



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 08:22 PM BST

PDB ID : 5JR2  
Title : Crystal structure of the EphA4 LBD in complex with APYd3 peptide inhibitor  
Authors : Lechtenberg, B.C.; Olson, E.J.; Pasquale, E.B.; Dawson, P.E.; Riedl, S.J.  
Deposited on : 2016-05-05  
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

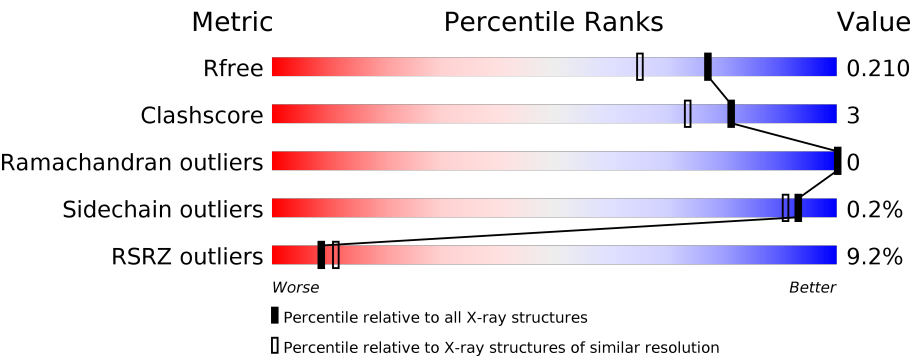
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

# 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 1.75 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))
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	179	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>
1	B	179	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>91%</div><div>8%</div><div>.</div></div>
1	C	179	<div><div>15%</div><div><div></div><div></div><div></div><div></div></div><div>93%</div><div>.</div><div>.</div></div>
1	D	179	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>96%</div><div>.</div><div>.</div></div>
2	E	13	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>85%</div><div>15%</div></div>
2	F	13	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>92%</div><div>8%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	13	<div><div></div><div>69%</div><div>31%</div></div>
2	H	13	<div><div>8%</div><div>92%</div><div>8%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7210 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ephrin type-A receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	11	0
			1521	956	259	297	9			
1	B	179	Total	C	N	O	S	0	20	0
			1593	1001	270	313	9			
1	C	175	Total	C	N	O	S	0	6	1
			1443	909	244	283	7			
1	D	176	Total	C	N	O	S	0	9	1
			1478	933	251	286	8			

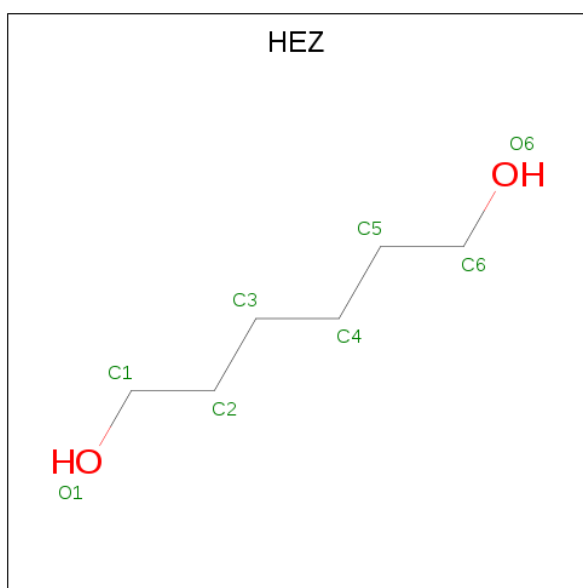
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP P54764
A	27	PRO	-	expression tag	UNP P54764
A	28	GLY	-	expression tag	UNP P54764
A	204	ALA	CYS	engineered mutation	UNP P54764
B	26	GLY	-	expression tag	UNP P54764
B	27	PRO	-	expression tag	UNP P54764
B	28	GLY	-	expression tag	UNP P54764
B	204	ALA	CYS	engineered mutation	UNP P54764
C	26	GLY	-	expression tag	UNP P54764
C	27	PRO	-	expression tag	UNP P54764
C	28	GLY	-	expression tag	UNP P54764
C	204	ALA	CYS	engineered mutation	UNP P54764
D	26	GLY	-	expression tag	UNP P54764
D	27	PRO	-	expression tag	UNP P54764
D	28	GLY	-	expression tag	UNP P54764
D	204	ALA	CYS	engineered mutation	UNP P54764

- Molecule 2 is a protein called APYd3 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	S	0	0	1
			98	63	17	16	2			
2	F	13	Total	C	N	O	S	0	0	1
			98	63	17	16	2			
2	G	13	Total	C	N	O	S	0	0	1
			98	63	17	16	2			
2	H	13	Total	C	N	O	S	0	0	1
			98	63	17	16	2			

- Molecule 3 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	167	Total	O	0	1
			168	168		
5	B	154	Total	O	0	3
			155	155		
5	C	159	Total	O	0	0
			159	159		
5	D	160	Total	O	0	0
			160	160		

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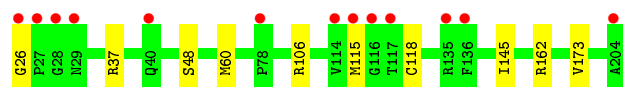
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	10	Total	O	0	0
			10	10		
5	F	15	Total	O	0	0
			15	15		
5	G	10	Total	O	0	0
			10	10		
5	H	10	Total	O	0	0
			10	10		

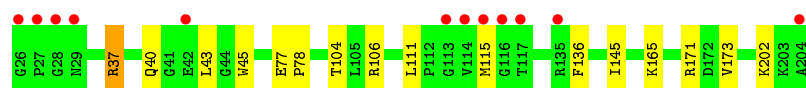
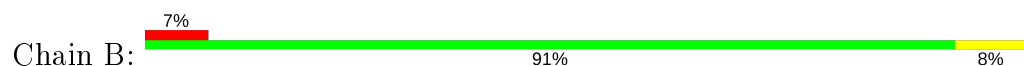
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

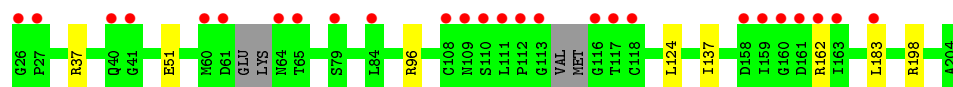
- Molecule 1: Ephrin type-A receptor 4



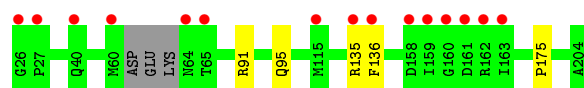
- Molecule 1: Ephrin type-A receptor 4



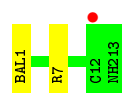
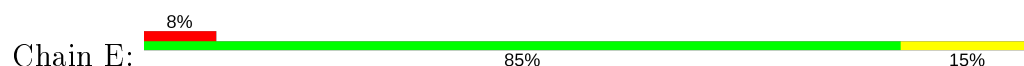
- Molecule 1: Ephrin type-A receptor 4



- Molecule 1: Ephrin type-A receptor 4

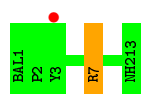
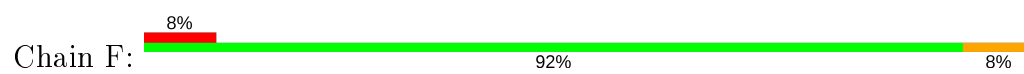


- Molecule 2: APYd3 peptide



- Molecule 2: APYd3 peptide

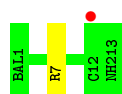
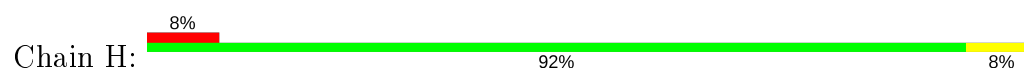




- Molecule 2: APYd3 peptide



- Molecule 2: APYd3 peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.14Å 84.47Å 127.89Å 90.00° 93.87° 90.00°	Depositor
Resolution (Å)	28.92 – 1.75 28.92 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.2 (28.92-1.75) 99.2 (28.92-1.75)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.170 , 0.204 0.179 , 0.210	Depositor DCC
$R_{free}$ test set	4103 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, BAL, HEZ, NH2

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	0.62	0/1549	0.86	2/2093 (0.1%)
1	B	0.64	0/1623	0.88	2/2195 (0.1%)
1	C	0.60	0/1469	0.84	3/1985 (0.2%)
1	D	0.61	0/1506	0.81	1/2036 (0.0%)
2	E	0.79	0/90	0.82	0/120
2	F	0.82	0/90	1.08	1/120 (0.8%)
2	G	0.71	0/90	0.69	0/120
2	H	0.62	0/90	0.67	0/120
All	All	0.63	0/6507	0.85	9/8789 (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
2	E	0	1
2	F	0	1
2	G	0	1
2	H	0	1
All	All	0	4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	7	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	37	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	37	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	C	37	ARG	NE-CZ-NH2	-5.81	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	37	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	C	96	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	171	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	D	91	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	7	ARG	Peptide
2	F	7	ARG	Peptide
2	G	7	ARG	Peptide
2	H	7	ARG	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1521	0	1473	10	0
1	B	1593	0	1531	14	0
1	C	1443	0	1389	6	0
1	D	1478	0	1431	3	0
2	E	98	0	85	0	0
2	F	98	0	85	0	0
2	G	98	0	85	2	0
2	H	98	0	85	0	0
3	A	16	0	28	1	0
3	B	24	0	42	3	0
3	C	8	0	14	1	0
4	A	18	0	24	0	0
4	B	18	0	24	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	168	0	0	7	1
5	B	155	0	0	2	0
5	C	159	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	160	0	0	2	0
5	E	10	0	0	0	0
5	F	15	0	0	0	0
5	G	10	0	0	1	0
5	H	10	0	0	0	0
All	All	7210	0	6312	34	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:CG	5:A:511:HOH:O	2.30	0.78
1:B:202:LYS:O	3:B:303:HEZ:H31	1.86	0.76
1:A:60:MET:SD	5:A:404:HOH:O	2.48	0.72
1:A:162:ARG:HG2	5:A:511:HOH:O	1.89	0.71
1:C:162:ARG:NH2	2:G:9:SER:OG	2.28	0.65
1:B:37:ARG:NH1	5:B:403:HOH:O	2.30	0.58
1:C:124:LEU:HD11	1:C:183[B]:LEU:HD11	1.85	0.58
1:B:45[B]:TRP:N	1:B:45[B]:TRP:CD1	2.70	0.57
2:G:1:BAL:N	5:G:102:HOH:O	2.29	0.57
1:B:145:ILE:HD13	1:B:173[B]:VAL:HG11	1.87	0.56
1:A:115[B]:MET:HE3	1:A:118:CYS:CB	2.37	0.56
1:B:145:ILE:CD1	1:B:173[B]:VAL:HG11	2.36	0.55
1:B:106:ARG:NH1	5:B:406:HOH:O	2.40	0.53
1:C:198:ARG:HD3	5:C:472:HOH:O	2.09	0.51
1:D:175:PRO:CB	5:D:475:HOH:O	2.60	0.50
1:D:135[A]:ARG:NH2	1:D:136[A]:PHE:HE2	2.11	0.49
1:A:162:ARG:HG3	5:A:511:HOH:O	2.03	0.48
1:B:40[B]:GLN:HG3	1:B:40[B]:GLN:O	2.12	0.48
1:C:162:ARG:NH1	5:C:404:HOH:O	2.47	0.48
1:A:145:ILE:CD1	1:A:173[B]:VAL:HG11	2.44	0.47
1:B:45[B]:TRP:N	1:B:45[B]:TRP:HD1	2.12	0.46
1:B:165:LYS:HE2	3:B:302:HEZ:H11	1.97	0.46
1:A:115[B]:MET:HE3	1:A:118:CYS:HB2	1.98	0.45
1:B:136:PHE:CD2	1:C:51:GLU:HB2	2.50	0.45
1:D:95:GLN:HG2	5:D:465:HOH:O	2.18	0.43
1:A:26:GLY:N	5:A:410:HOH:O	2.51	0.43
1:B:77[A]:GLU:OE1	1:B:78:PRO:HD2	2.18	0.43
1:C:137:ILE:O	3:C:301:HEZ:H51	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:301:HEZ:H12	5:A:520:HOH:O	2.19	0.42
1:B:43[B]:LEU:HD23	1:B:43[B]:LEU:HA	1.88	0.42
1:B:111:LEU:HB2	1:B:115[B]:MET:HE1	2.02	0.41
1:B:104:THR:OG1	3:B:302:HEZ:H61	2.20	0.41
1:A:145:ILE:HD13	1:A:173[B]:VAL:HG11	2.01	0.41
1:A:48[A]:SER:OG	5:A:401:HOH:O	2.13	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:554:HOH:O	5:C:491:HOH:O[1_455]	2.12	0.08

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	188/179 (105%)	176 (94%)	12 (6%)	0	100	100
1	B	197/179 (110%)	186 (94%)	11 (6%)	0	100	100
1	C	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
1	D	181/179 (101%)	171 (94%)	10 (6%)	0	100	100
2	E	10/13 (77%)	10 (100%)	0	0	100	100
2	F	10/13 (77%)	10 (100%)	0	0	100	100
2	G	10/13 (77%)	10 (100%)	0	0	100	100
2	H	10/13 (77%)	10 (100%)	0	0	100	100
All	All	781/768 (102%)	740 (95%)	41 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	168/158 (106%)	167 (99%)	1 (1%)	86	79
1	B	175/158 (111%)	175 (100%)	0	100	100
1	C	159/158 (101%)	159 (100%)	0	100	100
1	D	163/158 (103%)	163 (100%)	0	100	100
2	E	10/10 (100%)	10 (100%)	0	100	100
2	F	10/10 (100%)	10 (100%)	0	100	100
2	G	10/10 (100%)	10 (100%)	0	100	100
2	H	10/10 (100%)	10 (100%)	0	100	100
All	All	705/672 (105%)	704 (100%)	1 (0%)	93	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	$\# Z  > 2$
2	BAL	E	1	2	4,4,5	0.61	0	3,3,5	2.42	1 (33%)
2	BAL	F	1	2	4,4,5	0.50	0	3,3,5	0.94	0
2	BAL	H	1	2	4,4,5	0.47	0	3,3,5	0.62	0
2	BAL	H	8	2	4,4,5	0.31	0	3,3,5	1.09	0
2	BAL	E	8	2	4,4,5	0.23	0	3,3,5	0.90	0
2	BAL	F	8	2	4,4,5	0.39	0	3,3,5	1.03	0
2	BAL	G	8	2	4,4,5	0.46	0	3,3,5	1.72	1 (33%)
2	BAL	G	1	2	4,4,5	0.40	0	3,3,5	0.79	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
2	BAL	E	1	2	-	1/1/2/3	-
2	BAL	F	1	2	-	0/1/2/3	-
2	BAL	H	1	2	-	0/1/2/3	-
2	BAL	H	8	2	-	0/1/2/3	-
2	BAL	E	8	2	-	0/1/2/3	-
2	BAL	F	8	2	-	0/1/2/3	-
2	BAL	G	8	2	-	0/1/2/3	-
2	BAL	G	1	2	-	0/1/2/3	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	BAL	CB-CA-C	4.02	117.39	111.42
2	G	8	BAL	CB-CA-C	-2.76	107.33	111.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	BAL	C-CA-CB-N

There are no ring outliers.



1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	BAL	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 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	$\# Z  > 2$
3	HEZ	B	303	-	7,7,7	0.29	0	6,6,6	0.57	0
4	GOL	A	304	-	5,5,5	0.43	0	5,5,5	0.23	0
3	HEZ	A	302	-	7,7,7	0.20	0	6,6,6	0.52	0
4	GOL	B	306	-	5,5,5	0.71	0	5,5,5	0.98	0
4	GOL	A	303	-	5,5,5	0.15	0	5,5,5	0.38	0
3	HEZ	C	301	-	7,7,7	0.16	0	6,6,6	0.68	0
3	HEZ	A	301	-	7,7,7	0.18	0	6,6,6	0.41	0
3	HEZ	B	301	-	7,7,7	0.23	0	6,6,6	0.36	0
4	GOL	B	305	-	5,5,5	0.48	0	5,5,5	0.23	0
4	GOL	A	305	-	5,5,5	0.62	0	5,5,5	0.68	0
4	GOL	D	301	-	5,5,5	0.65	0	5,5,5	0.57	0
3	HEZ	B	302	-	7,7,7	0.68	0	6,6,6	0.57	0
4	GOL	C	302	-	5,5,5	0.40	0	5,5,5	0.57	0
4	GOL	B	304	-	5,5,5	0.43	0	5,5,5	0.24	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
3	HEZ	B	303	-	-	4/5/5/5	-
4	GOL	A	304	-	-	0/4/4/4	-
3	HEZ	A	302	-	-	3/5/5/5	-
4	GOL	B	306	-	-	2/4/4/4	-
4	GOL	A	303	-	-	2/4/4/4	-
3	HEZ	C	301	-	-	4/5/5/5	-
3	HEZ	A	301	-	-	0/5/5/5	-
3	HEZ	B	301	-	-	0/5/5/5	-
4	GOL	B	305	-	-	2/4/4/4	-
4	GOL	A	305	-	-	2/4/4/4	-
4	GOL	D	301	-	-	2/4/4/4	-
3	HEZ	B	302	-	-	1/5/5/5	-
4	GOL	C	302	-	-	0/4/4/4	-
4	GOL	B	304	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	305	GOL	O1-C1-C2-C3
4	B	304	GOL	O1-C1-C2-C3
4	B	306	GOL	O1-C1-C2-C3
4	A	303	GOL	O1-C1-C2-C3
4	B	305	GOL	O1-C1-C2-C3
4	D	301	GOL	O1-C1-C2-C3
3	B	303	HEZ	C3-C4-C5-C6
4	A	303	GOL	O1-C1-C2-O2
4	A	305	GOL	O1-C1-C2-O2
4	B	304	GOL	O1-C1-C2-O2
3	B	303	HEZ	C1-C2-C3-C4
4	B	306	GOL	O1-C1-C2-O2
4	B	305	GOL	O1-C1-C2-O2
3	B	302	HEZ	C2-C3-C4-C5
3	C	301	HEZ	O1-C1-C2-C3
3	C	301	HEZ	C4-C5-C6-O6
3	A	302	HEZ	C2-C3-C4-C5
3	C	301	HEZ	C2-C3-C4-C5
3	A	302	HEZ	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	302	HEZ	C3-C4-C5-C6
3	B	303	HEZ	O1-C1-C2-C3
3	C	301	HEZ	C3-C4-C5-C6
4	D	301	GOL	O1-C1-C2-O2
3	B	303	HEZ	C2-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	HEZ	1	0
3	C	301	HEZ	1	0
3	A	301	HEZ	1	0
3	B	302	HEZ	2	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<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	179/179 (100%)	0.31	13 (7%) 15 20	10, 18, 39, 52	0
1	B	179/179 (100%)	0.29	12 (6%) 17 23	10, 17, 38, 52	0
1	C	175/179 (97%)	0.83	26 (14%) 2 3	10, 19, 56, 71	0
1	D	176/179 (98%)	0.57	15 (8%) 10 14	10, 19, 44, 69	0
2	E	10/13 (76%)	0.25	1 (10%) 7 9	12, 20, 27, 32	0
2	F	10/13 (76%)	0.16	1 (10%) 7 9	11, 18, 27, 31	0
2	G	10/13 (76%)	0.11	0 100 100	17, 26, 30, 32	0
2	H	10/13 (76%)	0.49	1 (10%) 7 9	19, 24, 31, 33	0
All	All	749/768 (97%)	0.48	69 (9%) 9 11	10, 18, 43, 71	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136[A]	PHE	8.8
1	C	112	PRO	8.6
1	D	161	ASP	7.5
1	A	136	PHE	7.5
1	C	117	THR	7.1
1	B	114	VAL	7.1
1	B	27	PRO	6.1
1	C	111	LEU	5.9
1	C	64	ASN	5.6
1	A	204	ALA	5.6
1	C	116	GLY	5.4
1	A	27	PRO	5.2
1	C	26	GLY	4.8
1	C	118	CYS	4.5
1	A	117	THR	4.4
1	C	161	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	78	PRO	4.3
1	B	115[A]	MET	4.2
1	C	27	PRO	4.2
1	D	162	ARG	4.2
1	C	65	THR	4.2
1	D	159	ILE	4.1
1	D	64	ASN	4.1
1	C	108	CYS	4.0
1	C	158	ASP	4.0
1	C	160	GLY	4.0
1	D	158	ASP	3.9
1	A	114	VAL	3.9
1	C	159	ILE	3.8
1	C	113	GLY	3.8
1	B	117	THR	3.6
1	A	115[A]	MET	3.6
1	B	28	GLY	3.6
1	D	65	THR	3.6
1	C	109	ASN	3.5
1	C	162	ARG	3.5
1	D	135[A]	ARG	3.5
1	D	160	GLY	3.4
1	D	163	ILE	3.4
1	B	113	GLY	3.4
1	C	163	ILE	3.3
1	D	27	PRO	3.3
1	C	40	GLN	3.2
1	B	135	ARG	3.1
1	D	40	GLN	3.1
1	B	26	GLY	3.0
1	A	135	ARG	3.0
1	C	41	GLY	3.0
1	A	26	GLY	2.9
1	C	110	SER	2.9
1	B	204	ALA	2.9
2	F	3	TYR	2.8
1	D	60	MET	2.8
1	D	115	MET	2.7
1	D	26	GLY	2.7
1	A	116	GLY	2.7
1	C	61	ASP	2.7
1	B	29[A]	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	42[A]	GLU	2.6
1	C	84	LEU	2.6
1	A	29[A]	ASN	2.6
2	E	12	CYS	2.6
1	C	79	SER	2.4
1	B	116	GLY	2.4
1	C	60	MET	2.3
2	H	12	CYS	2.3
1	C	183[A]	LEU	2.2
1	A	40	GLN	2.2
1	A	28	GLY	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BAL	F	1	5/6	0.78	0.21	27,27,32,33	0
2	BAL	E	1	5/6	0.85	0.14	24,26,28,31	0
2	BAL	G	1	5/6	0.87	0.23	33,33,39,41	0
2	BAL	H	8	5/6	0.96	0.09	25,26,28,30	0
2	BAL	G	8	5/6	0.96	0.07	20,22,25,27	0
2	BAL	H	1	5/6	0.96	0.07	28,28,35,35	0
2	BAL	E	8	5/6	0.98	0.07	13,14,16,16	0
2	BAL	F	8	5/6	0.98	0.07	13,14,15,16	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	305	6/6	0.67	0.24	27,39,40,44	0
4	GOL	B	304	6/6	0.69	0.21	34,35,38,42	0
3	HEZ	B	302	8/8	0.76	0.20	23,35,43,44	0
4	GOL	A	303	6/6	0.79	0.16	38,42,45,47	0
4	GOL	B	305	6/6	0.82	0.19	24,34,37,42	0
3	HEZ	B	303	8/8	0.85	0.27	17,25,35,37	0
3	HEZ	C	301	8/8	0.85	0.18	29,38,45,46	0
3	HEZ	A	302	8/8	0.87	0.13	35,36,38,39	0
4	GOL	A	304	6/6	0.89	0.14	24,30,33,38	0
4	GOL	D	301	6/6	0.89	0.15	19,23,26,30	0
4	GOL	B	306	6/6	0.90	0.12	26,32,35,36	0
4	GOL	C	302	6/6	0.94	0.13	18,22,25,31	0
3	HEZ	B	301	8/8	0.96	0.09	15,15,17,17	0
3	HEZ	A	301	8/8	0.97	0.10	15,16,18,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.