wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:38 PM GMT

PDB ID	:	4YFL
Title	:	Crystal structure of VH1-46 germline-derived CD4-binding site-directed antibody 1B2530 in complex with HIV-1 clade A/E 93TH057 gp120
Authors	:	Acharya, P.; Zhou, T.; Moquin, S.; Kwong, P.D.
Deposited on	:	2015-02-25
Resolution	:	3.39 Å(reported)

This is a wwPDB X-ray Structure 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/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:

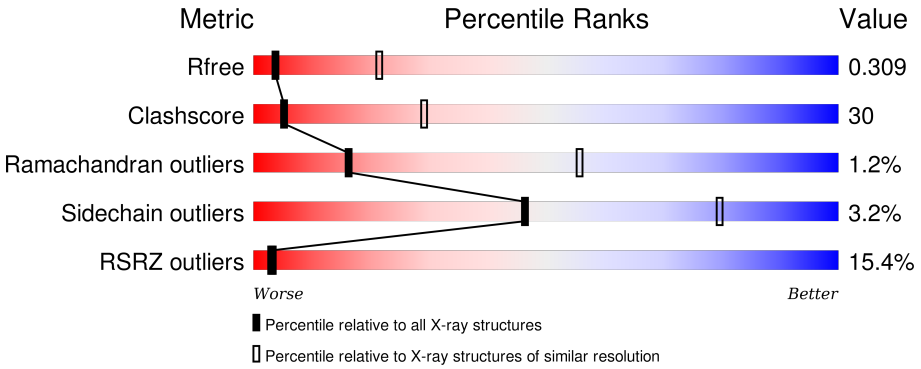
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1084 (3.46-3.30)
Clashscore	102246	1158 (3.46-3.30)
Ramachandran outliers	100387	1139 (3.46-3.30)
Sidechain outliers	100360	1138 (3.46-3.30)
RSRZ outliers	91569	1089 (3.46-3.30)

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	E	353	11% 55% 42%
1	G	353	11% 49% 47%
2	F	227	19% 42% 52%
2	H	227	15% 39% 56%
3	I	215	16% 47% 44% 7%

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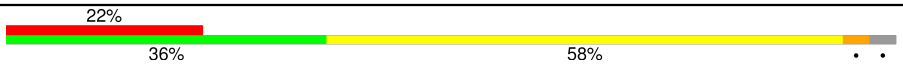
Mol	Chain	Length	Quality of chain
3	L	215	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23777 atoms, of which 11731 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 Envelope glycoprotein gp160,Envelope glycoprotein gp160,Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	347	Total	C	H	N	O	S	0	0	0
			5360	1700	2647	472	518	23			
1	E	347	Total	C	H	N	O	S	0	0	0
			5356	1700	2643	472	518	23			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	124	GLY	-	linker	UNP Q0ED31
G	198	GLY	-	linker	UNP Q0ED31
G	318	GLY	-	linker	UNP Q0ED31
G	319	GLY	-	linker	UNP Q0ED31
G	320	SER	-	linker	UNP Q0ED31
G	321	GLY	-	linker	UNP Q0ED31
G	322	SER	-	linker	UNP Q0ED31
G	323	GLY	-	linker	UNP Q0ED31
E	124	GLY	-	linker	UNP Q0ED31
E	198	GLY	-	linker	UNP Q0ED31
E	318	GLY	-	linker	UNP Q0ED31
E	319	GLY	-	linker	UNP Q0ED31
E	320	SER	-	linker	UNP Q0ED31
E	321	GLY	-	linker	UNP Q0ED31
E	322	SER	-	linker	UNP Q0ED31
E	323	GLY	-	linker	UNP Q0ED31

- Molecule 2 is a protein called 1B2530 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	223	Total	C	H	N	O	S	0	0	0
			3350	1069	1661	290	322	8			

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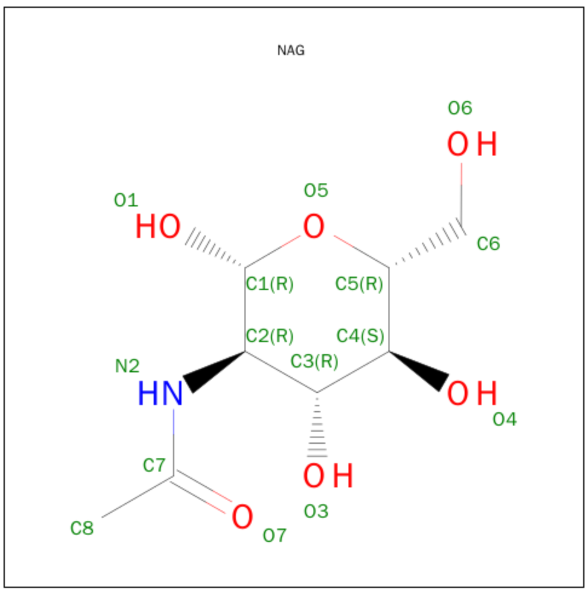
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	F	221	3329	1063	1651	288	319	8	0	0	0

- Molecule 3 is a protein called 1B2530 Light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	L	209	3020	964	1479	261	312	4	0	0	0
3	I	200	2914	932	1426	251	301	4	0	0	0

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	G	1	28	8	14	1	5	0	0
4	G	1	28	8	14	1	5	0	0
4	G	1	28	8	14	1	5	0	0
4	G	1	28	8	14	1	5	0	0
4	G	1	28	8	14	1	5	0	0
4	G	1	28	8	14	1	5	0	0

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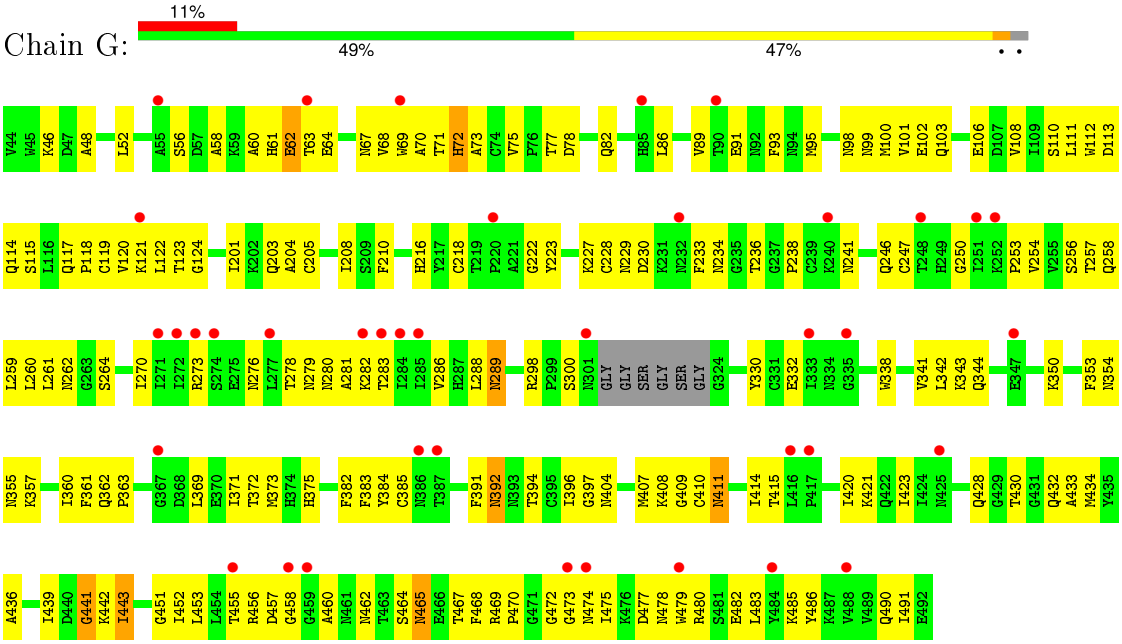
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	E	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	E	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	E	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	E	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	E	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	E	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	E	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	E	1	Total 28	C 8	H 14	N 1	O 5	0	0
4	E	1	Total 28	C 8	H 14	N 1	O 5	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.

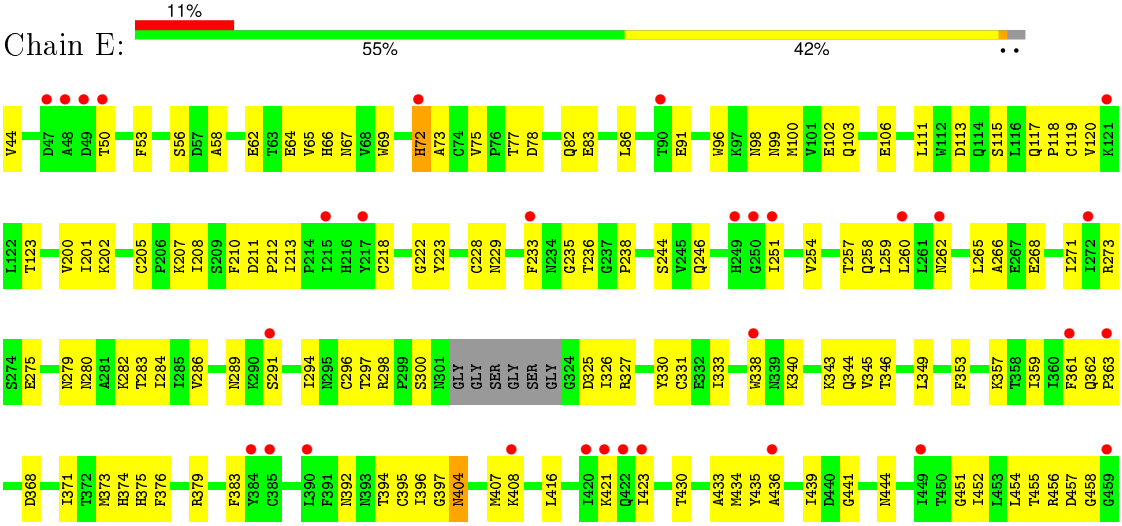
• Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160,Envelope glycoprotein gp160

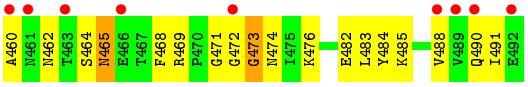
Chain G:



• Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160,Envelope glycoprotein gp160

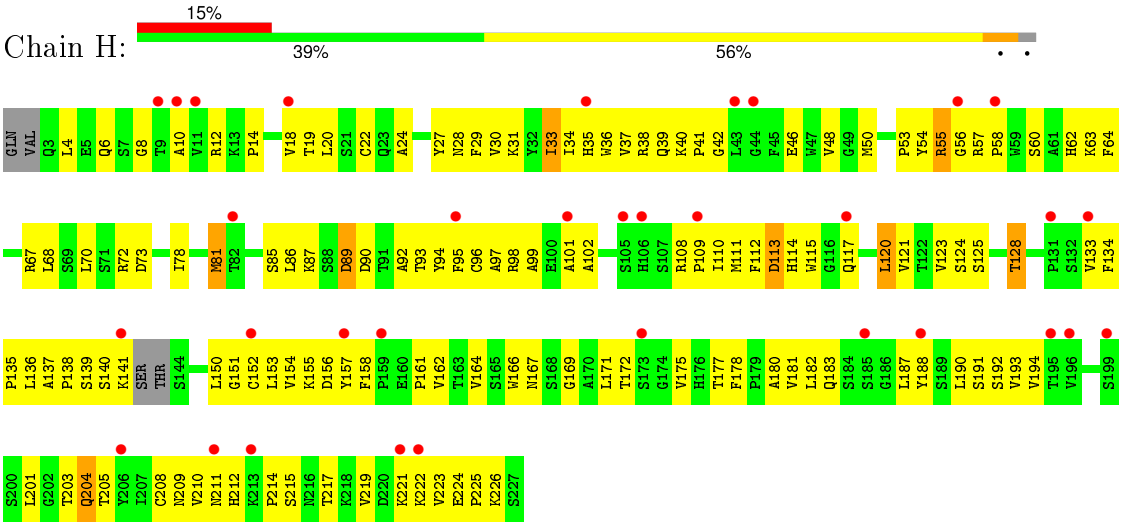
Chain E:





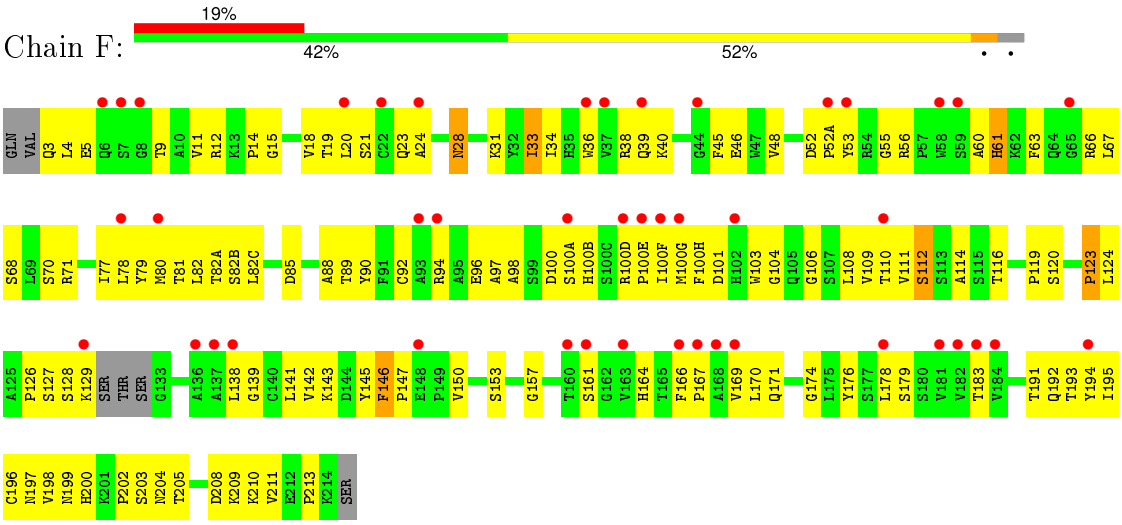
• Molecule 2: 1B2530 heavy chain

Chain H:



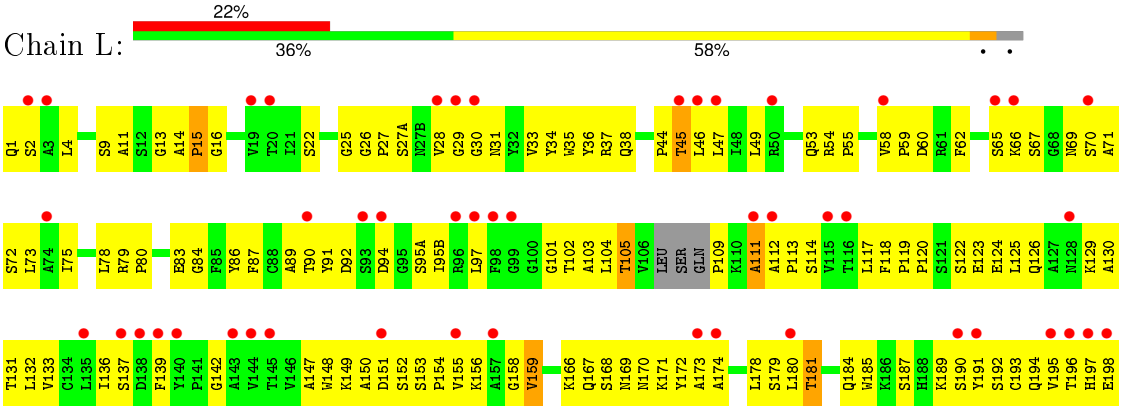
• Molecule 2: 1B2530 heavy chain

Chain F:



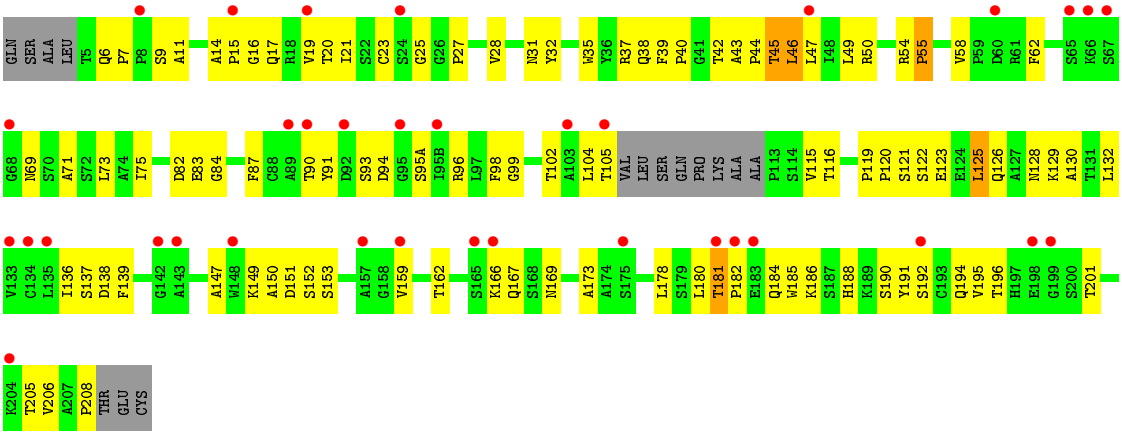
• Molecule 3: 1B2530 Light chain

Chain L:



• Molecule 3: 1B2530 Light chain

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.96Å 57.32Å 254.72Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	28.77 – 3.39 28.78 – 3.39	Depositor EDS
% Data completeness (in resolution range)	90.0 (28.77-3.39) 85.2 (28.78-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 3.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.268 , 0.326 0.272 , 0.309	Depositor DCC
R_{free} test set	1188 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	113.7	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 131.9	EDS
Estimated twinning fraction	0.408 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 24706 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23777	wwPDB-VP
Average B, all atoms (Å^2)	223.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: NAG

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	E	0.46	0/2770	0.94	2/3760 (0.1%)
1	G	0.49	0/2770	0.96	6/3760 (0.2%)
2	F	0.41	0/1722	0.70	0/2341
2	H	0.46	0/1733	0.78	0/2355
3	I	0.40	0/1527	0.72	0/2083
3	L	0.46	0/1580	0.79	1/2157 (0.0%)
All	All	0.46	0/12102	0.85	9/16456 (0.1%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	109	PRO	N-CA-CB	6.82	111.48	103.30
1	G	62	GLU	N-CA-C	-5.74	95.50	111.00
1	G	441	GLY	N-CA-C	5.70	127.34	113.10
1	G	411	ASN	N-CA-C	5.48	125.80	111.00
1	E	483	LEU	CA-CB-CG	5.40	127.72	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2713	2643	2644	117	0
1	G	2713	2647	2647	148	1
2	F	1678	1651	1651	125	0
2	H	1689	1661	1661	135	22
3	I	1488	1426	1426	92	0
3	L	1541	1479	1473	132	17
4	E	140	140	130	11	0
4	G	84	84	78	11	0
All	All	12046	11731	11710	723	24

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 30.

The worst 5 of 723 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)
2:F:3:GLN:N	2:F:24:ALA:HA	1.37	1.36
2:F:3:GLN:N	2:F:24:ALA:CA	2.17	1.08
1:E:113:ASP:O	1:E:117:GLN:NE2	2.01	0.93
2:F:5:GLU:OE2	2:F:23:GLN:OE1	1.88	0.92
2:F:5:GLU:CG	2:F:23:GLN:HB3	2.01	0.91

The worst 5 of 24 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)
2:H:63:LYS:C	3:L:152:SER:OG[2_656]	1.03	1.17
2:H:63:LYS:HA	3:L:152:SER:HG[2_656]	0.62	0.98
2:H:140:SER:HB2	2:H:182:LEU:HD12[2_646]	0.90	0.70
2:H:63:LYS:O	3:L:152:SER:OG[2_656]	1.62	0.58
2:H:63:LYS:CA	3:L:152:SER:HG[2_656]	1.06	0.54

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	E	343/353 (97%)	323 (94%)	18 (5%)	2 (1%)	30	71
1	G	343/353 (97%)	325 (95%)	15 (4%)	3 (1%)	21	63
2	F	217/227 (96%)	184 (85%)	31 (14%)	2 (1%)	21	63
2	H	219/227 (96%)	180 (82%)	35 (16%)	4 (2%)	11	47
3	I	196/215 (91%)	171 (87%)	21 (11%)	4 (2%)	9	45
3	L	205/215 (95%)	172 (84%)	29 (14%)	4 (2%)	9	45
All	All	1523/1590 (96%)	1355 (89%)	149 (10%)	19 (1%)	16	56

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	473	GLY
2	H	55	ARG
3	L	199	GLY
1	E	473	GLY
1	G	397	GLY

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	E	309/311 (99%)	303 (98%)	6 (2%)	65	86
1	G	309/311 (99%)	303 (98%)	6 (2%)	65	86
2	F	188/194 (97%)	177 (94%)	11 (6%)	24	63
2	H	190/194 (98%)	182 (96%)	8 (4%)	36	73
3	I	165/177 (93%)	159 (96%)	6 (4%)	42	77
3	L	168/177 (95%)	163 (97%)	5 (3%)	48	80
All	All	1329/1364 (97%)	1287 (97%)	42 (3%)	46	80

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	181	THR
1	E	404	ASN
3	I	104	LEU
1	E	44	VAL
1	E	200	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	23	GLN
3	I	6	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

16 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	NAG	E	501	-	14,14,15	0.22	0	15,19,21	0.81	1 (6%)
4	NAG	E	502	1	14,14,15	0.41	0	15,19,21	0.59	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	E	503	1	14,14,15	0.70	1 (7%)	15,19,21	0.42	0
4	NAG	E	504	1	14,14,15	0.80	1 (7%)	15,19,21	0.78	1 (6%)
4	NAG	E	505	1	14,14,15	0.27	0	15,19,21	0.96	1 (6%)
4	NAG	E	506	1	14,14,15	0.47	0	15,19,21	0.77	0
4	NAG	E	507	1	14,14,15	0.46	0	15,19,21	0.58	0
4	NAG	E	508	1	14,14,15	0.32	0	15,19,21	0.69	1 (6%)
4	NAG	E	509	1	14,14,15	0.37	0	15,19,21	1.77	2 (13%)
4	NAG	E	510	1	14,14,15	0.39	0	15,19,21	1.18	1 (6%)
4	NAG	G	501	1	14,14,15	0.53	0	15,19,21	0.97	1 (6%)
4	NAG	G	502	1	14,14,15	0.19	0	15,19,21	1.04	1 (6%)
4	NAG	G	503	1	14,14,15	0.67	1 (7%)	15,19,21	0.93	1 (6%)
4	NAG	G	504	1	14,14,15	0.47	0	15,19,21	0.33	0
4	NAG	G	505	1	14,14,15	0.49	0	15,19,21	0.48	0
4	NAG	G	506	1	14,14,15	0.45	0	15,19,21	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
4	NAG	E	501	-	-	0/6/23/26	0/1/1/1
4	NAG	E	502	1	-	0/6/23/26	0/1/1/1
4	NAG	E	503	1	-	0/6/23/26	0/1/1/1
4	NAG	E	504	1	-	0/6/23/26	0/1/1/1
4	NAG	E	505	1	-	0/6/23/26	0/1/1/1
4	NAG	E	506	1	-	0/6/23/26	0/1/1/1
4	NAG	E	507	1	-	0/6/23/26	0/1/1/1
4	NAG	E	508	1	-	0/6/23/26	0/1/1/1
4	NAG	E	509	1	-	0/6/23/26	0/1/1/1
4	NAG	E	510	1	-	0/6/23/26	0/1/1/1
4	NAG	G	501	1	-	0/6/23/26	0/1/1/1
4	NAG	G	502	1	-	0/6/23/26	0/1/1/1
4	NAG	G	503	1	-	0/6/23/26	0/1/1/1
4	NAG	G	504	1	-	0/6/23/26	0/1/1/1
4	NAG	G	505	1	-	0/6/23/26	0/1/1/1
4	NAG	G	506	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	503	NAG	O5-C1	2.12	1.47	1.43
4	E	503	NAG	C1-C2	2.28	1.55	1.52
4	E	504	NAG	C1-C2	2.88	1.56	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	504	NAG	C1-O5-C5	2.11	114.92	112.25
4	E	502	NAG	C1-O5-C5	2.14	114.96	112.25
4	E	508	NAG	C1-O5-C5	2.33	115.21	112.25
4	E	501	NAG	C1-O5-C5	2.94	115.98	112.25
4	E	505	NAG	C1-O5-C5	3.42	116.59	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	503	NAG	3	0
4	E	504	NAG	3	0
4	E	508	NAG	1	0
4	E	509	NAG	2	0
4	E	510	NAG	2	0
4	G	501	NAG	2	0
4	G	502	NAG	4	0
4	G	504	NAG	1	0
4	G	506	NAG	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, 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	E	347/353 (98%)	0.50	40 (11%)	6 7	71, 165, 396, 660	0
1	G	347/353 (98%)	0.38	39 (11%)	7 7	66, 154, 341, 695	0
2	F	221/227 (97%)	1.16	44 (19%)	1 2	94, 191, 520, 722	0
2	H	223/227 (98%)	0.51	33 (14%)	3 3	75, 173, 465, 632	0
3	I	200/215 (93%)	0.72	35 (17%)	2 2	91, 177, 486, 709	0
3	L	209/215 (97%)	1.18	48 (22%)	1 1	91, 183, 587, 723	0
All	All	1547/1590 (97%)	0.69	239 (15%)	3 3	66, 170, 481, 723	0

The worst 5 of 239 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	184	VAL	21.8
1	G	283	THR	21.7
2	F	182	VAL	19.8
3	L	97	LEU	18.4
3	I	134	CYS	16.6

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
4	NAG	G	502	14/15	0.83	0.25	0.31	81,133,246,246	0
4	NAG	G	506	14/15	0.95	0.21	0.29	96,186,232,279	0
4	NAG	G	501	14/15	0.79	0.28	0.27	98,157,226,334	0
4	NAG	G	504	14/15	0.89	0.22	0.11	98,144,250,250	0
4	NAG	E	508	14/15	0.83	0.21	0.05	97,126,157,181	0
4	NAG	E	501	14/15	0.92	0.24	0.02	71,103,199,199	0
4	NAG	G	503	14/15	0.90	0.28	-0.06	100,140,214,237	0
4	NAG	E	510	14/15	0.78	0.20	-0.16	74,153,204,223	0
4	NAG	E	507	14/15	0.89	0.17	-0.18	88,116,149,179	0
4	NAG	E	505	14/15	0.79	0.16	-0.49	117,155,206,210	0
4	NAG	E	502	14/15	0.93	0.18	-0.54	94,127,225,267	0
4	NAG	E	506	14/15	0.92	0.18	-0.60	117,150,180,183	0
4	NAG	G	505	14/15	0.89	0.13	-0.66	84,139,189,227	0
4	NAG	E	504	14/15	0.80	0.14	-0.69	98,148,184,193	0
4	NAG	E	509	14/15	0.92	0.15	-0.72	57,73,118,127	0
4	NAG	E	503	14/15	0.94	0.14	-	73,114,157,193	0

6.5 Other polymers

There are no such residues in this entry.