



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:45 PM GMT

PDB ID : 2Y3A  
Title : CRYSTAL STRUCTURE OF P110BETA IN COMPLEX WITH ICSH2 OF P85BETA AND THE DRUG GDC-0941  
Authors : Zhang, X.; Vadas, O.; Perisic, O.; Williams, R.L.  
Deposited on : 2010-12-20  
Resolution : 3.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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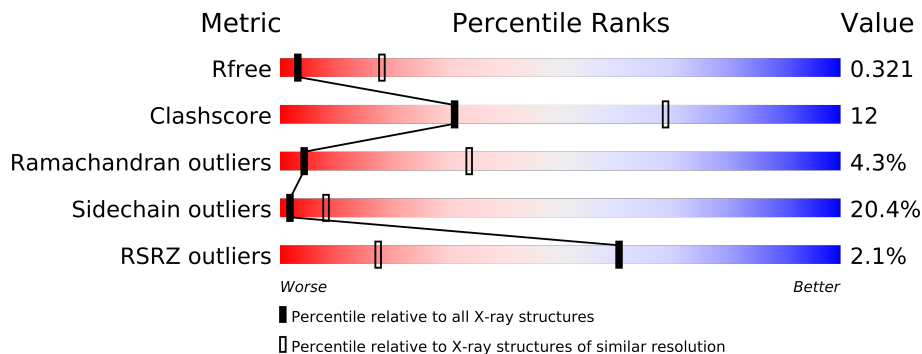
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.30 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	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1092	
2	B	302	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9848 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 PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE3-KINASE CATALYTIC SUBUNIT BETA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	976	Total	C	N	O	S	0	0	0
			7862	5047	1323	1443	49			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	EXPRESSION TAG	UNP Q8BTI9
A	-26	SER	-	EXPRESSION TAG	UNP Q8BTI9
A	-25	TYR	-	EXPRESSION TAG	UNP Q8BTI9
A	-24	TYR	-	EXPRESSION TAG	UNP Q8BTI9
A	-23	HIS	-	EXPRESSION TAG	UNP Q8BTI9
A	-22	HIS	-	EXPRESSION TAG	UNP Q8BTI9
A	-21	HIS	-	EXPRESSION TAG	UNP Q8BTI9
A	-20	HIS	-	EXPRESSION TAG	UNP Q8BTI9
A	-19	HIS	-	EXPRESSION TAG	UNP Q8BTI9
A	-18	HIS	-	EXPRESSION TAG	UNP Q8BTI9
A	-17	ASP	-	EXPRESSION TAG	UNP Q8BTI9
A	-16	TYR	-	EXPRESSION TAG	UNP Q8BTI9
A	-15	ASP	-	EXPRESSION TAG	UNP Q8BTI9
A	-14	ILE	-	EXPRESSION TAG	UNP Q8BTI9
A	-13	PRO	-	EXPRESSION TAG	UNP Q8BTI9
A	-12	THR	-	EXPRESSION TAG	UNP Q8BTI9
A	-11	THR	-	EXPRESSION TAG	UNP Q8BTI9
A	-10	GLU	-	EXPRESSION TAG	UNP Q8BTI9
A	-9	ASN	-	EXPRESSION TAG	UNP Q8BTI9
A	-8	LEU	-	EXPRESSION TAG	UNP Q8BTI9
A	-7	TYR	-	EXPRESSION TAG	UNP Q8BTI9
A	-6	PHE	-	EXPRESSION TAG	UNP Q8BTI9
A	-5	GLN	-	EXPRESSION TAG	UNP Q8BTI9
A	-4	GLY	-	EXPRESSION TAG	UNP Q8BTI9
A	-3	ALA	-	EXPRESSION TAG	UNP Q8BTI9
A	-2	MET	-	EXPRESSION TAG	UNP Q8BTI9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q8BTI9
A	0	SER	-	EXPRESSION TAG	UNP Q8BTI9
A	123	LEU	ARG	CONFLICT	UNP Q8BTI9

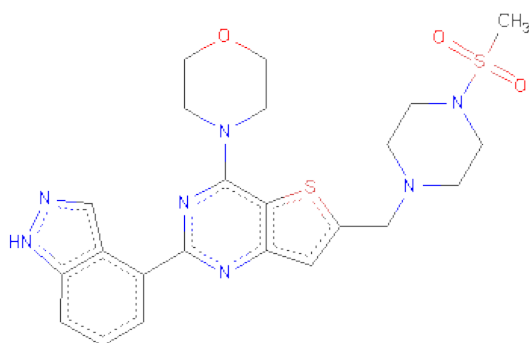
- Molecule 2 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE REGULATORY SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	0
			1951	1214	355	373	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	421	MET	-	EXPRESSION TAG	UNP O08908
B	422	SER	-	EXPRESSION TAG	UNP O08908

- Molecule 3 is 2-(1H-INDAZOL-4-YL)-6-{[4-(METHYLSULFONYL)PIPERAZIN-1-YL]METHYL}-4-MORPHOLIN-4-YL-THIENO[3,2-D]PYRIMIDINE (three-letter code: GD9) (formula: C<sub>23</sub>H<sub>27</sub>N<sub>7</sub>O<sub>3</sub>S<sub>2</sub>).



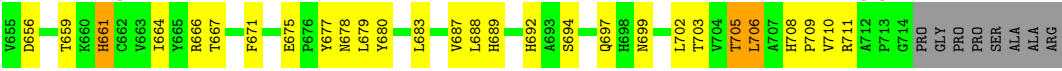
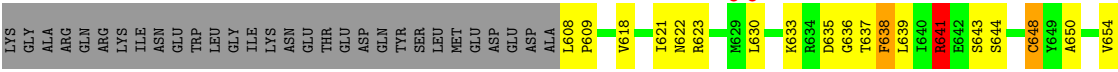
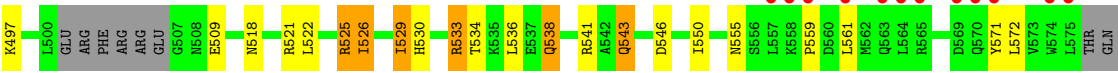
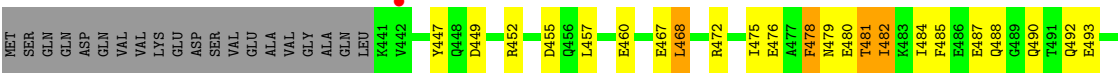
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			35	23	7	3	2		





● Molecule 2: PHOSPHATIDYLINOSITOL 3-KINASE REGULATORY SUBUNIT BETA

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.31 Å   134.31 Å   428.06 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	44.68 – 3.30 44.02 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (44.68-3.30) 96.6 (44.02-3.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 3.32 Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.234   ,   0.296 0.251   ,   0.321	Depositor DCC
$R_{free}$ test set	1761 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	99.7	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31   ,   109.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 34249 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: GD9

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	0.52	0/8028	0.82	1/10858 (0.0%)
2	B	0.51	0/1984	0.80	0/2665
All	All	0.52	0/10012	0.82	1/13523 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	752	LEU	C-N-CA	5.73	136.02	121.70

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	7862	0	7903	192	0
2	B	1951	0	1916	49	0
3	A	35	0	27	5	0
All	All	9848	0	9846	231	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 12.

All (231) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:661:ASN:HB2	1:A:665:GLY:H	1.35	0.91
2:B:475:ILE:HG23	2:B:536:LEU:HD23	1.54	0.89
1:A:448:SER:HA	1:A:489:PHE:HB2	1.57	0.87
1:A:969:ASN:HD21	1:A:971:GLU:HG3	1.40	0.87
1:A:1019:LYS:HA	1:A:1024:LEU:HD12	1.58	0.85
1:A:359:CYS:HB2	1:A:383:ILE:HD11	1.60	0.82
1:A:784:TYR:HB2	1:A:794:VAL:HG23	1.64	0.80
1:A:896:THR:HG23	1:A:962:ILE:HG12	1.71	0.73
1:A:797:ILE:HD11	1:A:847:VAL:HG23	1.71	0.72
1:A:54:TRP:HA	1:A:57:VAL:HG13	1.72	0.72
1:A:938:ASN:HB3	1:A:948:GLU:HB3	1.70	0.72
1:A:754:SER:HB2	1:A:762:LEU:HD13	1.71	0.71
1:A:171:PRO:HD2	1:A:662:ARG:HA	1.71	0.71
1:A:345:VAL:HG11	1:A:367:ILE:H	1.57	0.70
1:A:94:CYS:O	1:A:97:ARG:HG3	1.90	0.70
1:A:41:PRO:HG2	1:A:44:ALA:HB2	1.74	0.69
2:B:475:ILE:CG2	2:B:536:LEU:HD23	2.22	0.69
1:A:40:VAL:HG11	1:A:49:ILE:HG12	1.74	0.69
1:A:91:ARG:HD2	1:A:96:VAL:HB	1.75	0.68
1:A:147:ARG:HG3	1:A:694:ARG:HD3	1.77	0.66
1:A:713:LEU:HD21	1:A:782:LEU:HD11	1.78	0.66
1:A:906:SER:HB3	1:A:914:ARG:NH1	2.12	0.65
1:A:154:ILE:HD11	1:A:694:ARG:O	1.96	0.65
1:A:969:ASN:HB3	1:A:973:PHE:CZ	2.32	0.64
1:A:73:MET:HG2	1:A:108:ARG:HA	1.79	0.64
2:B:482:ILE:HD13	2:B:533:ARG:HH11	1.64	0.63
1:A:80:THR:O	1:A:82:VAL:N	2.29	0.63
1:A:77:VAL:HG21	2:B:481:THR:HG23	1.82	0.62
2:B:694:SER:HA	2:B:705:THR:HG22	1.81	0.62
1:A:998:PHE:HD1	1:A:1009:LEU:HD11	1.64	0.62
2:B:643:SER:OG	2:B:648:CYS:HB3	2.00	0.62
1:A:35:TYR:HB2	2:B:522:LEU:HD23	1.83	0.61
2:B:635:ASP:HB2	2:B:656:ASP:HA	1.81	0.60
1:A:110:CYS:C	1:A:112:PRO:HD2	2.22	0.60
1:A:674:SER:HA	1:A:839:GLY:HA2	1.84	0.60
1:A:906:SER:HA	1:A:911:ILE:HD12	1.84	0.59
1:A:210:PRO:O	1:A:258:ILE:HG13	2.02	0.59
1:A:703:LEU:O	1:A:707:VAL:HG23	2.01	0.59
2:B:467:GLU:HB3	2:B:543:GLN:HE22	1.67	0.59
1:A:434:TRP:HD1	1:A:460:PRO:HG3	1.68	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:629:LEU:HD22	1:A:657:ARG:HD3	1.85	0.59
1:A:46:ILE:HG22	1:A:89:GLU:HA	1.84	0.58
1:A:193:VAL:HG23	1:A:273:PRO:HB2	1.84	0.58
1:A:256:PRO:HG2	1:A:259:GLN:HB2	1.85	0.58
1:A:435:VAL:HG13	1:A:455:SER:HA	1.86	0.58
1:A:635:GLN:HE22	1:A:812:GLN:HE22	1.50	0.57
2:B:478:PHE:HB3	2:B:533:ARG:HD2	1.85	0.57
1:A:863:ASN:CB	1:A:870:PHE:HA	2.35	0.57
1:A:1012:VAL:HA	1:A:1015:ILE:HD12	1.87	0.57
1:A:215:ILE:HA	1:A:218:ASN:HD22	1.69	0.57
1:A:142:PHE:HE2	1:A:442:PHE:HD2	1.50	0.57
1:A:40:VAL:CG1	1:A:49:ILE:HG12	2.34	0.56
1:A:43:GLU:HB2	1:A:92:ARG:HE	1.69	0.56
1:A:347:VAL:HA	1:A:398:VAL:HG12	1.88	0.56
1:A:173:GLU:O	1:A:260:PHE:HA	2.06	0.56
1:A:476:ASN:HD22	1:A:478:TYR:H	1.52	0.56
1:A:1047:TRP:CE3	2:B:697:GLN:HB3	2.41	0.55
1:A:720:ILE:HD11	1:A:736:MET:HB2	1.89	0.55
1:A:808:MET:HE2	1:A:836:LEU:HD23	1.88	0.55
1:A:711:ASN:HA	1:A:714:LYS:HD2	1.87	0.55
1:A:959:ILE:HG21	2:B:677:TYR:HE1	1.71	0.55
1:A:574:ILE:HD11	1:A:585:LEU:HG	1.87	0.55
2:B:623:ARG:HG3	2:B:641:ARG:NH1	2.21	0.55
2:B:608:LEU:N	2:B:609:PRO:HD3	2.21	0.55
1:A:58:HIS:HA	1:A:63:PHE:HB3	1.89	0.55
1:A:195:VAL:HG12	1:A:275:PHE:HB2	1.89	0.55
2:B:638:PHE:CD1	2:B:706:LEU:HB3	2.41	0.55
1:A:259:GLN:HA	1:A:264:ARG:HH21	1.73	0.54
3:A:2058:GD9:S1	3:A:2058:GD9:H17	2.48	0.54
1:A:687:VAL:O	1:A:690:GLU:HG3	2.07	0.54
2:B:526:ILE:HD12	2:B:530:HIS:CD2	2.43	0.53
1:A:387:ASP:HB3	1:A:578:LYS:HA	1.90	0.53
1:A:628:GLU:O	1:A:631:GLN:HB2	2.09	0.53
1:A:329:ILE:HD12	1:A:489:PHE:HD1	1.73	0.53
1:A:35:TYR:H	2:B:518:ASN:HD21	1.55	0.53
2:B:699:ASN:HB3	2:B:702:LEU:HG	1.90	0.53
1:A:963:GLN:HG3	1:A:973:PHE:HE2	1.73	0.52
1:A:124:ILE:HG23	1:A:689:LEU:HD13	1.90	0.52
1:A:806:GLN:HG3	1:A:1006:LEU:HD12	1.92	0.52
1:A:683:VAL:O	1:A:687:VAL:HG23	2.10	0.52
1:A:130:GLU:O	1:A:134:LEU:HG	2.10	0.52
1:A:528:PHE:HA	1:A:531:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:781:TRP:CZ2	1:A:847:VAL:HG21	2.45	0.51
1:A:806:GLN:O	1:A:810:THR:HG23	2.11	0.51
1:A:54:TRP:O	1:A:57:VAL:HG22	2.10	0.51
2:B:641:ARG:HG3	2:B:650:ALA:HB3	1.93	0.51
1:A:138:GLU:HG3	1:A:442:PHE:CZ	2.46	0.50
1:A:766:TYR:HD2	1:A:785:SER:HB2	1.76	0.50
1:A:23:ALA:HA	1:A:41:PRO:HA	1.93	0.50
1:A:447:ARG:HH21	1:A:451:VAL:HG11	1.75	0.50
1:A:567:LEU:HD23	1:A:592:TRP:CG	2.47	0.50
1:A:387:ASP:HA	1:A:579:LEU:HG	1.93	0.50
1:A:120:ILE:HG22	1:A:128:LEU:HD21	1.94	0.50
1:A:914:ARG:HA	1:A:918:ASN:HD21	1.76	0.50
1:A:959:ILE:HG21	2:B:677:TYR:CE1	2.47	0.50
1:A:706:GLN:HE22	1:A:755:PRO:HA	1.77	0.49
1:A:652:ARG:O	1:A:656:GLU:HB2	2.12	0.49
1:A:963:GLN:HG3	1:A:973:PHE:CE2	2.48	0.49
1:A:280:CYS:O	1:A:283:ILE:HG13	2.12	0.49
1:A:706:GLN:NE2	1:A:755:PRO:HA	2.27	0.49
1:A:655:LEU:HD11	1:A:688:ILE:HG23	1.95	0.49
1:A:876:LEU:HD22	1:A:880:LYS:HE3	1.94	0.49
1:A:702:VAL:HA	1:A:705:LYS:HD2	1.93	0.49
1:A:614:ARG:O	1:A:618:VAL:HG22	2.11	0.49
1:A:244:VAL:HG22	1:A:247:ARG:HB2	1.95	0.49
2:B:482:ILE:HG13	2:B:529:ILE:HD11	1.95	0.48
1:A:504:LYS:O	1:A:508:LYS:HG3	2.13	0.48
1:A:963:GLN:O	1:A:964:GLN:HB2	2.13	0.48
1:A:782:LEU:HB2	1:A:796:VAL:HG12	1.95	0.48
1:A:810:THR:CG2	1:A:935:ILE:HG21	2.44	0.48
1:A:714:LYS:HG2	1:A:800:ASN:ND2	2.28	0.48
1:A:663:ARG:HH22	1:A:757:ASN:HD21	1.62	0.48
2:B:468:LEU:HD22	2:B:543:GLN:HE21	1.78	0.48
1:A:728:SER:HB3	1:A:731:LYS:HB2	1.96	0.48
1:A:540:PRO:HG2	1:A:995:ILE:HG13	1.96	0.48
1:A:24:ILE:HD13	1:A:42:ARG:HE	1.79	0.48
1:A:138:GLU:OE2	1:A:139:VAL:HG23	2.13	0.48
1:A:952:PHE:HE1	1:A:954:LEU:HG	1.77	0.48
1:A:658:ALA:HB1	1:A:665:GLY:HA2	1.96	0.47
2:B:630:LEU:HD22	2:B:654:VAL:HG23	1.96	0.47
1:A:78:ASN:ND2	1:A:79:GLN:H	2.12	0.47
3:A:2058:GD9:S1	3:A:2058:GD9:C17	3.03	0.47
2:B:637:THR:HG22	2:B:708:HIS:HB2	1.96	0.47
1:A:138:GLU:HG3	1:A:442:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:30:LEU:HD22	1:A:105:LEU:HD22	1.96	0.47
1:A:77:VAL:CG2	2:B:481:THR:HG23	2.44	0.47
1:A:436:ASN:O	1:A:473:VAL:HA	2.15	0.47
1:A:29:LEU:HD22	2:B:488:GLN:HG3	1.97	0.47
1:A:943:PHE:HA	2:B:455:ASP:CG	2.36	0.47
1:A:810:THR:HG21	1:A:935:ILE:HG21	1.97	0.46
1:A:54:TRP:HA	1:A:57:VAL:CG1	2.43	0.46
1:A:164:ASP:HA	1:A:167:LYS:HD2	1.97	0.46
1:A:478:TYR:OH	2:B:472:ARG:HB2	2.16	0.46
1:A:934:HIS:HB2	1:A:939:PHE:HB2	1.97	0.46
2:B:638:PHE:CE2	2:B:706:LEU:HD22	2.51	0.46
1:A:902:TYR:CD2	1:A:929:HIS:HD2	2.33	0.46
1:A:603:LEU:HA	1:A:608:TYR:CD2	2.51	0.46
1:A:535:ILE:HG23	1:A:548:GLU:OE1	2.16	0.46
1:A:60:TYR:O	1:A:63:PHE:HD2	1.99	0.46
1:A:27:ASP:HB2	1:A:102:VAL:HB	1.97	0.46
1:A:572:LEU:HD11	1:A:607:ASN:HB3	1.98	0.46
1:A:626:ASP:HB3	1:A:664:ILE:HD11	1.98	0.46
1:A:784:TYR:HB2	1:A:794:VAL:CG2	2.40	0.45
1:A:714:LYS:HG2	1:A:800:ASN:HD22	1.81	0.45
1:A:716:LEU:HA	1:A:719:LEU:HD23	1.98	0.45
2:B:475:ILE:HG23	2:B:536:LEU:CD2	2.38	0.45
1:A:716:LEU:HD11	1:A:740:LEU:HD22	1.97	0.45
1:A:26:VAL:HG21	1:A:103:LEU:HD12	1.99	0.45
1:A:80:THR:C	1:A:82:VAL:H	2.18	0.45
1:A:459:PHE:N	1:A:460:PRO:CD	2.80	0.45
1:A:142:PHE:HE2	1:A:442:PHE:CD2	2.32	0.45
2:B:485:PHE:O	2:B:488:GLN:HB2	2.17	0.45
1:A:728:SER:HB3	1:A:731:LYS:HD2	1.98	0.44
1:A:635:GLN:NE2	1:A:635:GLN:H	2.14	0.44
1:A:432:VAL:HB	2:B:555:ASN:HB3	1.99	0.44
1:A:863:ASN:HB2	1:A:870:PHE:HA	2.00	0.44
1:A:243:GLN:HB3	1:A:276:ILE:HG22	2.00	0.44
1:A:899:CYS:HA	1:A:927:LEU:HD22	2.00	0.44
2:B:623:ARG:HG2	2:B:661:HIS:ND1	2.33	0.44
1:A:158:VAL:HA	1:A:291:MET:SD	2.58	0.44
2:B:618:VAL:HB	2:B:621:ILE:HD12	1.99	0.44
2:B:480:GLU:O	2:B:484:ILE:HD12	2.18	0.43
1:A:749:LEU:O	1:A:765:LEU:HD11	2.18	0.43
1:A:437:THR:HA	1:A:473:VAL:HG23	1.99	0.43
2:B:623:ARG:HE	2:B:661:HIS:HB2	1.82	0.43
1:A:911:ILE:O	1:A:914:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:630:LEU:HA	2:B:633:LYS:HD2	1.99	0.43
1:A:151:GLU:HA	1:A:154:ILE:HD12	2.01	0.43
1:A:592:TRP:CD1	1:A:593:PRO:HD2	2.54	0.43
1:A:401:VAL:HA	2:B:559:PRO:HG3	2.00	0.43
1:A:434:TRP:CD1	1:A:460:PRO:HG3	2.52	0.43
1:A:567:LEU:O	1:A:571:LEU:HG	2.19	0.43
1:A:952:PHE:CE1	1:A:954:LEU:HG	2.54	0.43
1:A:31:PRO:HD3	1:A:105:LEU:HD23	2.01	0.43
1:A:851:SER:HA	1:A:922:LYS:HA	2.01	0.43
2:B:525:ARG:O	2:B:529:ILE:HG23	2.18	0.43
1:A:192:VAL:O	1:A:273:PRO:HD2	2.18	0.43
1:A:196:HIS:HB3	1:A:203:VAL:HG23	2.00	0.43
1:A:97:ARG:HH22	1:A:711:ASN:HB3	1.84	0.42
1:A:196:HIS:HB3	1:A:203:VAL:HA	2.00	0.42
1:A:805:ARG:HG2	1:A:805:ARG:H	1.68	0.42
1:A:717:ASN:HB2	1:A:780:LEU:HD21	2.00	0.42
1:A:398:VAL:HG23	1:A:432:VAL:HA	2.00	0.42
1:A:604:LEU:HD23	1:A:614:ARG:HD3	2.01	0.42
1:A:829:ARG:HG3	1:A:894:GLU:HG2	2.01	0.42
1:A:880:LYS:HG2	1:A:888:LEU:HD11	2.00	0.42
2:B:630:LEU:HB3	2:B:654:VAL:CG2	2.50	0.42
1:A:914:ARG:HH21	1:A:953:ILE:HD12	1.84	0.42
1:A:816:LEU:HD23	1:A:994:PHE:CE1	2.55	0.42
1:A:828:LEU:HA	1:A:897:LEU:HB2	2.01	0.42
1:A:154:ILE:HA	1:A:157:LEU:HD12	2.02	0.42
1:A:435:VAL:HG11	1:A:453:LEU:HB3	2.02	0.42
1:A:343:VAL:HG11	1:A:399:TYR:CE2	2.54	0.42
1:A:627:GLU:OE2	1:A:662:ARG:NH1	2.52	0.42
1:A:808:MET:HE2	1:A:837:ALA:H	1.84	0.42
1:A:678:THR:HA	1:A:679:PRO:HD2	1.77	0.42
1:A:705:LYS:HD3	1:A:752:LEU:HB3	2.02	0.42
1:A:207:GLN:CD	1:A:207:GLN:H	2.23	0.42
2:B:472:ARG:HA	2:B:475:ILE:HG12	2.01	0.41
1:A:808:MET:CE	1:A:837:ALA:H	2.33	0.41
1:A:321:TRP:HE1	1:A:579:LEU:HD12	1.85	0.41
1:A:565:GLN:H	1:A:565:GLN:HG3	1.51	0.41
3:A:2058:GD9:N2	3:A:2058:GD9:H23	2.35	0.41
1:A:340:GLU:HB3	1:A:343:VAL:O	2.20	0.41
1:A:556:ARG:HD2	1:A:588:LEU:HD11	2.03	0.41
1:A:336:LYS:HE3	1:A:483:THR:HB	2.01	0.41
1:A:343:VAL:HG11	1:A:399:TYR:HE2	1.85	0.41
2:B:671:PHE:O	2:B:680:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:326:PRO:HA	1:A:384:ASN:HA	2.01	0.41
1:A:605:ASP:HB3	1:A:1000:LEU:HD23	2.03	0.41
1:A:27:ASP:OD1	2:B:525:ARG:HD3	2.21	0.41
3:A:2058:GD9:H23	3:A:2058:GD9:H14	2.01	0.41
1:A:663:ARG:HB2	1:A:758:PRO:HG2	2.01	0.41
1:A:34:ILE:HD11	1:A:62:MET:HB2	2.02	0.41
1:A:478:TYR:CZ	2:B:472:ARG:HD2	2.56	0.41
1:A:756:LEU:HD23	1:A:836:LEU:HB2	2.03	0.41
1:A:663:ARG:HH22	1:A:757:ASN:ND2	2.18	0.41
1:A:100:LEU:HD12	1:A:100:LEU:HA	1.81	0.41
2:B:522:LEU:O	2:B:526:ILE:HG23	2.21	0.41
1:A:969:ASN:O	2:B:675:GLU:CG	2.69	0.40
1:A:144:ARG:HG2	1:A:147:ARG:HH12	1.86	0.40
2:B:538:GLN:HE21	2:B:541:ARG:HH22	1.69	0.40
3:A:2058:GD9:C6	3:A:2058:GD9:C12	2.99	0.40
1:A:757:ASN:HD22	1:A:760:VAL:H	1.69	0.40
1:A:444:GLY:HA3	1:A:499:TYR:CD1	2.56	0.40
2:B:487:GLU:HA	2:B:490:GLN:CD	2.42	0.40
1:A:804:LEU:O	1:A:808:MET:HB2	2.22	0.40
2:B:687:VAL:HG13	2:B:706:LEU:HD11	2.04	0.40
1:A:134:LEU:C	1:A:136:ASP:H	2.25	0.40
1:A:567:LEU:HD13	1:A:571:LEU:HD11	2.03	0.40
1:A:775:SER:O	1:A:778:LYS:HD3	2.22	0.40

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	966/1092 (88%)	818 (85%)	105 (11%)	43 (4%)	4	32
2	B	230/302 (76%)	202 (88%)	20 (9%)	8 (4%)	6	41
All	All	1196/1394 (86%)	1020 (85%)	125 (10%)	51 (4%)	4	34

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	63	PHE
1	A	81	ALA
1	A	492	ASN
1	A	546	GLU
1	A	661	ASN
1	A	967	THR
2	B	709	PRO
2	B	711	ARG
1	A	135	LYS
1	A	198	GLU
1	A	322	ASP
1	A	324	ASN
1	A	663	ARG
1	A	746	ARG
1	A	753	GLN
1	A	787	ARG
1	A	863	ASN
1	A	869	ALA
1	A	885	GLY
1	A	966	LYS
2	B	447	TYR
2	B	705	THR
1	A	184	ASP
1	A	344	LYS
1	A	466	MET
1	A	942	LYS
1	A	970	THR
1	A	1009	LEU
2	B	636	GLY
2	B	703	THR
1	A	160	LEU
1	A	367	ILE
1	A	674	SER
1	A	700	MET
1	A	724	ALA
2	B	571	TYR
1	A	70	ASP
1	A	111	ASP
1	A	112	PRO
1	A	347	VAL
1	A	603	LEU
1	A	332	VAL

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Mol	Chain	Res	Type
1	A	539	ASP
1	A	679	PRO
2	B	641	ARG
1	A	471	GLY
1	A	490	PRO
1	A	767	VAL
1	A	725	VAL
1	A	363	VAL

### 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	871/976 (89%)	695 (80%)	176 (20%)	2	8
2	B	212/268 (79%)	167 (79%)	45 (21%)	1	7
All	All	1083/1244 (87%)	862 (80%)	221 (20%)	2	8

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	15	ASP
1	A	17	GLN
1	A	25	SER
1	A	26	VAL
1	A	43	GLU
1	A	45	THR
1	A	46	ILE
1	A	47	SER
1	A	53	LEU
1	A	54	TRP
1	A	63	PHE
1	A	69	ILE
1	A	73	MET
1	A	77	VAL
1	A	84	GLU
1	A	86	LEU

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Mol	Chain	Res	Type
1	A	89	GLU
1	A	90	THR
1	A	91	ARG
1	A	93	LEU
1	A	97	ARG
1	A	100	LEU
1	A	102	VAL
1	A	108	ARG
1	A	116	LEU
1	A	126	LYS
1	A	135	LYS
1	A	138	GLU
1	A	140	ASN
1	A	141	GLU
1	A	179	LEU
1	A	181	ASN
1	A	182	LEU
1	A	186	LEU
1	A	202	ASP
1	A	203	VAL
1	A	205	SER
1	A	207	GLN
1	A	215	ILE
1	A	224	LYS
1	A	226	LEU
1	A	238	CYS
1	A	241	VAL
1	A	244	VAL
1	A	248	VAL
1	A	257	LEU
1	A	268	MET
1	A	269	ASN
1	A	271	THR
1	A	276	ILE
1	A	277	LEU
1	A	280	CYS
1	A	291	MET
1	A	294	ILE
1	A	330	THR
1	A	331	LEU
1	A	336	LYS
1	A	341	GLU

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Mol	Chain	Res	Type
1	A	345	VAL
1	A	347	VAL
1	A	351	LEU
1	A	357	LEU
1	A	363	VAL
1	A	364	SER
1	A	377	GLU
1	A	385	ILE
1	A	388	LEU
1	A	390	ARG
1	A	394	LEU
1	A	435	VAL
1	A	446	LEU
1	A	450	ASP
1	A	455	SER
1	A	464	GLU
1	A	465	GLU
1	A	476	ASN
1	A	485	LEU
1	A	495	GLN
1	A	505	ILE
1	A	512	LEU
1	A	529	LEU
1	A	532	LEU
1	A	538	ARG
1	A	540	PRO
1	A	541	LEU
1	A	543	GLN
1	A	546	GLU
1	A	555	LEU
1	A	556	ARG
1	A	565	GLN
1	A	577	ASN
1	A	595	LEU
1	A	615	GLU
1	A	633	LEU
1	A	634	LEU
1	A	637	VAL
1	A	650	LEU
1	A	657	ARG
1	A	660	ASP
1	A	661	ASN

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Mol	Chain	Res	Type
1	A	663	ARG
1	A	668	LEU
1	A	674	SER
1	A	681	VAL
1	A	700	MET
1	A	701	LYS
1	A	710	LEU
1	A	712	LYS
1	A	719	LEU
1	A	731	LYS
1	A	736	MET
1	A	742	GLN
1	A	743	SER
1	A	747	GLU
1	A	752	LEU
1	A	753	GLN
1	A	761	ILE
1	A	765	LEU
1	A	768	GLU
1	A	776	LYS
1	A	778	LYS
1	A	780	LEU
1	A	781	TRP
1	A	787	ARG
1	A	796	VAL
1	A	803	ASP
1	A	805	ARG
1	A	806	GLN
1	A	808	MET
1	A	814	LEU
1	A	815	ARG
1	A	836	LEU
1	A	847	VAL
1	A	849	SER
1	A	853	THR
1	A	854	ILE
1	A	859	LEU
1	A	875	LEU
1	A	876	LEU
1	A	886	ASP
1	A	888	LEU
1	A	890	ARG

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Mol	Chain	Res	Type
1	A	896	THR
1	A	897	LEU
1	A	917	ASP
1	A	919	ILE
1	A	921	VAL
1	A	927	LEU
1	A	930	ILE
1	A	931	ASP
1	A	934	HIS
1	A	938	ASN
1	A	947	ARG
1	A	948	GLU
1	A	949	ARG
1	A	964	GLN
1	A	970	THR
1	A	973	PHE
1	A	995	ILE
1	A	1003	THR
1	A	1021	SER
1	A	1027	SER
1	A	1028	GLU
1	A	1032	LEU
1	A	1033	LYS
1	A	1034	GLN
1	A	1036	LYS
1	A	1037	GLN
1	A	1041	GLU
1	A	1046	SER
1	A	1048	THR
1	A	1050	LYS
1	A	1053	TRP
1	A	1054	MET
1	A	1057	THR
2	B	449	ASP
2	B	452	ARG
2	B	457	LEU
2	B	460	GLU
2	B	468	LEU
2	B	476	GLU
2	B	478	PHE
2	B	479	ASN
2	B	481	THR

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Mol	Chain	Res	Type
2	B	482	ILE
2	B	492	GLN
2	B	493	GLU
2	B	497	LYS
2	B	509	GLU
2	B	521	ARG
2	B	525	ARG
2	B	526	ILE
2	B	529	ILE
2	B	533	ARG
2	B	534	THR
2	B	538	GLN
2	B	543	GLN
2	B	546	ASP
2	B	550	ILE
2	B	561	LEU
2	B	572	LEU
2	B	622	ASN
2	B	638	PHE
2	B	639	LEU
2	B	641	ARG
2	B	644	SER
2	B	648	CYS
2	B	659	THR
2	B	661	HIS
2	B	664	ILE
2	B	666	ARG
2	B	667	THR
2	B	678	ASN
2	B	679	LEU
2	B	683	LEU
2	B	688	LEU
2	B	689	HIS
2	B	692	HIS
2	B	706	LEU
2	B	710	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	323	ASN

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Mol	Chain	Res	Type
1	A	325	ASN
1	A	445	GLN
1	A	476	ASN
1	A	557	GLN
1	A	590	GLN
1	A	635	GLN
1	A	638	GLN
1	A	661	ASN
1	A	737	HIS
1	A	860	ASN
1	A	871	ASN
1	A	929	HIS
1	A	960	HIS
2	B	518	ASN
2	B	530	HIS
2	B	538	GLN
2	B	543	GLN
2	B	622	ASN
2	B	625	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is 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	GD9	A	2058	-	40,40,40	1.81	9 (22%)	54,59,59	4.57	24 (44%)

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	GD9	A	2058	-	-	0/18/36/36	0/2/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2058	GD9	C6-C5	-4.32	1.31	1.35
3	A	2058	GD9	C17-N3	4.28	1.53	1.46
3	A	2058	GD9	C13-S2	3.68	1.83	1.75
3	A	2058	GD9	C5-S1	3.22	1.78	1.73
3	A	2058	GD9	C12-N4	2.88	1.54	1.47
3	A	2058	GD9	C23-N7	-2.72	1.28	1.33
3	A	2058	GD9	C14-N3	2.59	1.50	1.46
3	A	2058	GD9	C8-C3	-2.38	1.45	1.48
3	A	2058	GD9	C3-N1	-2.23	1.29	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2058	GD9	C23-N7-N6	27.63	112.02	104.27
3	A	2058	GD9	N1-C3-N2	-7.25	121.27	126.10
3	A	2058	GD9	O2-S2-N5	-5.63	101.26	106.98
3	A	2058	GD9	C4-N2-C3	5.57	125.48	116.16
3	A	2058	GD9	C5-C7-N4	-4.61	107.01	113.70
3	A	2058	GD9	C11-C12-N4	4.32	119.13	110.61
3	A	2058	GD9	C13-S2-N5	3.75	111.08	107.62
3	A	2058	GD9	C7-C5-S1	3.72	127.03	120.77
3	A	2058	GD9	C7-C5-C6	-3.70	120.19	126.87
3	A	2058	GD9	O1-S2-O2	3.68	123.82	118.68
3	A	2058	GD9	C12-N4-C9	3.64	117.90	108.86
3	A	2058	GD9	C3-N1-C2	3.52	118.88	116.25
3	A	2058	GD9	C16-C17-N3	3.44	116.64	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2058	GD9	C17-N3-C14	3.40	118.66	111.67
3	A	2058	GD9	C8-C22-C21	3.19	120.58	118.32
3	A	2058	GD9	C1-C4-N2	-2.71	114.36	120.67
3	A	2058	GD9	C7-N4-C12	2.71	115.77	111.07
3	A	2058	GD9	C6-C2-C1	2.64	112.19	110.48
3	A	2058	GD9	O1-S2-C13	-2.61	105.03	108.77
3	A	2058	GD9	N2-C4-N3	2.58	119.63	116.97
3	A	2058	GD9	O1-S2-N5	-2.41	104.53	106.98
3	A	2058	GD9	C15-C14-N3	2.29	114.44	110.05
3	A	2058	GD9	C11-N5-C10	2.29	114.99	112.16
3	A	2058	GD9	C10-C9-N4	2.09	114.74	110.61

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	976/1092 (89%)	0.12	7 (0%) 84 42	65, 116, 192, 219	0
2	B	236/302 (78%)	0.37	18 (7%) 14 4	80, 138, 215, 231	0
All	All	1212/1394 (86%)	0.17	25 (2%) 60 17	65, 119, 195, 231	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	THR	5.0
2	B	557	LEU	3.9
2	B	712	ALA	3.7
1	A	340	GLU	3.4
2	B	558	LYS	3.0
2	B	570	GLN	3.0
2	B	713	PRO	2.8
2	B	571	TYR	2.8
2	B	630	LEU	2.7
2	B	561	LEU	2.6
2	B	575	LEU	2.6
2	B	442	VAL	2.5
2	B	563	GLN	2.5
2	B	565	ARG	2.5
1	A	348	ARG	2.5
2	B	574	TRP	2.4
2	B	564	LEU	2.4
1	A	494	LYS	2.3
2	B	559	PRO	2.3
1	A	662	ARG	2.2
2	B	629	MET	2.2
1	A	1055	ALA	2.2
2	B	569	ASP	2.2
1	A	349	ALA	2.1

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
2	B	662	CYS	2.1

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

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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
3	GD9	A	2058	35/35	0.23	-0.34	67,97,129,130	0

## 6.5 Other polymers

There are no such residues in this entry.