



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:19 PM GMT

PDB ID : 3F5P  
Title : Complex Structure of Insulin-like Growth Factor Receptor and 3-Cyanoquinoline Inhibitor  
Authors : Xu, W.; Miller, L.M.; Mayer, S.C.; Berger, D.M.; Boschelli, D.H.; Boschelli, F.  
Deposited on : 2008-11-04  
Resolution : 2.90 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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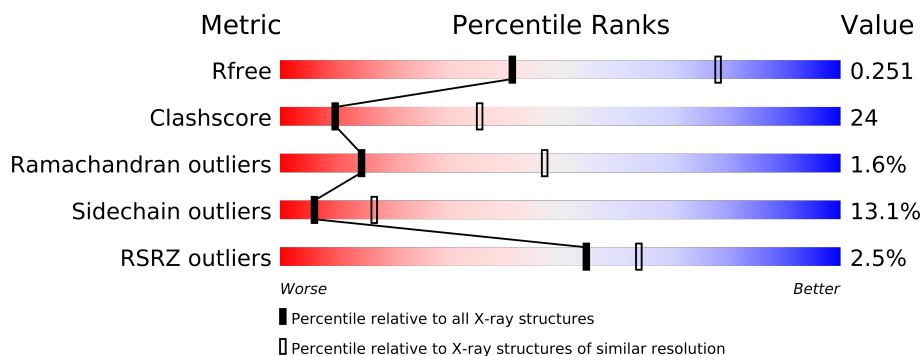
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	308	
1	B	308	
1	C	308	
1	D	308	
1	E	308	
1	F	308	
1	G	308	
1	H	308	
1	I	308	
1	J	308	
1	K	308	
1	L	308	
1	M	308	
1	R	308	

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Mol	Chain	Length	Quality of chain
1	S	308	
1	T	308	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39086 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.

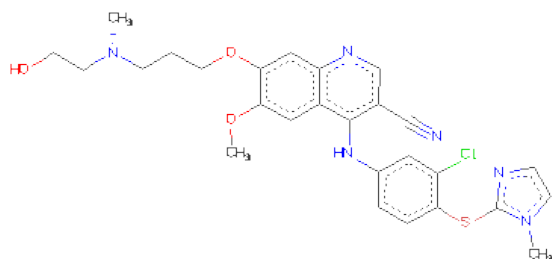
- Molecule 1 is a protein called Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	P	S	0	0	0
			2420	1530	400	464	3	23			
1	B	301	Total	C	N	O	P	S	0	0	0
			2408	1525	399	460	2	22			
1	C	304	Total	C	N	O	P	S	0	0	0
			2420	1531	402	463	2	22			
1	D	300	Total	C	N	O	P	S	0	0	0
			2399	1520	398	457	2	22			
1	E	302	Total	C	N	O	P	S	0	0	0
			2405	1522	399	460	2	22			
1	F	302	Total	C	N	O	P	S	0	0	0
			2412	1529	399	460	2	22			
1	G	302	Total	C	N	O	P	S	0	0	0
			2416	1532	400	460	2	22			
1	H	302	Total	C	N	O	P	S	0	0	0
			2416	1530	400	461	2	23			
1	I	297	Total	C	N	O	P	S	0	0	0
			2380	1508	395	453	2	22			
1	J	296	Total	C	N	O	P	S	0	0	0
			2369	1500	393	452	2	22			
1	K	296	Total	C	N	O	P	S	0	0	0
			2369	1500	393	452	2	22			
1	M	298	Total	C	N	O	P	S	0	0	0
			2381	1508	395	454	2	22			
1	L	296	Total	C	N	O	P	S	0	0	0
			2369	1500	393	452	2	22			
1	R	297	Total	C	N	O	P	S	0	0	0
			2376	1505	394	453	2	22			
1	S	298	Total	C	N	O	P	S	0	0	0
			2386	1511	396	455	2	22			
1	T	298	Total	C	N	O	P	S	0	0	0
			2386	1511	396	455	2	22			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	979	GLY	-	EXPRESSION TAG	UNP P08069
A	980	SER	-	EXPRESSION TAG	UNP P08069
B	979	GLY	-	EXPRESSION TAG	UNP P08069
B	980	SER	-	EXPRESSION TAG	UNP P08069
C	979	GLY	-	EXPRESSION TAG	UNP P08069
C	980	SER	-	EXPRESSION TAG	UNP P08069
D	979	GLY	-	EXPRESSION TAG	UNP P08069
D	980	SER	-	EXPRESSION TAG	UNP P08069
E	979	GLY	-	EXPRESSION TAG	UNP P08069
E	980	SER	-	EXPRESSION TAG	UNP P08069
F	979	GLY	-	EXPRESSION TAG	UNP P08069
F	980	SER	-	EXPRESSION TAG	UNP P08069
G	979	GLY	-	EXPRESSION TAG	UNP P08069
G	980	SER	-	EXPRESSION TAG	UNP P08069
H	979	GLY	-	EXPRESSION TAG	UNP P08069
H	980	SER	-	EXPRESSION TAG	UNP P08069
I	979	GLY	-	EXPRESSION TAG	UNP P08069
I	980	SER	-	EXPRESSION TAG	UNP P08069
J	979	GLY	-	EXPRESSION TAG	UNP P08069
J	980	SER	-	EXPRESSION TAG	UNP P08069
K	979	GLY	-	EXPRESSION TAG	UNP P08069
K	980	SER	-	EXPRESSION TAG	UNP P08069
M	979	GLY	-	EXPRESSION TAG	UNP P08069
M	980	SER	-	EXPRESSION TAG	UNP P08069
L	979	GLY	-	EXPRESSION TAG	UNP P08069
L	980	SER	-	EXPRESSION TAG	UNP P08069
R	979	GLY	-	EXPRESSION TAG	UNP P08069
R	980	SER	-	EXPRESSION TAG	UNP P08069
S	979	GLY	-	EXPRESSION TAG	UNP P08069
S	980	SER	-	EXPRESSION TAG	UNP P08069
T	979	GLY	-	EXPRESSION TAG	UNP P08069
T	980	SER	-	EXPRESSION TAG	UNP P08069

- Molecule 2 is 4-[[3-CHLORO-4-(1-METHYLMIDAZOL-2-YL)SULFANYL-PHENYL]AMINO]-7-[3-(2-HYDROXYETHYL-METHYL-AMINO)PROPOXY]-6-METHOXY-QUINOLINE-3-CARBONITRILE (three-letter code: 741) (formula: C<sub>27</sub>H<sub>29</sub>ClN<sub>6</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	B	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	C	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	D	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	E	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	F	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	G	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	H	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	I	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	J	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	K	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	M	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	L	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	R	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	S	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	T	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0

- Molecule 3 is water.

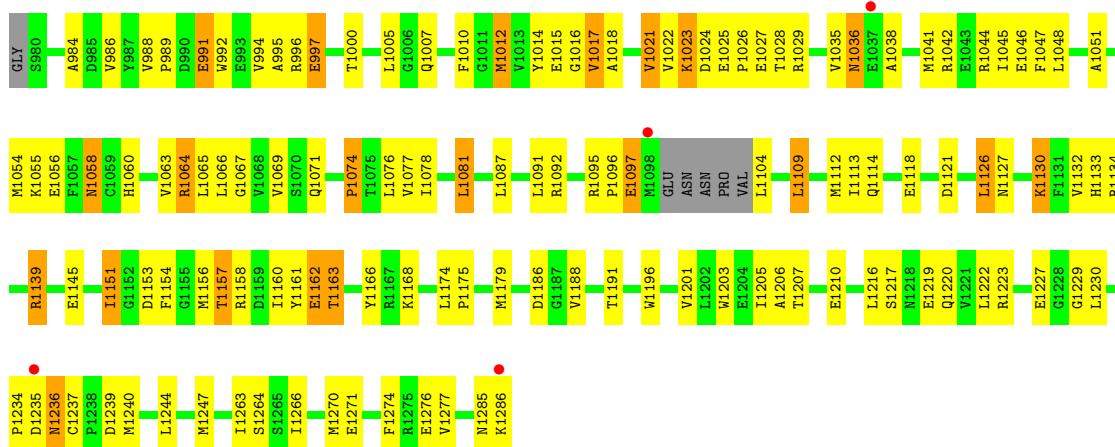
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	O 5	0	0
3	B	19	Total 19	O 19	0	0
3	C	18	Total 18	O 18	0	0
3	D	7	Total 7	O 7	0	0
3	E	1	Total 1	O 1	0	0
3	F	4	Total 4	O 4	0	0
3	G	14	Total 14	O 14	0	0
3	H	19	Total 19	O 19	0	0
3	I	19	Total 19	O 19	0	0
3	J	29	Total 29	O 29	0	0
3	K	1	Total 1	O 1	0	0
3	M	1	Total 1	O 1	0	0
3	L	6	Total 6	O 6	0	0
3	R	16	Total 16	O 16	0	0
3	S	6	Total 6	O 6	0	0
3	T	1	Total 1	O 1	0	0

### 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.

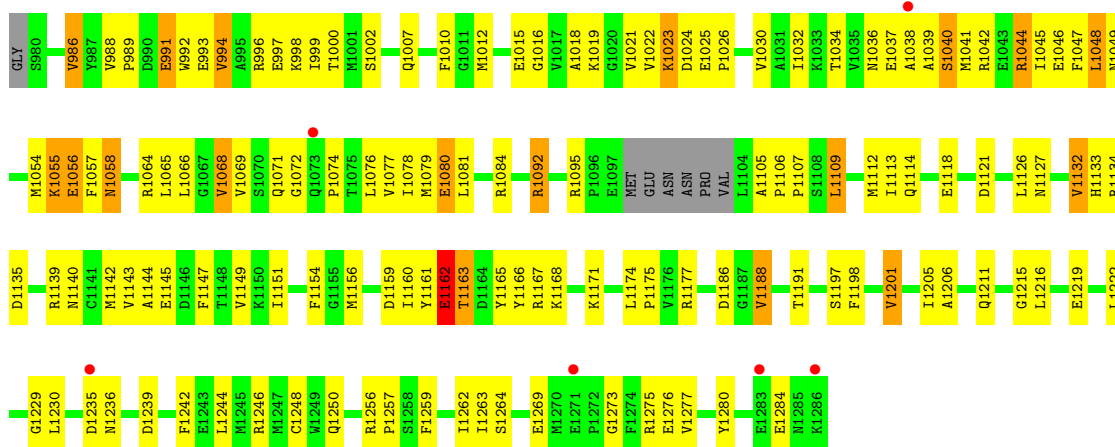
- Molecule 1: Insulin-like growth factor 1 receptor

Chain A: 



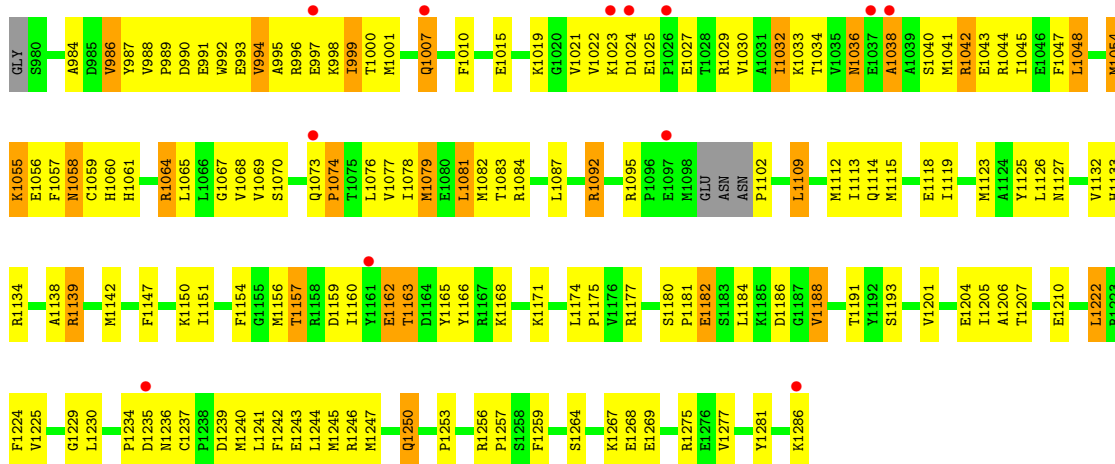
- Molecule 1: Insulin-like growth factor 1 receptor

Chain B: 



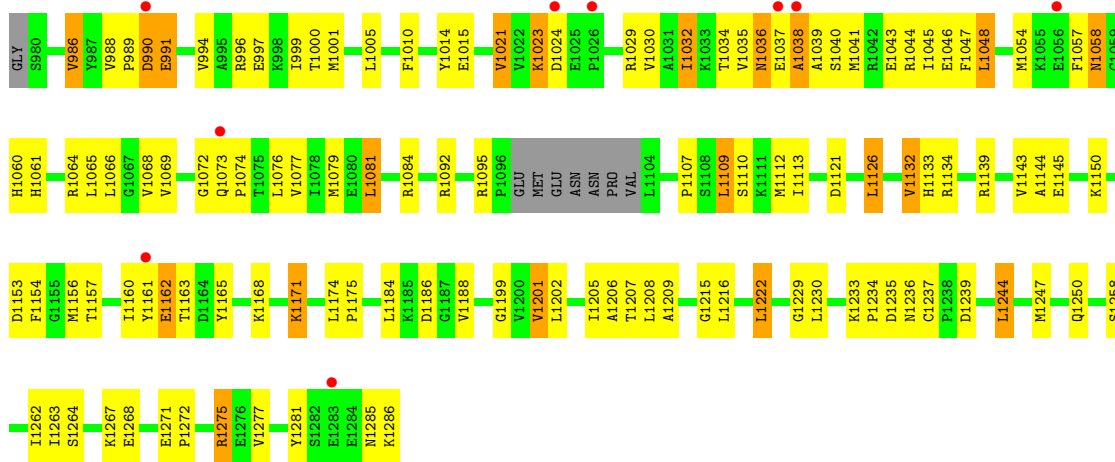
- Molecule 1: Insulin-like growth factor 1 receptor

Chain C: 



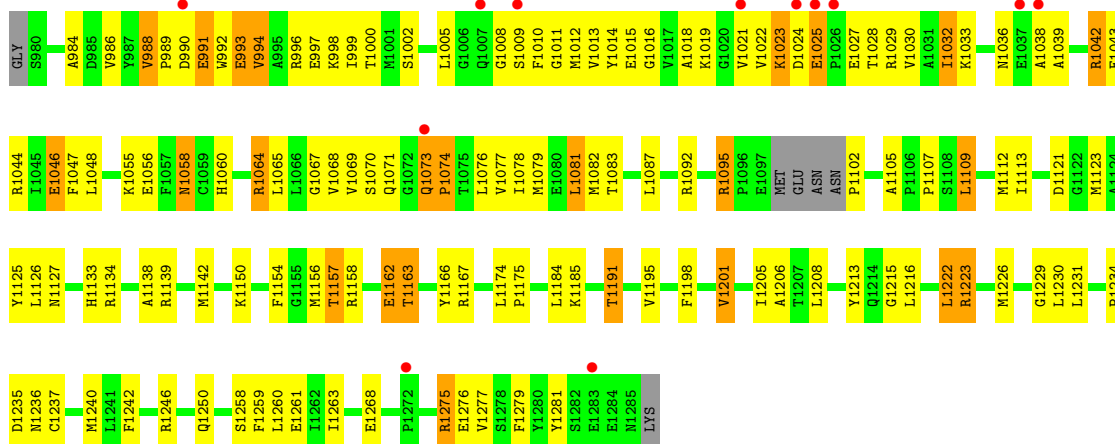
• Molecule 1: Insulin-like growth factor 1 receptor

Chain D:



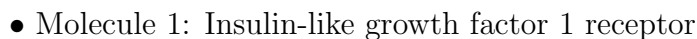
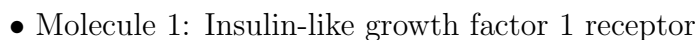
• Molecule 1: Insulin-like growth factor 1 receptor

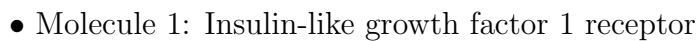
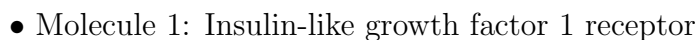
Chain E:



• Molecule 1: Insulin-like growth factor 1 receptor

Age Group	Percentage
18-29	90%
30-49	83%
50-64	70%
65+	56%

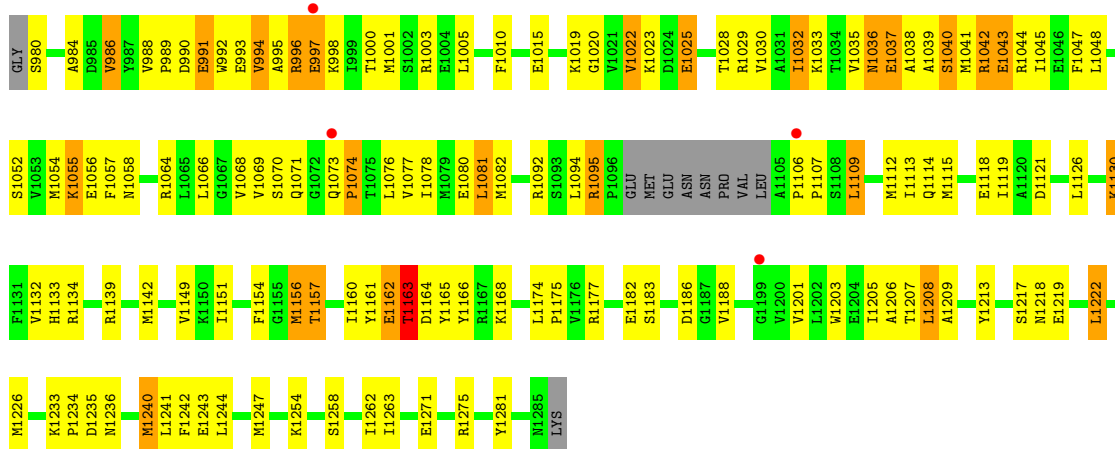




Age Group	Percentage
18-24	~5%
25-34	~45%
35-44	~35%
45-54	~10%
55-64	~5%
65-74	~1%
75-84	~1%
85+	~1%

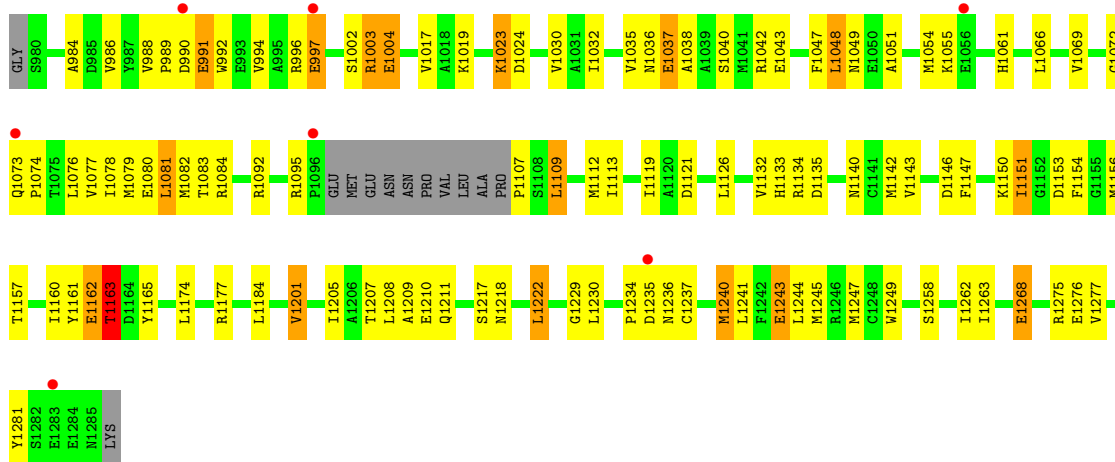


1:



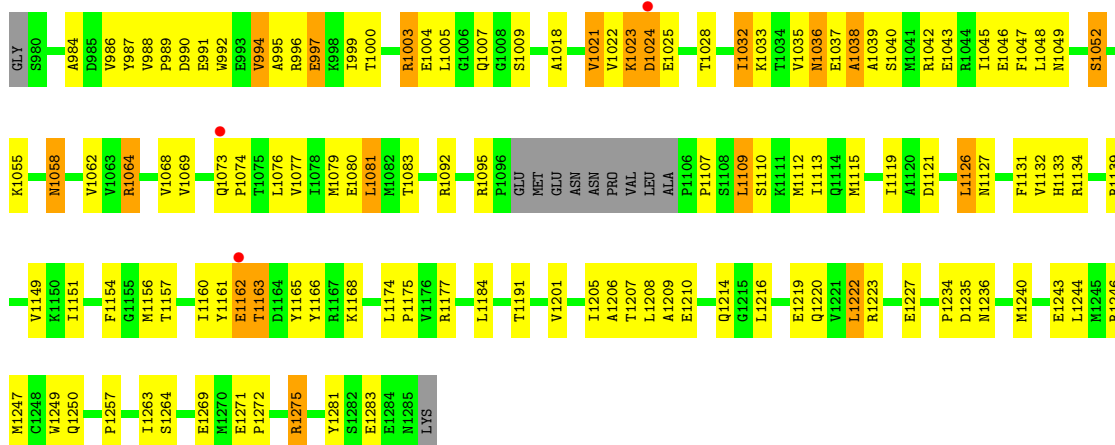
• Molecule 1: Insulin-like growth factor 1 receptor

Chain L:

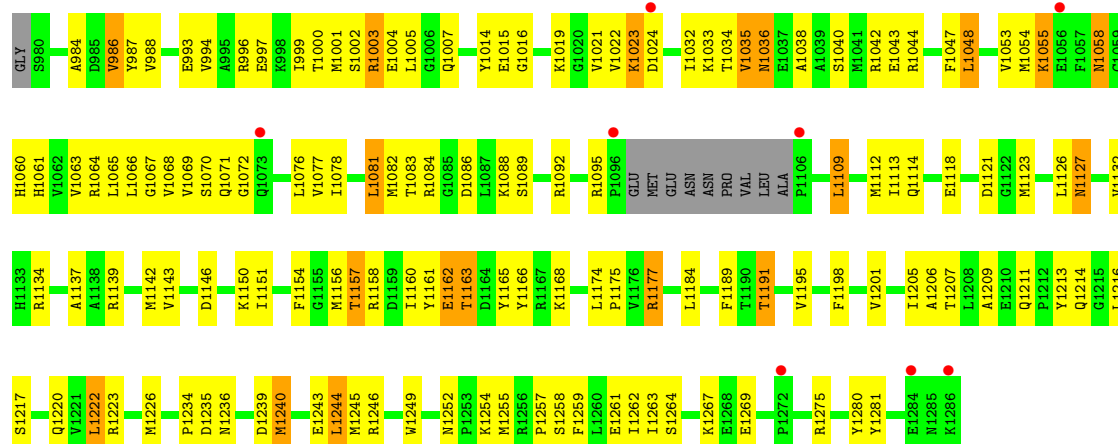


• Molecule 1: Insulin-like growth factor 1 receptor

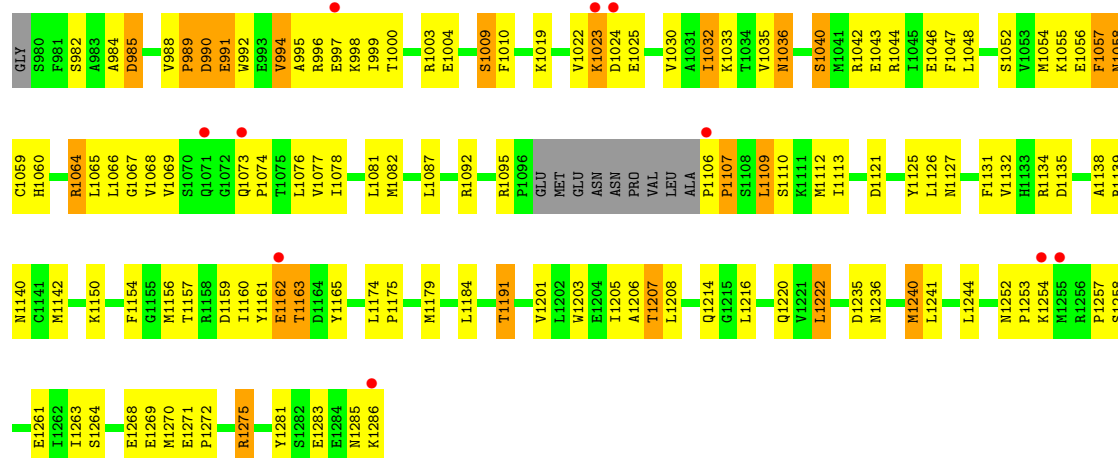
Chain R:



• Molecule 1: Insulin-like growth factor 1 receptor

Chain S: 

- Molecule 1: Insulin-like growth factor 1 receptor

Chain T: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.34Å 137.02Å 178.99Å 90.00° 110.36° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.99-2.90) 97.1 (19.99-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.88Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.210 , 0.258 0.206 , 0.251	Depositor DCC
$R_{free}$ test set	6716 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 18.7	EDS
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 133592 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	39086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.03 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.1640e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities 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: 741, PTR

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	0.40	0/2418	0.57	0/3255
1	B	0.39	0/2410	0.55	0/3245
1	C	0.39	0/2422	0.56	1/3262 (0.0%)
1	D	0.39	0/2401	0.55	1/3233 (0.0%)
1	E	0.39	0/2407	0.58	1/3244 (0.0%)
1	F	0.39	0/2415	0.57	0/3255
1	G	0.37	0/2419	0.53	0/3259
1	H	0.37	0/2418	0.55	0/3255
1	I	0.46	1/2382 (0.0%)	0.59	0/3207
1	J	0.39	0/2370	0.55	0/3191
1	K	0.41	0/2370	0.56	0/3191
1	L	0.38	0/2370	0.54	0/3191
1	M	0.40	0/2383	0.56	0/3211
1	R	0.39	0/2378	0.55	0/3203
1	S	0.39	0/2388	0.56	0/3214
1	T	0.42	0/2388	0.58	0/3214
All	All	0.40	1/38339 (0.0%)	0.56	3/51630 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1254	LYS	CE-NZ	-5.91	1.34	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1102	PRO	N-CA-CB	6.57	111.19	103.30
1	C	1102	PRO	N-CA-CB	6.10	110.62	103.30
1	D	1048	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2420	0	2358	111	0
1	B	2408	0	2349	110	0
1	C	2420	0	2346	145	0
1	D	2399	0	2343	112	0
1	E	2405	0	2331	125	0
1	F	2412	0	2353	112	0
1	G	2416	0	2364	118	0
1	H	2416	0	2358	112	0
1	I	2380	0	2326	139	0
1	J	2369	0	2308	104	0
1	K	2369	0	2308	102	0
1	L	2369	0	2308	87	0
1	M	2381	0	2319	126	0
1	R	2376	0	2315	114	0
1	S	2386	0	2328	118	0
1	T	2386	0	2328	114	0
2	A	38	0	29	5	0
2	B	38	0	29	3	0
2	C	38	0	29	2	0
2	D	38	0	29	1	0
2	E	38	0	29	5	0
2	F	38	0	29	5	0
2	G	38	0	29	2	0
2	H	38	0	29	4	0
2	I	38	0	29	9	0
2	J	38	0	29	2	0
2	K	38	0	29	2	0
2	L	38	0	29	3	0
2	M	38	0	29	1	0
2	R	38	0	29	6	0
2	S	38	0	29	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	38	0	29	3	0
3	A	5	0	0	0	0
3	B	19	0	0	1	0
3	C	18	0	0	2	0
3	D	7	0	0	3	0
3	E	1	0	0	1	0
3	F	4	0	0	1	0
3	G	14	0	0	0	0
3	H	19	0	0	1	0
3	I	19	0	0	0	0
3	J	29	0	0	7	0
3	K	1	0	0	0	0
3	L	6	0	0	0	0
3	M	1	0	0	0	0
3	R	16	0	0	3	0
3	S	6	0	0	0	0
3	T	1	0	0	0	0
All	All	39086	0	37806	1849	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 24.

The worst 5 of 1849 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:1254:LYS:HE3	1:I:1254:LYS:N	1.61	1.13
1:C:1092:ARG:HG3	1:C:1092:ARG:HH11	0.99	1.13
1:K:989:PRO:HG2	1:K:992:TRP:HD1	1.09	1.11
1:H:1023:LYS:H	1:H:1023:LYS:HD2	1.17	1.09
1:M:996:ARG:HH12	1:M:1074:PRO:HD2	0.93	1.09

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	295/308 (96%)	267 (90%)	22 (8%)	6 (2%)	11	40
1	B	294/308 (96%)	273 (93%)	17 (6%)	4 (1%)	16	52
1	C	297/308 (96%)	271 (91%)	20 (7%)	6 (2%)	11	40
1	D	293/308 (95%)	271 (92%)	18 (6%)	4 (1%)	16	52
1	E	295/308 (96%)	271 (92%)	20 (7%)	4 (1%)	16	52
1	F	295/308 (96%)	268 (91%)	21 (7%)	6 (2%)	11	40
1	G	295/308 (96%)	275 (93%)	16 (5%)	4 (1%)	16	52
1	H	295/308 (96%)	265 (90%)	22 (8%)	8 (3%)	8	30
1	I	290/308 (94%)	272 (94%)	15 (5%)	3 (1%)	22	63
1	J	289/308 (94%)	266 (92%)	20 (7%)	3 (1%)	22	63
1	K	289/308 (94%)	266 (92%)	17 (6%)	6 (2%)	11	39
1	L	289/308 (94%)	270 (93%)	16 (6%)	3 (1%)	22	63
1	M	291/308 (94%)	268 (92%)	14 (5%)	9 (3%)	7	26
1	R	290/308 (94%)	268 (92%)	19 (7%)	3 (1%)	22	63
1	S	291/308 (94%)	264 (91%)	24 (8%)	3 (1%)	22	63
1	T	291/308 (94%)	265 (91%)	21 (7%)	5 (2%)	14	45
All	All	4679/4928 (95%)	4300 (92%)	302 (6%)	77 (2%)	14	47

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1097	GLU
1	C	1055	LYS
1	C	1163	THR
1	D	1038	ALA
1	D	1163	THR

### 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	259/265 (98%)	228 (88%)	31 (12%)	7	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	258/265 (97%)	217 (84%)	41 (16%)	4	10
1	C	257/265 (97%)	222 (86%)	35 (14%)	5	15
1	D	257/265 (97%)	231 (90%)	26 (10%)	11	32
1	E	256/265 (97%)	219 (86%)	37 (14%)	5	13
1	F	259/265 (98%)	223 (86%)	36 (14%)	5	14
1	G	260/265 (98%)	223 (86%)	37 (14%)	5	13
1	H	259/265 (98%)	226 (87%)	33 (13%)	6	18
1	I	256/265 (97%)	212 (83%)	44 (17%)	3	8
1	J	254/265 (96%)	230 (91%)	24 (9%)	13	36
1	K	254/265 (96%)	224 (88%)	30 (12%)	8	22
1	L	254/265 (96%)	226 (89%)	28 (11%)	9	26
1	M	255/265 (96%)	220 (86%)	35 (14%)	5	15
1	R	255/265 (96%)	223 (88%)	32 (12%)	7	19
1	S	256/265 (97%)	223 (87%)	33 (13%)	6	17
1	T	256/265 (97%)	220 (86%)	36 (14%)	5	14
All	All	4105/4240 (97%)	3567 (87%)	538 (13%)	6	17

5 of 538 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	986	VAL
1	I	1157	THR
1	S	1239	ASP
1	H	1036	ASN
1	H	1240	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	1060	HIS
1	J	1007	GLN
1	T	1036	ASN
1	H	1071	GLN
1	I	1036	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

48 non-standard protein/DNA/RNA residues 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$
1	PTR	A	1161	1	16,16,17	5.00	3 (18%)	20,22,24	1.51	1 (5%)
1	PTR	A	1165	1	16,16,17	4.75	3 (18%)	20,22,24	1.04	1 (5%)
1	PTR	A	1166	1	16,16,17	4.61	2 (12%)	20,22,24	2.40	1 (5%)
1	PTR	B	1161	1	12,12,17	5.40	3 (25%)	13,15,24	2.66	1 (7%)
1	PTR	B	1165	1	16,16,17	4.67	2 (12%)	20,22,24	1.64	1 (5%)
1	PTR	B	1166	1	16,16,17	4.83	4 (25%)	20,22,24	1.60	1 (5%)
1	PTR	C	1161	1	12,12,17	5.60	3 (25%)	13,15,24	1.77	1 (7%)
1	PTR	C	1165	1	16,16,17	4.65	3 (18%)	20,22,24	1.03	1 (5%)
1	PTR	C	1166	1	16,16,17	4.60	2 (12%)	20,22,24	2.42	1 (5%)
1	PTR	D	1161	1	12,12,17	5.27	2 (16%)	13,15,24	2.38	1 (7%)
1	PTR	D	1165	1	16,16,17	4.81	3 (18%)	20,22,24	0.97	1 (5%)
1	PTR	D	1166	1	16,16,17	4.62	2 (12%)	20,22,24	1.58	1 (5%)
1	PTR	E	1161	1	12,12,17	5.18	3 (25%)	13,15,24	2.34	1 (7%)
1	PTR	E	1165	1	16,16,17	4.69	3 (18%)	20,22,24	1.03	1 (5%)
1	PTR	E	1166	1	16,16,17	4.78	2 (12%)	20,22,24	1.52	1 (5%)
1	PTR	F	1161	1	12,12,17	5.37	2 (16%)	13,15,24	2.47	1 (7%)
1	PTR	F	1165	1	16,16,17	4.86	3 (18%)	20,22,24	1.02	2 (10%)
1	PTR	F	1166	1	16,16,17	4.42	2 (12%)	20,22,24	1.92	1 (5%)
1	PTR	G	1161	1	12,12,17	5.41	3 (25%)	13,15,24	2.53	1 (7%)
1	PTR	G	1165	1	16,16,17	5.00	3 (18%)	20,22,24	0.94	1 (5%)
1	PTR	G	1166	1	16,16,17	4.36	3 (18%)	20,22,24	1.72	1 (5%)
1	PTR	H	1161	1	12,12,17	5.44	3 (25%)	13,15,24	2.46	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PTR	H	1165	1	16,16,17	4.78	3 (18%)	20,22,24	1.05	1 (5%)
1	PTR	H	1166	1	16,16,17	4.70	3 (18%)	20,22,24	1.96	1 (5%)
1	PTR	I	1161	1	12,12,17	5.50	3 (25%)	13,15,24	1.91	1 (7%)
1	PTR	I	1165	1	16,16,17	4.78	3 (18%)	20,22,24	0.95	1 (5%)
1	PTR	I	1166	1	16,16,17	4.77	3 (18%)	20,22,24	2.36	3 (15%)
1	PTR	J	1161	1	12,12,17	5.07	3 (25%)	13,15,24	2.70	1 (7%)
1	PTR	J	1165	1	16,16,17	4.44	3 (18%)	20,22,24	0.60	0
1	PTR	J	1166	1	16,16,17	4.73	2 (12%)	20,22,24	1.76	2 (10%)
1	PTR	K	1161	1	12,12,17	5.66	3 (25%)	13,15,24	1.40	1 (7%)
1	PTR	K	1165	1	16,16,17	4.75	3 (18%)	20,22,24	1.29	1 (5%)
1	PTR	K	1166	1	16,16,17	4.80	3 (18%)	20,22,24	2.13	1 (5%)
1	PTR	L	1161	1	12,12,17	5.44	2 (16%)	13,15,24	2.31	1 (7%)
1	PTR	L	1165	1	16,16,17	4.83	3 (18%)	20,22,24	0.91	1 (5%)
1	PTR	L	1166	1	16,16,17	4.64	3 (18%)	20,22,24	1.91	1 (5%)
1	PTR	M	1161	1	12,12,17	5.59	3 (25%)	13,15,24	2.06	1 (7%)
1	PTR	M	1165	1	16,16,17	4.63	3 (18%)	20,22,24	0.96	1 (5%)
1	PTR	M	1166	1	16,16,17	4.72	5 (31%)	20,22,24	1.60	6 (30%)
1	PTR	R	1161	1	12,12,17	5.27	3 (25%)	13,15,24	2.29	1 (7%)
1	PTR	R	1165	1	16,16,17	4.70	3 (18%)	20,22,24	1.09	1 (5%)
1	PTR	R	1166	1	16,16,17	4.72	3 (18%)	20,22,24	1.91	1 (5%)
1	PTR	S	1161	1	12,12,17	5.51	3 (25%)	13,15,24	2.38	1 (7%)
1	PTR	S	1165	1	16,16,17	4.56	3 (18%)	20,22,24	1.02	1 (5%)
1	PTR	S	1166	1	16,16,17	4.55	3 (18%)	20,22,24	2.04	1 (5%)
1	PTR	T	1161	1	12,12,17	5.35	3 (25%)	13,15,24	2.43	1 (7%)
1	PTR	T	1165	1	16,16,17	4.85	3 (18%)	20,22,24	0.82	1 (5%)
1	PTR	T	1166	1	16,16,17	4.59	2 (12%)	20,22,24	1.98	1 (5%)

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
1	PTR	A	1161	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1161	1	-	0/4/6/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	B	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	C	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	C	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	C	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	D	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	E	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	E	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	E	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	F	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	F	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	F	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	G	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	G	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	G	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	H	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	H	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	H	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	I	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	I	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	I	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	J	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	J	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	J	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	K	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	K	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	K	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	L	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	L	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	L	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	M	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	M	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	M	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	R	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	R	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	R	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	S	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	S	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	S	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	T	1161	1	-	0/4/6/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	T	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	T	1166	1	-	0/9/11/13	0/1/1/1

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	1161	PTR	O-C	19.11	1.24	1.11
1	C	1161	PTR	O-C	18.96	1.24	1.11
1	M	1161	PTR	O-C	18.88	1.24	1.11
1	G	1165	PTR	O-C	18.64	1.24	1.11
1	S	1161	PTR	O-C	18.63	1.24	1.11

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1166	PTR	C-CA-N	-10.52	103.32	113.83
1	A	1166	PTR	C-CA-N	-10.35	103.49	113.83
1	I	1166	PTR	C-CA-N	-9.78	104.06	113.83
1	J	1161	PTR	C-CA-N	-9.31	104.53	113.83
1	B	1161	PTR	C-CA-N	-9.13	104.71	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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
2	741	A	1	-	41,41,41	1.01	2 (4%)	56,56,56	2.43	21 (37%)
2	741	B	2	-	41,41,41	0.98	2 (4%)	56,56,56	2.56	23 (41%)
2	741	C	3	-	41,41,41	1.00	2 (4%)	56,56,56	2.36	21 (37%)
2	741	D	4	-	41,41,41	1.09	2 (4%)	56,56,56	2.44	24 (42%)
2	741	E	5	-	41,41,41	1.06	2 (4%)	56,56,56	2.31	20 (35%)
2	741	F	6	-	41,41,41	1.06	2 (4%)	56,56,56	2.49	22 (39%)
2	741	G	7	-	41,41,41	0.99	2 (4%)	56,56,56	2.61	22 (39%)
2	741	H	8	-	41,41,41	0.98	2 (4%)	56,56,56	2.62	22 (39%)
2	741	I	9	-	41,41,41	0.96	2 (4%)	56,56,56	2.41	22 (39%)
2	741	J	10	-	41,41,41	1.10	3 (7%)	56,56,56	2.40	22 (39%)
2	741	K	11	-	41,41,41	0.98	1 (2%)	56,56,56	2.57	21 (37%)
2	741	L	13	-	41,41,41	1.13	4 (9%)	56,56,56	2.55	21 (37%)
2	741	M	12	-	41,41,41	0.99	2 (4%)	56,56,56	2.34	18 (32%)
2	741	R	14	-	41,41,41	1.17	4 (9%)	56,56,56	2.39	20 (35%)
2	741	S	15	-	41,41,41	1.00	2 (4%)	56,56,56	2.60	26 (46%)
2	741	T	16	-	41,41,41	0.98	3 (7%)	56,56,56	2.60	24 (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
2	741	A	1	-	-	0/22/22/22	0/2/4/4
2	741	B	2	-	-	0/22/22/22	0/2/4/4
2	741	C	3	-	-	0/22/22/22	0/2/4/4
2	741	D	4	-	-	0/22/22/22	0/2/4/4
2	741	E	5	-	-	0/22/22/22	0/2/4/4
2	741	F	6	-	-	0/22/22/22	0/2/4/4
2	741	G	7	-	-	0/22/22/22	0/2/4/4
2	741	H	8	-	-	0/22/22/22	0/2/4/4
2	741	I	9	-	-	0/22/22/22	0/2/4/4
2	741	J	10	-	-	0/22/22/22	0/2/4/4
2	741	K	11	-	-	0/22/22/22	0/2/4/4
2	741	L	13	-	-	0/22/22/22	0/2/4/4
2	741	M	12	-	-	0/22/22/22	0/2/4/4
2	741	R	14	-	-	0/22/22/22	0/2/4/4
2	741	S	15	-	-	0/22/22/22	0/2/4/4
2	741	T	16	-	-	0/22/22/22	0/2/4/4

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	13	741	C3-C2	2.81	1.41	1.36
2	C	3	741	C3-C2	2.80	1.41	1.36
2	D	4	741	C3-C2	2.73	1.41	1.36
2	R	14	741	C3-C2	2.72	1.41	1.36
2	L	13	741	C6-C1	2.65	1.41	1.36

The worst 5 of 349 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	16	741	O11-C1-C6	-8.58	114.45	125.25
2	H	8	741	C10-C9-C32	7.26	125.79	119.54
2	J	10	741	O11-C1-C6	-7.17	116.22	125.25
2	L	13	741	O11-C1-C6	-7.10	116.31	125.25
2	B	2	741	O11-C1-C6	-7.09	116.32	125.25

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	302/308 (98%)	-0.21	4 (1%) 74 82	18, 36, 79, 100	0
1	B	301/308 (97%)	-0.19	6 (1%) 62 71	22, 39, 77, 98	0
1	C	304/308 (98%)	-0.13	12 (3%) 37 45	20, 42, 82, 108	0
1	D	300/308 (97%)	-0.14	9 (3%) 48 57	23, 41, 79, 106	0
1	E	302/308 (98%)	-0.01	12 (3%) 36 43	26, 45, 83, 105	0
1	F	302/308 (98%)	-0.06	13 (4%) 34 40	22, 43, 85, 108	0
1	G	302/308 (98%)	-0.20	5 (1%) 67 76	23, 42, 75, 100	0
1	H	302/308 (98%)	-0.10	14 (4%) 31 38	24, 43, 84, 107	0
1	I	297/308 (96%)	-0.29	3 (1%) 79 86	18, 32, 61, 84	0
1	J	296/308 (96%)	-0.25	4 (1%) 72 80	26, 39, 69, 92	0
1	K	296/308 (96%)	-0.14	3 (1%) 79 86	26, 41, 72, 93	0
1	L	296/308 (96%)	-0.21	7 (2%) 56 65	24, 41, 75, 92	0
1	M	298/308 (96%)	-0.20	4 (1%) 74 82	25, 40, 72, 88	0
1	R	297/308 (96%)	-0.26	3 (1%) 79 86	19, 38, 73, 94	0
1	S	298/308 (96%)	-0.03	8 (2%) 52 61	29, 46, 79, 110	0
1	T	298/308 (96%)	-0.14	10 (3%) 43 51	23, 41, 71, 86	0
All	All	4791/4928 (97%)	-0.16	117 (2%) 54 65	18, 41, 77, 110	0

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	1073	GLN	6.8
1	K	1073	GLN	6.2
1	S	1073	GLN	4.8
1	M	1073	GLN	4.7
1	D	1037	GLU	4.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	PTR	D	1161	12/17	0.36	2.32	58,65,81,83	0
1	PTR	B	1161	12/17	0.31	2.11	44,69,80,81	0
1	PTR	C	1161	12/17	0.35	1.66	50,67,81,88	0
1	PTR	F	1165	16/17	0.21	1.19	40,50,73,73	0
1	PTR	H	1161	12/17	0.29	1.18	53,70,78,81	0
1	PTR	C	1165	16/17	0.19	1.15	32,46,60,63	0
1	PTR	F	1161	12/17	0.30	1.12	58,72,85,88	0
1	PTR	G	1161	12/17	0.28	1.09	49,60,71,73	0
1	PTR	A	1165	16/17	0.19	1.00	37,44,59,61	0
1	PTR	A	1161	16/17	0.29	0.99	46,81,114,234	0
1	PTR	E	1161	12/17	0.24	0.81	53,68,76,81	0
1	PTR	J	1161	12/17	0.27	0.80	46,64,81,87	0
1	PTR	S	1165	16/17	0.23	0.66	36,47,64,66	0
1	PTR	H	1165	16/17	0.18	0.59	40,48,55,56	0
1	PTR	L	1161	12/17	0.26	0.58	50,67,82,86	0
1	PTR	K	1161	12/17	0.24	0.49	43,69,87,92	0
1	PTR	D	1165	16/17	0.18	0.20	42,51,63,63	0
1	PTR	E	1165	16/17	0.17	0.18	38,46,51,61	0
1	PTR	M	1161	12/17	0.24	0.17	49,64,81,84	0
1	PTR	T	1161	12/17	0.23	0.15	47,71,82,84	0
1	PTR	R	1161	12/17	0.24	0.12	45,59,74,76	0
1	PTR	I	1161	12/17	0.22	0.11	39,64,80,83	0
1	PTR	I	1165	16/17	0.18	0.09	32,44,64,66	0
1	PTR	T	1165	16/17	0.22	0.08	37,53,63,67	0
1	PTR	B	1165	16/17	0.17	-0.09	34,44,63,68	0
1	PTR	J	1165	16/17	0.16	-0.12	32,45,57,64	0
1	PTR	M	1166	16/17	0.16	-0.13	32,39,69,78	0
1	PTR	M	1165	16/17	0.18	-0.13	37,48,61,64	0
1	PTR	L	1165	16/17	0.18	-0.13	40,47,66,72	0
1	PTR	S	1161	12/17	0.18	-0.19	51,61,68,68	0
1	PTR	G	1165	16/17	0.17	-0.35	40,48,56,57	0
1	PTR	R	1165	16/17	0.16	-0.49	33,44,64,64	0
1	PTR	K	1165	16/17	0.16	-0.49	35,45,53,57	0
1	PTR	L	1166	16/17	0.12	-0.81	36,39,55,56	0
1	PTR	F	1166	16/17	0.12	-1.00	36,38,50,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PTR	T	1166	16/17	0.14	-1.00	38,44,54,55	0
1	PTR	I	1166	16/17	0.13	-1.04	27,33,45,48	0
1	PTR	S	1166	16/17	0.12	-1.17	33,38,52,55	0
1	PTR	K	1166	16/17	0.12	-1.18	29,38,47,48	0
1	PTR	J	1166	16/17	0.12	-1.20	26,31,44,44	0
1	PTR	B	1166	16/17	0.11	-1.28	32,35,46,48	0
1	PTR	G	1166	16/17	0.11	-1.32	30,37,45,48	0
1	PTR	E	1166	16/17	0.09	-1.74	27,31,39,43	0
1	PTR	R	1166	16/17	0.10	-1.79	29,34,44,48	0
1	PTR	C	1166	16/17	0.09	-1.86	30,33,38,42	0
1	PTR	D	1166	16/17	0.09	-2.15	31,37,47,56	0
1	PTR	A	1166	16/17	0.08	-2.45	28,32,40,49	0
1	PTR	H	1166	16/17	0.09	-3.44	29,34,41,49	0

## 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	741	R	14	38/38	0.22	0.69	24,34,59,304	0
2	741	B	2	38/38	0.19	0.23	31,36,59,84	0
2	741	D	4	38/38	0.19	0.02	31,41,57,78	0
2	741	J	10	38/38	0.16	-0.01	20,30,48,69	0
2	741	H	8	38/38	0.19	-0.14	33,44,53,60	0
2	741	G	7	38/38	0.17	-0.17	31,38,48,54	0
2	741	K	11	38/38	0.15	-0.21	29,36,52,59	0
2	741	A	1	38/38	0.17	-0.23	24,33,51,60	0
2	741	S	15	38/38	0.15	-0.29	27,42,67,77	0
2	741	E	5	38/38	0.20	-0.33	40,45,57,58	0
2	741	L	13	38/38	0.14	-0.33	24,30,44,51	0
2	741	M	12	38/38	0.15	-0.35	23,27,58,64	0
2	741	C	3	38/38	0.17	-0.41	32,39,55,84	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	741	I	9	38/38	0.14	-0.48	17,21,34,53	0
2	741	T	16	38/38	0.14	-0.50	22,28,43,56	0
2	741	F	6	38/38	0.16	-0.78	33,41,55,58	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.