



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:06 PM GMT

PDB ID : 4ZLT  
Title : Crystal structure of viral chemokine binding protein R17 in complex with CCL3  
Authors : Lubman, O.Y.; Fremont, D.H.  
Deposited on : 2015-05-01  
Resolution : 3.00 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  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

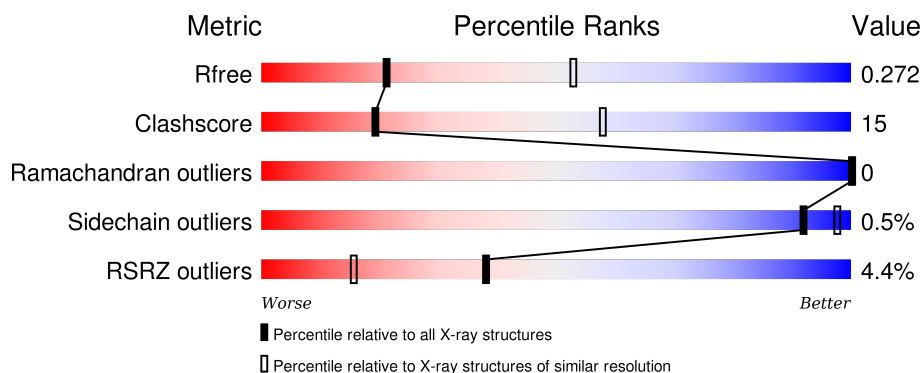
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	420	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>23%</div> <div>10%</div> </div> </div>
1	B	420	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>28%</div> <div>10%</div> </div> </div>
2	F	70	<div> <div></div> <div> <div></div> <div>53%</div> <div>36%</div> <div>11%</div> </div> </div>
2	L	70	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>27%</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7086 atoms, of which 53 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	379	Total	C	H	N	O	S	0	0	0
			2999	1906	1	498	574	20			
1	A	376	Total	C	H	N	O	S	0	0	0
			2972	1890	1	491	570	20			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	333	ASP	LYS	engineered mutation	UNP E9M5R0
B	335	GLU	ARG	engineered mutation	UNP E9M5R0
B	336	GLU	ARG	engineered mutation	UNP E9M5R0
B	337	ASP	LYS	engineered mutation	UNP E9M5R0
B	413	HIS	-	expression tag	UNP E9M5R0
B	414	HIS	-	expression tag	UNP E9M5R0
B	415	HIS	-	expression tag	UNP E9M5R0
B	416	HIS	-	expression tag	UNP E9M5R0
B	417	HIS	-	expression tag	UNP E9M5R0
B	418	HIS	-	expression tag	UNP E9M5R0
B	419	HIS	-	expression tag	UNP E9M5R0
B	420	HIS	-	expression tag	UNP E9M5R0
A	333	ASP	LYS	engineered mutation	UNP E9M5R0
A	335	GLU	ARG	engineered mutation	UNP E9M5R0
A	336	GLU	ARG	engineered mutation	UNP E9M5R0
A	337	ASP	LYS	engineered mutation	UNP E9M5R0
A	413	HIS	-	expression tag	UNP E9M5R0
A	414	HIS	-	expression tag	UNP E9M5R0
A	415	HIS	-	expression tag	UNP E9M5R0
A	416	HIS	-	expression tag	UNP E9M5R0
A	417	HIS	-	expression tag	UNP E9M5R0
A	418	HIS	-	expression tag	UNP E9M5R0
A	419	HIS	-	expression tag	UNP E9M5R0
A	420	HIS	-	expression tag	UNP E9M5R0

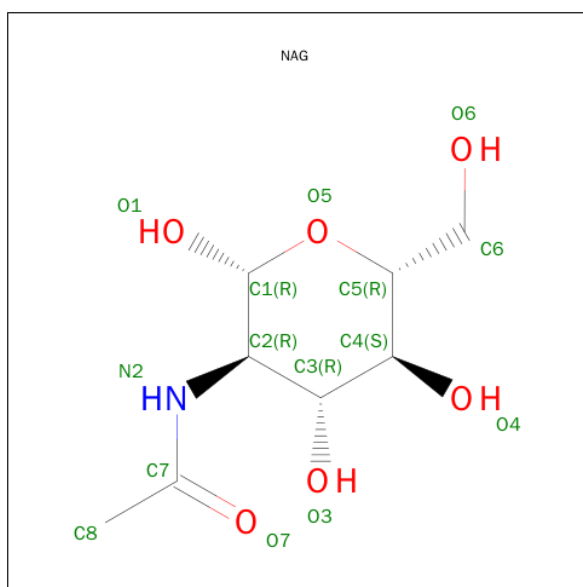
- Molecule 2 is a protein called C-C motif chemokine 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	62	Total	C	N	O	S	0	0	0
			504	321	84	95	4			
2	L	62	Total	C	N	O	S	0	0	0
			504	321	84	95	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	MET	-	expression tag	UNP P10855
F	26	ALA	ASP	engineered mutation	UNP P10855
L	0	MET	-	expression tag	UNP P10855
L	26	ALA	ASP	engineered mutation	UNP P10855

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

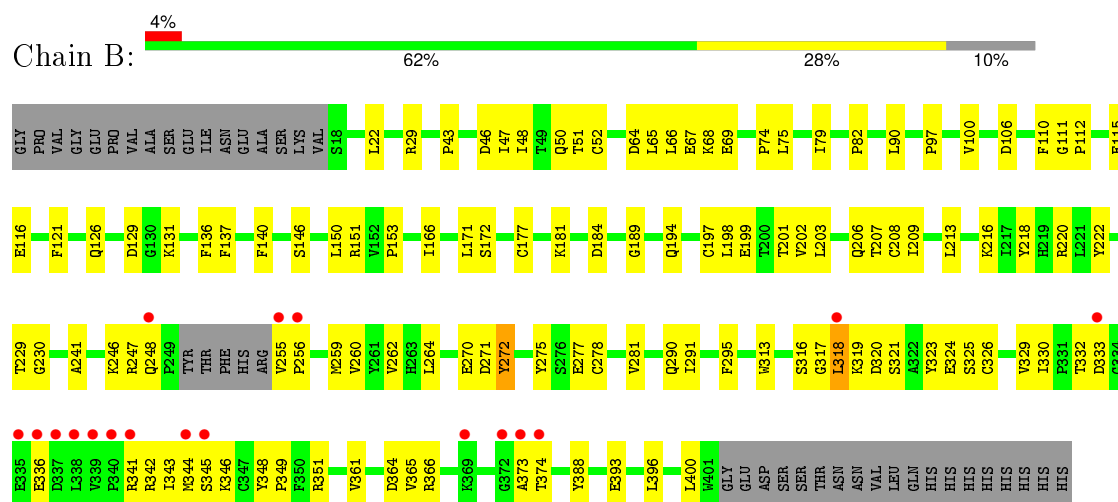


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

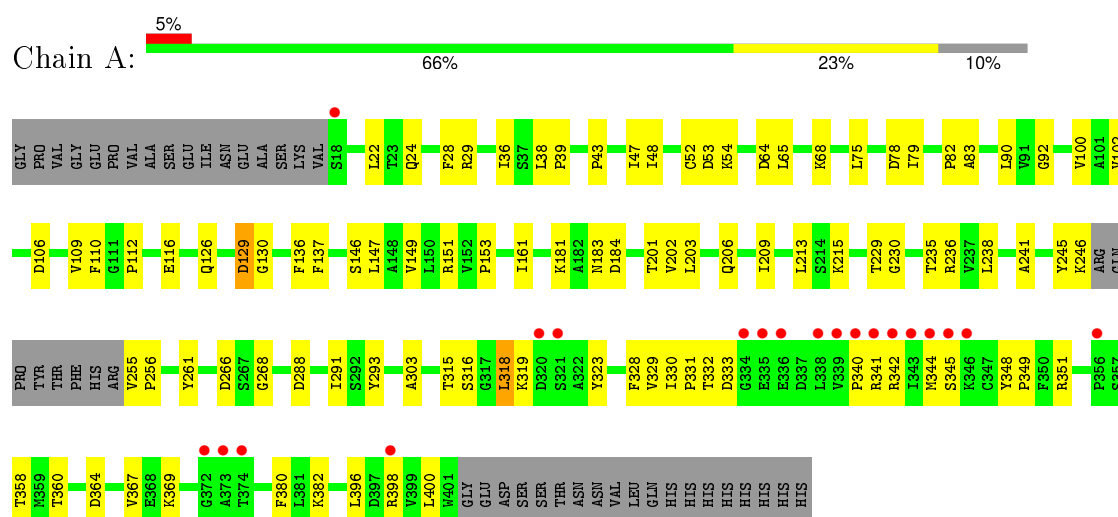
### 3 Residue-property plots

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.

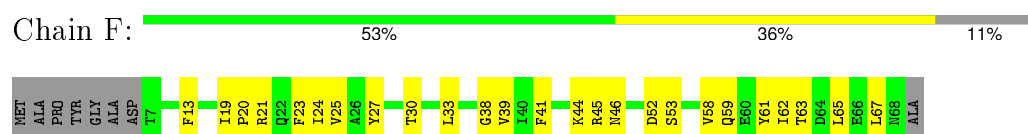
#### • Molecule 1: Putative uncharacterized protein



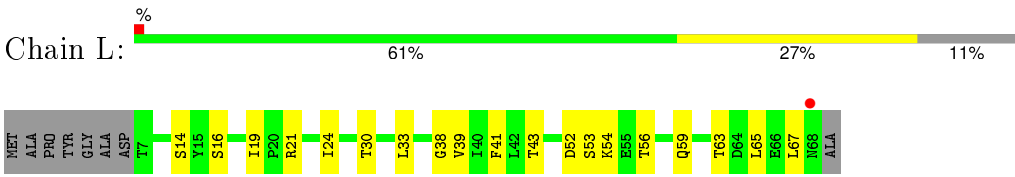
#### • Molecule 1: Putative uncharacterized protein



#### • Molecule 2: C-C motif chemokine 3



● Molecule 2: C-C motif chemokine 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.49Å 109.48Å 210.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 3.00 49.25 – 2.76	Depositor EDS
% Data completeness (in resolution range)	93.1 (49.25-3.00) 80.1 (49.25-2.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.59 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.215 , 0.274 0.213 , 0.272	Depositor DCC
$R_{free}$ test set	1617 reflections (7.47%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.7	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 26.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 26825 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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, 0.375 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	A	0.28	0/3035	0.45	0/4114
1	B	0.29	0/3063	0.45	0/4152
2	F	0.28	0/515	0.40	0/698
2	L	0.30	0/515	0.43	0/698
All	All	0.28	0/7128	0.44	0/9662

There are no bond length outliers.

There are no bond angle outliers.

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	A	2971	1	2926	87	0
1	B	2998	1	2953	102	1
2	F	504	0	492	19	0
2	L	504	0	492	16	0
3	A	28	26	26	1	0
3	B	28	25	26	0	0
All	All	7033	53	6915	211	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 15.



All (211) 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:318:LEU:H	1:A:318:LEU:HD23	1.31	0.93
2:L:19:ILE:HD11	2:L:24:ILE:HD11	1.53	0.90
1:B:318:LEU:HG	1:B:319:LYS:H	1.36	0.89
1:B:75:LEU:HD12	1:B:146:SER:HB2	1.56	0.86
1:A:255:VAL:HG13	1:A:256:PRO:HD3	1.65	0.79
2:L:24:ILE:HD12	2:L:41:PHE:HB3	1.63	0.79
1:B:318:LEU:HD23	1:B:318:LEU:H	1.48	0.78
1:A:201:THR:HG22	1:A:203:LEU:H	1.49	0.77
1:A:28:PHE:HE1	1:A:331:PRO:HG3	1.49	0.76
1:A:106:ASP:HB3	1:A:153:PRO:HG2	1.66	0.76
1:A:291:ILE:HD12	1:A:396:LEU:HD23	1.66	0.76
1:B:201:THR:HG22	1:B:203:LEU:H	1.50	0.76
1:B:106:ASP:HB3	1:B:153:PRO:HG2	1.66	0.76
1:B:201:THR:HG21	1:B:203:LEU:HG	1.69	0.75
1:B:342:ARG:NH1	1:B:346:LYS:HG2	2.03	0.73
1:B:65:LEU:CD1	1:B:209:ILE:HD11	2.20	0.72
1:B:202:VAL:HG12	1:B:246:LYS:HE3	1.70	0.71
1:B:65:LEU:HD12	1:B:209:ILE:HD11	1.73	0.70
1:B:201:THR:CG2	1:B:203:LEU:HG	2.21	0.70
2:L:39:VAL:HG23	2:L:53:SER:HB3	1.74	0.68
1:A:28:PHE:CE1	1:A:331:PRO:HG3	2.28	0.68
1:B:97:PRO:HG2	1:B:100:VAL:HG23	1.76	0.68
1:A:68:LYS:HD2	1:A:151:ARG:HH21	1.60	0.67
1:A:245:TYR:CE1	2:L:33:LEU:HD21	2.30	0.67
1:A:201:THR:CG2	1:A:203:LEU:HG	2.25	0.67
1:B:199:GLU:HA	1:B:206:GLN:HE22	1.60	0.66
1:A:65:LEU:HD12	1:A:209:ILE:HD11	1.76	0.66
1:B:202:VAL:CG1	1:B:246:LYS:HE3	2.25	0.66
1:A:316:SER:HB2	1:A:400:LEU:H	1.60	0.66
1:B:97:PRO:HG2	1:B:100:VAL:CG2	2.25	0.66
1:B:275:TYR:CD1	1:B:278:CYS:HB2	2.31	0.65
1:A:29:ARG:HD3	1:A:53:ASP:OD1	1.97	0.65
1:B:342:ARG:HH11	1:B:346:LYS:HG2	1.61	0.65
2:F:24:ILE:HD12	2:F:41:PHE:HB3	1.78	0.64
1:B:336:GLU:HB2	1:B:341:ARG:NH1	2.13	0.64
1:A:202:VAL:CG1	1:A:246:LYS:HE3	2.28	0.64
1:B:317:GLY:HA3	1:B:321:SER:HB2	1.78	0.64
1:A:268:GLY:HA2	2:L:16:SER:HB2	1.79	0.63
1:A:110:PHE:HB3	1:A:116:GLU:HA	1.79	0.63
1:A:201:THR:HB	1:A:206:GLN:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:VAL:HB	1:B:256:PRO:HD3	1.81	0.63
1:A:330:ILE:HG12	1:A:340:PRO:HA	1.81	0.63
1:A:106:ASP:HB3	1:A:153:PRO:CG	2.28	0.62
1:A:65:LEU:CD1	1:A:209:ILE:HD11	2.29	0.62
1:B:202:VAL:HG23	2:F:33:LEU:O	2.00	0.62
1:B:199:GLU:HA	1:B:206:GLN:NE2	2.15	0.62
1:B:112:PRO:HD2	1:B:140:PHE:CD1	2.35	0.62
1:B:129:ASP:OD2	1:B:131:LYS:HE2	2.00	0.62
1:A:328:PHE:HE1	1:A:342:ARG:HG2	1.65	0.61
1:B:318:LEU:HB2	2:F:25:VAL:HG12	1.82	0.61
1:B:64:ASP:O	1:B:65:LEU:HD23	2.00	0.60
1:A:328:PHE:CE1	1:A:342:ARG:HG2	2.37	0.60
2:L:21:ARG:NH2	2:L:65:LEU:HD23	2.17	0.60
1:B:106:ASP:HB3	1:B:153:PRO:CG	2.32	0.59
2:F:19:ILE:HD11	2:F:24:ILE:HD11	1.85	0.59
1:A:201:THR:HG21	1:A:203:LEU:HG	1.84	0.58
1:B:198:LEU:HD13	2:F:13:PHE:CZ	2.38	0.58
1:B:270:GLU:HG2	1:B:271:ASP:N	2.19	0.58
2:L:19:ILE:CD1	2:L:24:ILE:HD11	2.31	0.58
1:B:319:LYS:HG3	1:B:320:ASP:N	2.19	0.57
1:B:316:SER:HB2	1:B:400:LEU:HB3	1.86	0.57
1:A:293:TYR:OH	1:A:396:LEU:HG	2.05	0.57
1:A:255:VAL:N	1:A:256:PRO:HD2	2.20	0.57
1:A:245:TYR:CE2	1:A:256:PRO:HG2	2.39	0.57
1:A:92:GLY:HA3	1:A:136:PHE:CZ	2.41	0.56
1:A:48:ILE:HA	1:A:52:CYS:SG	2.45	0.56
1:B:318:LEU:CB	2:F:25:VAL:HG12	2.35	0.56
1:B:348:TYR:HB2	1:B:349:PRO:HD3	1.87	0.56
1:B:121:PHE:CE2	1:B:136:PHE:HB3	2.41	0.56
1:B:48:ILE:HA	1:B:52:CYS:SG	2.46	0.56
2:F:27:TYR:CZ	2:F:62:ILE:HG23	2.40	0.56
1:A:126:GLN:O	1:A:130:GLY:N	2.39	0.55
1:A:255:VAL:CG1	1:A:256:PRO:HD3	2.33	0.55
2:L:63:THR:O	2:L:67:LEU:HD13	2.07	0.55
1:A:161:ILE:HD12	1:A:161:ILE:N	2.21	0.55
1:A:64:ASP:O	1:A:65:LEU:HD23	2.07	0.55
2:F:30:THR:HG23	2:F:38:GLY:O	2.07	0.55
1:B:79:ILE:HG21	1:B:82:PRO:HB3	1.88	0.55
1:A:126:GLN:HE21	1:A:129:ASP:HB2	1.72	0.54
1:A:241:ALA:O	1:A:261:TYR:HA	2.07	0.54
1:B:110:PHE:HB3	1:B:116:GLU:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ALA:HB3	1:A:323:TYR:OH	2.07	0.54
1:B:172:SER:HB3	1:B:325:SER:OG	2.07	0.54
1:B:46:ASP:OD2	1:B:126:GLN:NE2	2.41	0.54
1:B:291:ILE:HD12	1:B:396:LEU:HD23	1.89	0.54
1:B:295:PHE:CE1	1:B:361:VAL:HB	2.43	0.54
1:A:380:PHE:CE2	1:A:382:LYS:HB2	2.43	0.53
1:A:318:LEU:HD23	1:A:318:LEU:N	2.13	0.53
1:A:318:LEU:HD12	1:A:319:LYS:HD2	1.91	0.52
1:A:181:LYS:HE2	1:A:184:ASP:OD1	2.08	0.52
2:F:52:ASP:O	2:F:58:VAL:HG21	2.09	0.52
1:B:111:GLY:HA3	1:B:140:PHE:CE1	2.45	0.51
1:B:318:LEU:HG	1:B:319:LYS:N	2.17	0.51
2:F:20:PRO:HG2	2:F:23:PHE:CD2	2.45	0.51
1:B:351:ARG:HB3	1:B:364:ASP:HB2	1.93	0.51
1:B:247:ARG:NH1	2:L:52:ASP:OD2	2.44	0.51
1:A:351:ARG:HB3	1:A:364:ASP:HB2	1.91	0.51
2:F:39:VAL:HG23	2:F:53:SER:HB3	1.93	0.50
1:A:183:ASN:OD1	3:A:501:NAG:H4	2.12	0.50
1:B:344:MET:HG3	1:B:345:SER:N	2.26	0.50
1:B:272:TYR:CD1	1:B:275:TYR:HB3	2.46	0.50
1:B:115:GLU:HG2	1:B:260:VAL:CG1	2.42	0.50
1:B:74:PRO:HG3	1:B:213:LEU:HD11	1.94	0.50
1:A:78:ASP:OD2	1:A:215:LYS:NZ	2.44	0.50
1:B:345:SER:O	1:B:346:LYS:HG3	2.12	0.49
1:B:218:TYR:HD2	1:B:388:TYR:CD2	2.29	0.49
1:A:348:TYR:HB2	1:A:349:PRO:HD3	1.93	0.49
1:A:315:THR:O	1:A:315:THR:HG23	2.12	0.49
1:B:29:ARG:HH11	1:B:51:THR:HA	1.77	0.49
1:B:201:THR:HG22	1:B:202:VAL:N	2.27	0.49
1:A:75:LEU:HD12	1:A:146:SER:HB2	1.95	0.49
1:A:202:VAL:HG13	1:A:246:LYS:HE3	1.94	0.49
1:A:68:LYS:HB2	1:A:151:ARG:NH2	2.27	0.49
1:B:198:LEU:N	1:B:198:LEU:HD12	2.28	0.48
1:A:79:ILE:CG2	1:A:82:PRO:HA	2.43	0.48
1:B:281:VAL:O	1:B:281:VAL:HG13	2.14	0.48
1:A:245:TYR:HE1	2:L:33:LEU:HD21	1.78	0.48
1:A:331:PRO:CG	1:A:341:ARG:HE	2.26	0.48
1:B:90:LEU:O	1:B:137:PHE:HA	2.13	0.48
1:B:318:LEU:CG	1:B:319:LYS:H	2.16	0.48
1:B:275:TYR:CE2	2:F:44:LYS:HD3	2.48	0.48
1:A:255:VAL:HG13	1:A:256:PRO:CD	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:VAL:O	1:A:341:ARG:HB2	2.14	0.48
1:A:344:MET:HG3	1:A:345:SER:H	1.78	0.47
1:A:68:LYS:HD2	1:A:151:ARG:NH2	2.28	0.47
1:B:329:VAL:HG23	1:B:343:ILE:HD11	1.96	0.47
1:B:275:TYR:HD1	1:B:278:CYS:HB2	1.75	0.47
1:B:313:TRP:HA	1:B:324:GLU:O	2.13	0.47
1:B:172:SER:HB2	1:B:326:CYS:C	2.34	0.47
1:A:90:LEU:O	1:A:137:PHE:HA	2.15	0.47
1:A:255:VAL:N	1:A:256:PRO:CD	2.77	0.47
2:F:19:ILE:HB	2:F:20:PRO:HD2	1.96	0.47
2:F:61:TYR:O	2:F:65:LEU:HG	2.15	0.47
1:B:332:THR:O	1:B:333:ASP:HB2	2.15	0.47
1:B:203:LEU:HD11	1:B:262:VAL:HG23	1.96	0.47
1:B:247:ARG:HB2	2:L:54:LYS:O	2.15	0.47
1:A:79:ILE:CG2	1:A:82:PRO:HG3	2.45	0.47
1:A:38:LEU:HA	1:A:39:PRO:C	2.35	0.46
1:B:129:ASP:OD2	1:B:131:LYS:HG3	2.15	0.46
1:B:270:GLU:HG2	1:B:271:ASP:H	1.80	0.46
1:A:201:THR:HG22	1:A:202:VAL:N	2.30	0.46
1:A:236:ARG:NE	1:A:238:LEU:HD21	2.31	0.46
1:B:316:SER:HB2	1:B:400:LEU:H	1.80	0.46
1:A:36:ILE:CD1	1:A:47:ILE:HG23	2.46	0.46
1:B:272:TYR:CE1	1:B:275:TYR:HB3	2.51	0.46
1:B:220:ARG:HD2	1:B:222:TYR:OH	2.15	0.46
1:B:319:LYS:HG3	1:B:320:ASP:H	1.79	0.46
1:A:201:THR:HG22	1:A:203:LEU:HG	1.97	0.46
1:B:318:LEU:HD23	1:B:318:LEU:N	2.25	0.45
1:B:202:VAL:HG12	1:B:202:VAL:O	2.16	0.45
1:A:396:LEU:HD12	1:A:396:LEU:N	2.31	0.45
1:A:109:VAL:HA	1:A:149:VAL:O	2.16	0.45
1:B:330:ILE:HD12	1:B:330:ILE:N	2.31	0.45
1:A:112:PRO:HG3	1:A:146:SER:HB3	1.98	0.45
1:B:317:GLY:HA3	1:B:321:SER:CB	2.44	0.45
1:B:171:LEU:HD21	1:B:323:TYR:O	2.17	0.45
1:B:68:LYS:HB2	1:B:151:ARG:NH2	2.32	0.45
1:B:90:LEU:HD21	1:B:150:LEU:HD11	1.99	0.45
1:A:92:GLY:HA3	1:A:136:PHE:CE1	2.52	0.45
1:A:229:THR:HG22	1:A:230:GLY:N	2.31	0.45
1:B:229:THR:HG22	1:B:230:GLY:N	2.32	0.45
1:A:24:GLN:OE1	1:A:54:LYS:HE3	2.17	0.44
1:A:100:VAL:HG12	1:A:102:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:GLN:NE2	1:B:207:THR:HG23	2.33	0.44
1:A:36:ILE:HD11	1:A:47:ILE:HG23	1.99	0.44
1:A:358:THR:O	1:A:360:THR:HG23	2.17	0.44
1:B:373:ALA:O	1:B:374:THR:HB	2.17	0.44
1:B:344:MET:HG3	1:B:345:SER:H	1.82	0.44
1:B:166:ILE:O	1:B:177:CYS:HA	2.17	0.44
1:B:66:LEU:O	1:B:67:GLU:HB2	2.18	0.44
2:F:46:ASN:ND2	2:F:46:ASN:O	2.51	0.44
1:A:332:THR:O	1:A:333:ASP:HB2	2.18	0.44
1:A:79:ILE:CG2	1:A:82:PRO:CA	2.96	0.44
1:B:69:GLU:O	1:B:151:ARG:HA	2.18	0.44
2:F:21:ARG:NH2	2:F:65:LEU:HD23	2.34	0.43
1:B:290:GLN:HA	1:B:365:VAL:O	2.18	0.43
1:B:22:LEU:HG	1:B:189:GLY:CA	2.49	0.43
1:A:147:LEU:HD21	1:A:238:LEU:HD13	2.00	0.43
1:A:79:ILE:HG23	1:A:82:PRO:HA	2.01	0.43
2:F:59:GLN:O	2:F:63:THR:HG23	2.18	0.43
2:F:63:THR:O	2:F:67:LEU:HD13	2.18	0.43
1:A:79:ILE:HG21	1:A:82:PRO:HG3	2.01	0.43
1:A:266:ASP:OD1	2:L:14:SER:OG	2.30	0.42
1:A:344:MET:HG3	1:A:345:SER:N	2.34	0.42
1:B:396:LEU:HD12	1:B:396:LEU:N	2.34	0.42
1:A:22:LEU:HB2	1:A:215:LYS:HA	2.02	0.42
1:A:213:LEU:O	1:A:235:THR:HA	2.20	0.42
1:A:202:VAL:O	1:A:202:VAL:HG12	2.18	0.42
1:B:393:GLU:OE2	2:F:45:ARG:NH2	2.49	0.42
1:B:201:THR:HG22	1:B:203:LEU:HG	2.01	0.41
1:B:348:TYR:O	1:B:366:ARG:HD3	2.20	0.41
1:A:303:ALA:CB	1:A:332:THR:HG21	2.50	0.41
1:B:248:GLN:CG	2:L:56:THR:HG22	2.50	0.41
1:B:241:ALA:HB2	1:B:264:LEU:HD11	2.02	0.41
1:B:181:LYS:HE2	1:B:184:ASP:OD1	2.19	0.41
1:B:197:CYS:SG	1:B:208:CYS:N	2.93	0.41
1:B:218:TYR:HD2	1:B:388:TYR:CE2	2.39	0.41
1:B:324:GLU:HB3	1:B:349:PRO:HG2	2.02	0.41
1:B:374:THR:O	1:B:374:THR:HG22	2.21	0.41
1:B:255:VAL:HB	1:B:256:PRO:CD	2.47	0.41
1:B:43:PRO:O	1:B:47:ILE:HG13	2.20	0.41
2:L:59:GLN:O	2:L:63:THR:HG23	2.21	0.41
1:B:116:GLU:HB3	1:B:259:MET:H	1.84	0.41
1:A:43:PRO:O	1:A:47:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ASP:HB3	1:A:369:LYS:HD3	2.02	0.41
1:A:303:ALA:HB3	1:A:332:THR:HG21	2.02	0.40
1:A:367:VAL:HG21	1:A:398:ARG:HD2	2.03	0.40
2:L:24:ILE:HD13	2:L:43:THR:HG22	2.03	0.40
1:A:331:PRO:HG2	1:A:341:ARG:HE	1.86	0.40
1:B:29:ARG:HD2	1:B:50:GLN:O	2.20	0.40
2:L:30:THR:HG23	2:L:38:GLY:O	2.21	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)
1:B:216:LYS:NZ	1:B:277:GLU:OE1[3_555]	2.07	0.13

## 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	372/420 (89%)	351 (94%)	21 (6%)	0	100	100
1	B	375/420 (89%)	356 (95%)	19 (5%)	0	100	100
2	F	60/70 (86%)	59 (98%)	1 (2%)	0	100	100
2	L	60/70 (86%)	60 (100%)	0	0	100	100
All	All	867/980 (88%)	826 (95%)	41 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	332/371 (90%)	330 (99%)	2 (1%)	90	97
1	B	335/371 (90%)	333 (99%)	2 (1%)	90	97
2	F	58/62 (94%)	58 (100%)	0	100	100
2	L	58/62 (94%)	58 (100%)	0	100	100
All	All	783/866 (90%)	779 (100%)	4 (0%)	92	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	272	TYR
1	B	318	LEU
1	A	129	ASP
1	A	318	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	126	GLN
1	A	126	GLN
2	F	46	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 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	NAG	A	501	-	14,14,15	1.34	3 (21%)	15,19,21	1.05	0
3	NAG	A	502	1	14,14,15	1.33	3 (21%)	15,19,21	1.14	2 (13%)
3	NAG	B	501	1	14,14,15	1.34	3 (21%)	15,19,21	1.43	3 (20%)
3	NAG	B	502	1	14,14,15	1.33	3 (21%)	15,19,21	1.29	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	501	-	-	0/6/23/26	0/1/1/1
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	NAG	B	501	1	-	0/6/23/26	0/1/1/1
3	NAG	B	502	1	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	NAG	C2-N2	-2.61	1.41	1.46
3	B	502	NAG	C2-N2	-2.59	1.41	1.46
3	A	502	NAG	C2-N2	-2.59	1.41	1.46
3	A	501	NAG	C2-N2	-2.56	1.41	1.46
3	B	501	NAG	C1-C2	-2.48	1.48	1.52
3	A	501	NAG	C1-C2	-2.41	1.49	1.52
3	A	502	NAG	C1-C2	-2.36	1.49	1.52
3	B	502	NAG	C1-C2	-2.12	1.49	1.52
3	B	502	NAG	C7-N2	2.63	1.44	1.34
3	A	502	NAG	C7-N2	2.66	1.44	1.34
3	B	501	NAG	C7-N2	2.68	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	NAG	C7-N2	2.69	1.44	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NAG	C2-N2-C7	-2.46	119.91	123.11
3	A	502	NAG	C2-N2-C7	-2.20	120.25	123.11
3	B	502	NAG	C2-N2-C7	-2.11	120.36	123.11
3	B	501	NAG	C8-C7-N2	2.00	119.94	116.10
3	A	502	NAG	C8-C7-N2	2.06	120.04	116.10
3	B	502	NAG	C1-O5-C5	2.90	116.40	112.14
3	B	501	NAG	C1-O5-C5	3.62	117.46	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	NAG	1	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	376/420 (89%)	-0.06	20 (5%) 30 12	31, 55, 119, 192	0
1	B	379/420 (90%)	-0.10	18 (4%) 35 14	26, 49, 114, 147	0
2	F	62/70 (88%)	-0.17	0 100 100	48, 71, 90, 118	0
2	L	62/70 (88%)	-0.29	1 (1%) 74 47	37, 56, 85, 111	0
All	All	879/980 (89%)	-0.10	39 (4%) 38 16	26, 53, 114, 192	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	GLY	6.0
1	A	335	GLU	5.6
1	A	373	ALA	5.5
1	A	334	GLY	5.4
1	A	336	GLU	4.9
1	A	344	MET	4.7
1	B	256	PRO	4.5
1	A	340	PRO	4.3
1	B	337	ASP	4.1
1	A	342	ARG	4.1
1	B	339	VAL	4.0
1	B	338	LEU	3.8
1	B	374	THR	3.8
1	B	336	GLU	3.7
1	A	345	SER	3.6
1	B	255	VAL	3.3
1	B	369	LYS	3.2
1	B	373	ALA	3.2
1	A	341	ARG	3.2
1	A	374	THR	3.2
1	B	341	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	340	PRO	3.0
1	B	372	GLY	3.0
1	B	248	GLN	2.9
1	B	335	GLU	2.8
1	B	333	ASP	2.7
1	A	343	ILE	2.6
1	B	318	LEU	2.6
1	A	338	LEU	2.4
2	L	68	ASN	2.4
1	A	346	LYS	2.4
1	A	339	VAL	2.3
1	B	345	SER	2.2
1	A	321	SER	2.2
1	A	320	ASP	2.1
1	A	18	SER	2.1
1	A	356	PRO	2.1
1	B	344	MET	2.0
1	A	398	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	501	14/15	0.75	0.21	-	98,115,130,133	0
3	NAG	A	501	14/15	0.64	0.46	-	151,164,206,206	0
3	NAG	B	502	14/15	0.78	0.25	-	93,111,129,138	0
3	NAG	A	502	14/15	0.83	0.26	-	96,110,132,135	0

## 6.5 Other polymers

There are no such residues in this entry.