22	0/1/1/1
5	MAN	A	508	5	-	0/2/19/22	0/1/1/1
5	MAN	A	509	5	-	0/2/19/22	0/1/1/1
5	MAN	A	510	5	-	0/2/19/22	0/1/1/1
9	NAG	A	511	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	512	9	-	0/6/23/26	0/1/1/1
9	NAG	A	513	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	514	9	-	0/6/23/26	0/1/1/1
5	NAG	E	501	1,5	-	1/6/23/26	0/1/1/1
5	NAG	E	502	5	-	0/6/23/26	0/1/1/1
5	BMA	E	503	5	-	0/2/19/22	0/1/1/1
5	MAN	E	504	5	-	0/2/19/22	0/1/1/1
5	MAN	E	505	5	-	0/2/19/22	0/1/1/1
5	MAN	E	506	5	-	0/2/19/22	0/1/1/1
5	MAN	E	507	5	-	0/2/19/22	0/1/1/1
5	MAN	E	508	5	-	0/2/19/22	0/1/1/1
5	MAN	E	509	5	-	0/2/19/22	0/1/1/1
5	MAN	E	510	5	-	0/2/19/22	0/1/1/1
5	NAG	K	501	1,5	-	1/6/23/26	0/1/1/1
5	NAG	K	502	5	-	0/6/23/26	0/1/1/1
5	BMA	K	503	5	-	0/2/19/22	0/1/1/1
5	MAN	K	504	5	-	0/2/19/22	0/1/1/1
5	MAN	K	505	5	-	0/2/19/22	0/1/1/1
5	MAN	K	506	5	-	0/2/19/22	0/1/1/1
5	MAN	K	507	5	-	0/2/19/22	0/1/1/1
5	MAN	K	508	5	-	0/2/19/22	0/1/1/1
5	MAN	K	509	5	-	0/2/19/22	0/1/1/1
5	MAN	K	510	5	-	0/2/19/22	0/1/1/1
5	NAG	O	501	1,5	-	1/6/23/26	0/1/1/1
5	NAG	O	502	5	-	0/6/23/26	0/1/1/1
5	BMA	O	503	5	-	0/2/19/22	0/1/1/1
5	MAN	O	504	5	-	0/2/19/22	0/1/1/1
5	MAN	O	505	5	-	0/2/19/22	0/1/1/1
5	MAN	O	506	5	-	0/2/19/22	0/1/1/1
5	MAN	O	507	5	-	0/2/19/22	0/1/1/1
5	MAN	O	508	5	-	0/2/19/22	0/1/1/1
5	MAN	O	509	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	O	510	5	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	503	BMA	O2-C2	-2.28	1.38	1.43
5	A	503	BMA	O2-C2	-2.26	1.38	1.43
5	O	503	BMA	O2-C2	-2.26	1.38	1.43
5	E	503	BMA	O2-C2	-2.25	1.38	1.43
5	E	509	MAN	O5-C5	-2.02	1.42	1.45

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	503	BMA	O3-C3-C2	-13.14	85.88	109.74
5	O	503	BMA	O3-C3-C2	-13.11	85.94	109.74
5	A	503	BMA	O3-C3-C2	-13.10	85.96	109.74
5	K	503	BMA	O3-C3-C2	-13.10	85.95	109.74
5	E	503	BMA	O3-C3-C4	9.83	132.32	110.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	501	NAG	O7-C7-N2-C2
5	K	501	NAG	O7-C7-N2-C2
5	A	501	NAG	O7-C7-N2-C2
5	O	501	NAG	O7-C7-N2-C2

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	A	515	1	12,14,15	0.58	0	15,19,21	0.88	1 (6%)
6	NAG	A	516	1	12,14,15	0.50	0	15,19,21	0.79	1 (6%)
6	NAG	A	517	1	12,14,15	0.33	0	15,19,21	0.41	0
6	NAG	A	518	1	12,14,15	0.57	0	15,19,21	0.52	0
6	NAG	A	519	1	12,14,15	0.33	0	15,19,21	0.45	0
6	NAG	A	520	1	12,14,15	0.64	0	15,19,21	0.98	1 (6%)
8	GOL	D	301	-	5,5,5	0.19	0	5,5,5	0.26	0
6	NAG	E	511	1	12,14,15	0.69	0	15,19,21	1.08	2 (13%)
6	NAG	E	512	1	12,14,15	0.34	0	15,19,21	0.63	0
6	NAG	E	513	1	12,14,15	0.44	0	15,19,21	0.57	0
6	NAG	E	514	1	12,14,15	0.58	0	15,19,21	1.15	2 (13%)
6	NAG	E	515	1	12,14,15	0.52	0	15,19,21	0.97	1 (6%)
6	NAG	E	516	1	12,14,15	0.45	0	15,19,21	0.56	0
6	NAG	E	517	1	12,14,15	0.33	0	15,19,21	0.40	0
6	NAG	E	518	1	12,14,15	0.36	0	15,19,21	0.38	0
8	GOL	J	301	-	5,5,5	0.19	0	5,5,5	0.26	0
6	NAG	K	511	1	12,14,15	0.45	0	15,19,21	0.57	0
6	NAG	K	512	1	12,14,15	0.37	0	15,19,21	0.50	0
6	NAG	K	513	1	12,14,15	0.29	0	15,19,21	0.45	0
6	NAG	K	514	1	12,14,15	0.55	0	15,19,21	0.66	0
6	NAG	K	515	1	12,14,15	0.57	0	15,19,21	0.86	1 (6%)
8	GOL	N	301	-	5,5,5	0.20	0	5,5,5	0.27	0
6	NAG	O	511	1	12,14,15	0.40	0	15,19,21	0.41	0
6	NAG	O	512	1	12,14,15	0.52	0	15,19,21	0.59	0
6	NAG	O	513	1	12,14,15	0.37	0	15,19,21	0.75	0
6	NAG	O	514	1	12,14,15	0.41	0	15,19,21	0.93	0
6	NAG	O	515	1	12,14,15	0.62	0	15,19,21	0.80	1 (6%)
6	NAG	O	516	1	12,14,15	0.42	0	15,19,21	0.48	0
6	NAG	O	517	1	12,14,15	0.48	0	15,19,21	0.48	0
8	GOL	Q	301	-	5,5,5	0.19	0	5,5,5	0.26	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	NAG	A	515	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	516	1	-	0/6/23/26	0/1/1/1
6	NAG	A	517	1	-	0/6/23/26	0/1/1/1
6	NAG	A	518	1	-	0/6/23/26	0/1/1/1
6	NAG	A	519	1	-	0/6/23/26	0/1/1/1
6	NAG	A	520	1	-	0/6/23/26	0/1/1/1
8	GOL	D	301	-	-	0/4/4/4	0/0/0/0
6	NAG	E	511	1	-	0/6/23/26	0/1/1/1
6	NAG	E	512	1	-	0/6/23/26	0/1/1/1
6	NAG	E	513	1	-	0/6/23/26	0/1/1/1
6	NAG	E	514	1	-	0/6/23/26	0/1/1/1
6	NAG	E	515	1	-	0/6/23/26	0/1/1/1
6	NAG	E	516	1	-	0/6/23/26	0/1/1/1
6	NAG	E	517	1	-	0/6/23/26	0/1/1/1
6	NAG	E	518	1	-	0/6/23/26	0/1/1/1
8	GOL	J	301	-	-	0/4/4/4	0/0/0/0
6	NAG	K	511	1	-	0/6/23/26	0/1/1/1
6	NAG	K	512	1	-	0/6/23/26	0/1/1/1
6	NAG	K	513	1	-	0/6/23/26	0/1/1/1
6	NAG	K	514	1	-	0/6/23/26	0/1/1/1
6	NAG	K	515	1	-	0/6/23/26	0/1/1/1
8	GOL	N	301	-	-	0/4/4/4	0/0/0/0
6	NAG	O	511	1	-	0/6/23/26	0/1/1/1
6	NAG	O	512	1	-	0/6/23/26	0/1/1/1
6	NAG	O	513	1	-	0/6/23/26	0/1/1/1
6	NAG	O	514	1	-	0/6/23/26	0/1/1/1
6	NAG	O	515	1	-	0/6/23/26	0/1/1/1
6	NAG	O	516	1	-	0/6/23/26	0/1/1/1
6	NAG	O	517	1	-	0/6/23/26	0/1/1/1
8	GOL	Q	301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	520	NAG	C2-N2-C7	-3.06	119.69	123.39
6	E	514	NAG	O5-C5-C4	-2.94	106.93	110.65
6	E	511	NAG	O5-C5-C4	-2.87	107.02	110.65
6	E	515	NAG	O5-C5-C4	-2.59	107.36	110.65
6	A	516	NAG	O5-C5-C4	-2.54	107.43	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	302/309 (97%)	0.12	5 (1%) 67 21	34, 62, 99, 136	0
1	E	303/309 (98%)	0.15	5 (1%) 67 21	19, 44, 96, 113	0
1	K	303/309 (98%)	0.15	1 (0%) 91 61	25, 64, 97, 121	0
1	O	303/309 (98%)	0.08	1 (0%) 91 61	23, 46, 82, 111	0
2	B	175/184 (95%)	0.23	3 (1%) 67 21	31, 71, 111, 124	0
2	F	175/184 (95%)	0.35	4 (2%) 57 15	25, 53, 120, 138	0
2	H	176/184 (95%)	0.42	3 (1%) 67 21	36, 83, 124, 133	0
2	L	173/184 (94%)	0.39	4 (2%) 57 15	50, 94, 121, 131	0
3	C	210/214 (98%)	0.05	1 (0%) 88 49	31, 54, 81, 97	0
3	I	210/214 (98%)	-0.16	0 100 100	25, 42, 63, 78	0
3	M	210/214 (98%)	-0.13	0 100 100	18, 30, 47, 55	0
3	P	210/214 (98%)	-0.05	0 100 100	18, 42, 76, 90	0
4	D	225/236 (95%)	0.10	2 (0%) 81 36	28, 54, 101, 115	0
4	J	226/236 (95%)	-0.01	0 100 100	19, 38, 71, 93	0
4	N	228/236 (96%)	-0.02	0 100 100	18, 32, 66, 89	0
4	Q	228/236 (96%)	-0.01	1 (0%) 90 55	21, 47, 92, 104	0
All	All	3657/3772 (96%)	0.09	30 (0%) 83 38	18, 51, 103, 138	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	142	LYS	5.1
2	F	107	HIS	4.3
2	L	167	LYS	3.6
1	A	240	LYS	3.6
2	F	108	LEU	3.4

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	NAG	A	512	14/15	0.27	-	65,95,105,112	0
5	MAN	O	507	11/12	0.31	-	66,71,76,77	0
5	BMA	A	503	11/12	0.20	-	33,38,50,54	0
5	MAN	E	507	11/12	0.26	-	76,79,85,86	0
5	MAN	O	504	11/12	0.19	-	51,56,62,63	0
5	NAG	A	502	14/15	0.22	-	30,37,45,47	0
5	MAN	K	505	11/12	0.19	-	63,66,75,79	0
5	NAG	O	502	14/15	0.18	-	33,38,40,41	0
5	NAG	K	502	14/15	0.18	-	33,40,46,50	0
5	MAN	A	509	11/12	0.19	-	25,31,40,49	0
5	MAN	E	504	11/12	0.21	-	56,60,67,70	0
5	MAN	A	505	11/12	0.18	-	58,70,79,79	0
5	MAN	E	505	11/12	0.17	-	57,63,70,71	0
5	MAN	O	506	11/12	0.34	-	61,77,86,93	0
5	MAN	O	508	11/12	0.16	-	38,48,57,62	0
5	MAN	K	507	11/12	0.25	-	68,72,83,83	0
5	MAN	E	506	11/12	0.27	-	52,64,75,77	0
5	MAN	O	509	11/12	0.15	-	42,46,51,53	0
5	MAN	A	510	11/12	0.18	-	26,30,36,37	0
5	NAG	E	502	14/15	0.23	-	25,30,35,37	0
5	BMA	E	503	11/12	0.19	-	21,28,44,45	0
5	BMA	O	503	11/12	0.17	-	35,43,53,56	0
5	MAN	A	504	11/12	0.19	-	53,57,68,69	0
5	MAN	A	506	11/12	0.28	-	60,75,83,88	0
9	NAG	A	513	14/15	0.23	-	79,89,102,102	0
5	MAN	K	509	11/12	0.17	-	33,39,46,46	0
5	MAN	E	508	11/12	0.17	-	20,24,30,33	0
5	MAN	K	510	11/12	0.15	-	38,42,52,55	0
5	MAN	O	510	11/12	0.15	-	39,42,48,52	0
5	NAG	K	501	14/15	0.20	-	33,44,51,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	NAG	A	511	14/15	0.18	-	56,69,74,79	0
5	MAN	E	510	11/12	0.22	-	26,32,37,43	0
9	NAG	A	514	14/15	0.31	-	106,116,124,125	0
5	MAN	A	507	11/12	0.30	-	61,73,82,83	0
5	NAG	O	501	14/15	0.28	-	30,38,44,44	0
5	MAN	A	508	11/12	0.17	-	24,29,34,41	0
5	MAN	E	509	11/12	0.18	-	20,24,30,31	0
5	NAG	E	501	14/15	0.19	-	24,27,34,38	0
5	MAN	K	508	11/12	0.25	-	35,40,51,55	0
5	NAG	A	501	14/15	0.19	-	32,40,51,53	0
5	MAN	K	504	11/12	0.20	-	53,62,69,70	0
5	BMA	K	503	11/12	0.17	-	38,46,53,59	0
5	MAN	O	505	11/12	0.21	-	67,74,78,81	0
5	MAN	K	506	11/12	0.25	-	64,77,80,81	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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	GOL	N	301	6/6	0.24	-	44,47,53,55	0
7	CL	E	519	1/1	0.34	-	53,53,53,53	0
6	NAG	O	516	14/15	0.38	-	71,79,83,84	0
7	CL	K	516	1/1	0.19	-	70,70,70,70	0
6	NAG	K	514	14/15	0.28	-	74,87,92,98	0
8	GOL	D	301	6/6	0.30	-	52,55,56,66	0
6	NAG	E	516	14/15	0.36	-	42,56,65,70	0
6	NAG	O	513	14/15	0.25	-	48,62,70,78	0
6	NAG	A	516	14/15	0.23	-	79,96,104,107	0
7	CL	O	518	1/1	0.16	-	54,54,54,54	0
6	NAG	O	512	14/15	0.24	-	55,63,72,75	0
6	NAG	K	511	14/15	0.19	-	78,90,99,100	0
6	NAG	K	512	14/15	0.24	-	53,56,63,74	0
6	NAG	O	514	14/15	0.24	-	51,58,67,74	0
6	NAG	A	517	14/15	0.42	-	89,104,113,114	0
6	NAG	K	513	14/15	0.22	-	65,74,80,91	0
6	NAG	A	519	14/15	0.38	-	76,85,90,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	E	512	14/15	0.20	-	65,77,88,100	0
6	NAG	E	518	14/15	0.23	-	73,82,86,88	0
6	NAG	A	515	14/15	0.24	-	46,56,64,78	0
6	NAG	O	515	14/15	0.32	-	49,61,87,87	0
6	NAG	K	515	14/15	0.18	-	47,64,76,78	0
6	NAG	E	517	14/15	0.30	-	52,61,69,70	0
6	NAG	E	513	14/15	0.17	-	48,55,60,65	0
6	NAG	E	514	14/15	0.27	-	51,56,59,60	0
6	NAG	O	517	14/15	0.30	-	69,81,97,99	0
6	NAG	A	520	14/15	0.16	-	63,72,78,83	0
6	NAG	E	515	14/15	0.32	-	44,56,63,63	0
8	GOL	J	301	6/6	0.30	-	58,62,66,70	0
6	NAG	E	511	14/15	0.25	-	32,40,50,52	0
6	NAG	O	511	14/15	0.19	-	39,43,52,64	0
6	NAG	A	518	14/15	0.21	-	58,62,80,82	0
8	GOL	Q	301	6/6	0.31	-	48,52,56,59	0
7	CL	A	521	1/1	0.11	-	55,55,55,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.