



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2020 – 06:14 PM EDT

PDB ID : 6XAG
Title : Apo BRAF dimer bound to 14-3-3
Authors : Liao, N.P.D.; Hymowitz, S.G.; Sudhamsu, J.
Deposited on : 2020-06-04
Resolution : 3.30 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 2.14.6
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) : 2.14.6

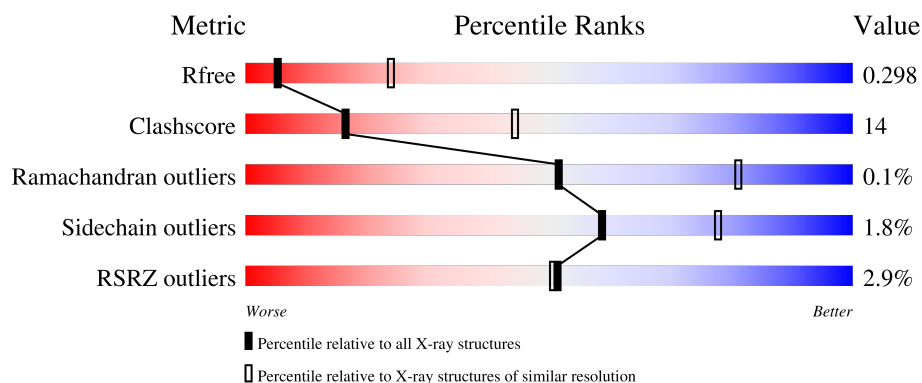
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	232	 73% 26% .
1	B	232	 7% 66% 29% . .
2	C	290	 % 68% 26% . 5%
2	D	290	 3% 71% 23% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8063 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 14-3-3 protein zeta/delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	1	0
			1843	1154	309	370	10			
1	B	223	Total	C	N	O	S	0	0	0
			1787	1121	302	354	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P63104
A	0	SER	-	expression tag	UNP P63104
B	-1	GLY	-	expression tag	UNP P63104
B	0	SER	-	expression tag	UNP P63104

- Molecule 2 is a protein called Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	276	Total	C	N	O	P S	0	0	0
			2202	1388	396	404	1 13			
2	D	278	Total	C	N	O	P S	0	0	0
			2227	1408	398	407	1 13			

There are 30 discrepancies between the modelled and reference sequences:

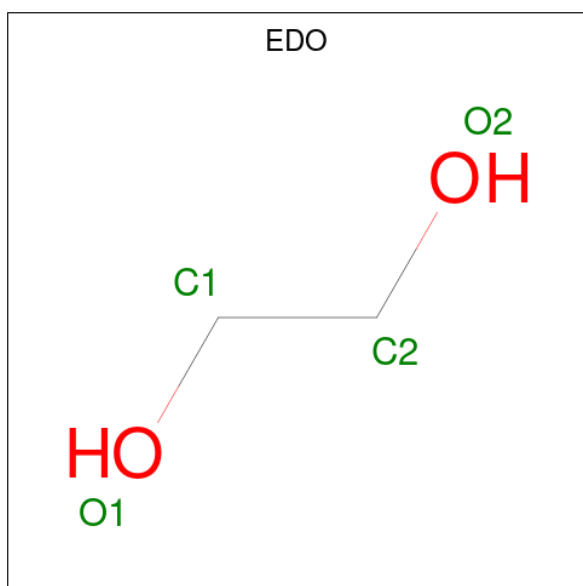
Chain	Residue	Modelled	Actual	Comment	Reference
C	446	GLY	-	expression tag	UNP P15056
C	543	ALA	ILE	conflict	UNP P15056
C	544	SER	ILE	conflict	UNP P15056
C	551	LYS	ILE	conflict	UNP P15056
C	562	ARG	GLN	conflict	UNP P15056
C	588	ASN	LEU	conflict	UNP P15056
C	630	SER	LYS	conflict	UNP P15056
C	667	GLU	PHE	conflict	UNP P15056

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	673	SER	TYR	conflict	UNP P15056
C	688	ARG	ALA	conflict	UNP P15056
C	706	SER	LEU	conflict	UNP P15056
C	709	ARG	GLN	conflict	UNP P15056
C	713	GLU	SER	conflict	UNP P15056
C	716	GLU	LEU	conflict	UNP P15056
C	720	GLU	SER	conflict	UNP P15056
D	446	GLY	-	expression tag	UNP P15056
D	543	ALA	ILE	conflict	UNP P15056
D	544	SER	ILE	conflict	UNP P15056
D	551	LYS	ILE	conflict	UNP P15056
D	562	ARG	GLN	conflict	UNP P15056
D	588	ASN	LEU	conflict	UNP P15056
D	630	SER	LYS	conflict	UNP P15056
D	667	GLU	PHE	conflict	UNP P15056
D	673	SER	TYR	conflict	UNP P15056
D	688	ARG	ALA	conflict	UNP P15056
D	706	SER	LEU	conflict	UNP P15056
D	709	ARG	GLN	conflict	UNP P15056
D	713	GLU	SER	conflict	UNP P15056
D	716	GLU	LEU	conflict	UNP P15056
D	720	GLU	SER	conflict	UNP P15056

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

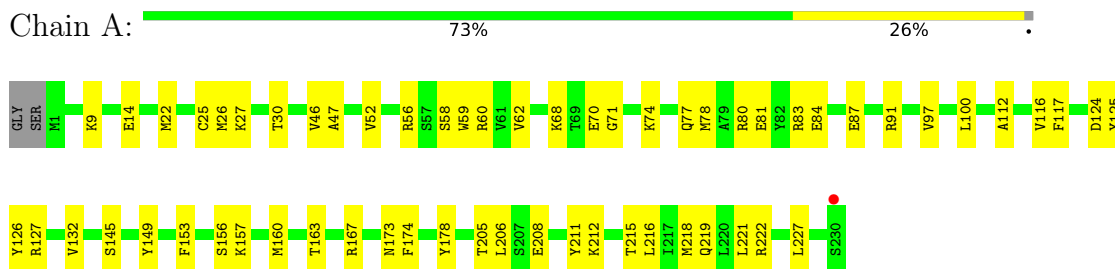


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		

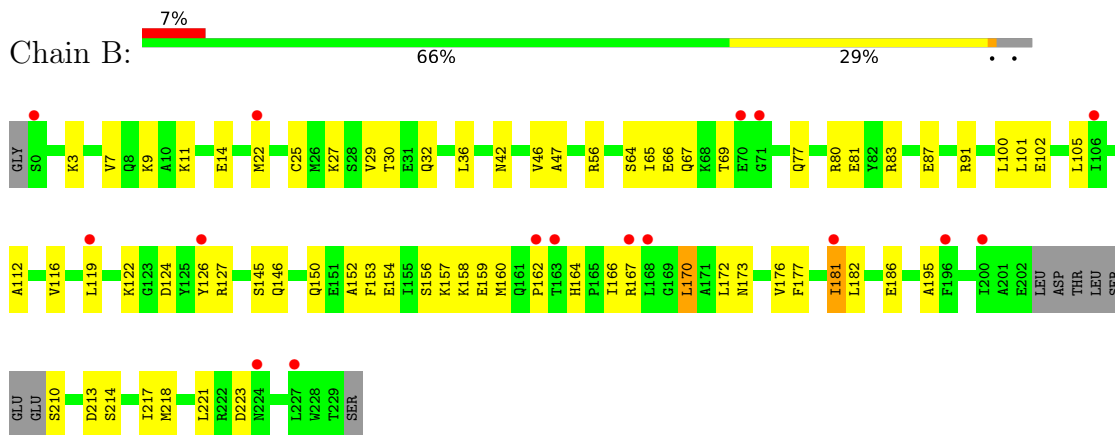
3 Residue-property plots

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.

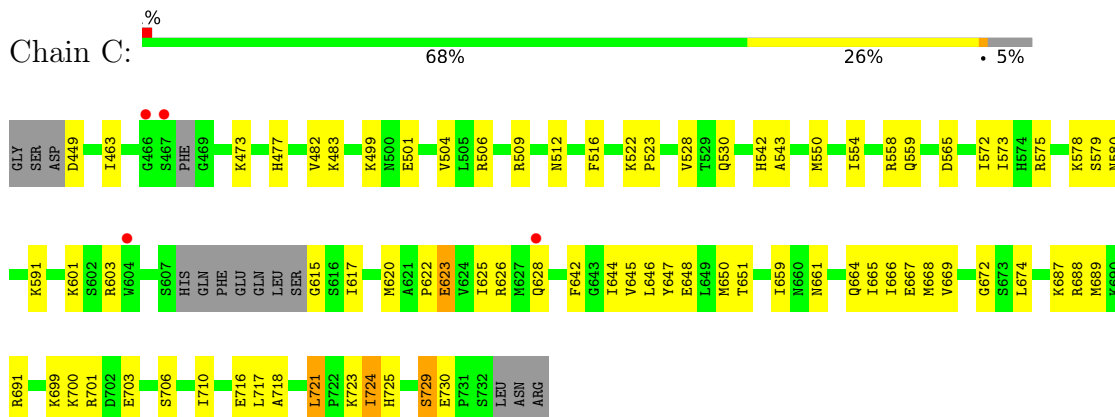
- Molecule 1: 14-3-3 protein zeta/delta



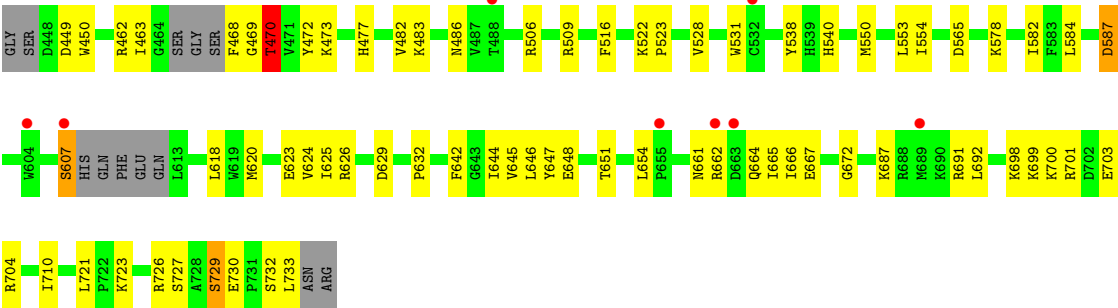
- Molecule 1: 14-3-3 protein zeta/delta



- Molecule 2: Serine/threonine-protein kinase B-raf



● Molecule 2: Serine/threonine-protein kinase B-raf



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.50Å 115.75Å 153.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.33 – 3.30 92.33 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.3 (92.33-3.30) 94.3 (92.33-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.17.1-3660_final	Depositor
R, R_{free}	0.250 , 0.300 0.249 , 0.298	Depositor DCC
R_{free} test set	658 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	109.6	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8063	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, SEP

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	0.27	0/1868	0.50	0/2510
1	B	0.34	0/1811	0.58	0/2432
2	C	0.35	0/2236	0.60	0/3010
2	D	0.31	0/2262	0.60	0/3046
All	All	0.32	0/8177	0.58	0/10998

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 [i](#)

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	1843	0	1825	43	0
1	B	1787	0	1782	60	0
2	C	2202	0	2217	77	0
2	D	2227	0	2243	74	0
3	D	4	0	6	2	0
All	All	8063	0	8073	231	0

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 14.

All (231) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:462:ARG:HB2	2:D:472:TYR:CE1	1.85	1.09
2:D:701:ARG:HA	2:D:704:ARG:NH2	1.72	1.04
2:D:462:ARG:HB2	2:D:472:TYR:HE1	1.33	0.92
2:C:625:ILE:HD13	2:C:669:VAL:HG21	1.55	0.88
1:B:66:GLU:OE2	1:B:80:ARG:HA	1.74	0.87
2:C:625:ILE:CD1	2:C:669:VAL:HG21	2.05	0.87
1:B:223:ASP:OD2	2:C:723:LYS:HG2	1.75	0.86
1:B:124:ASP:O	1:B:127:ARG:HB3	1.76	0.85
1:A:205:THR:O	1:A:205:THR:HG22	1.74	0.85
1:B:172:LEU:HD23	2:C:730:GLU:HB3	1.59	0.83
2:D:623:GLU:HB3	2:D:626:ARG:HH21	1.42	0.83
2:C:659:ILE:CD1	2:C:668:MET:HE1	2.08	0.83
1:B:223:ASP:HB3	2:C:724:ILE:HG13	1.59	0.83
2:D:462:ARG:HA	2:D:472:TYR:CD1	2.15	0.81
1:B:223:ASP:HB3	2:C:724:ILE:CG1	2.10	0.81
2:D:623:GLU:HA	2:D:626:ARG:HE	1.46	0.78
2:C:659:ILE:HD13	2:C:668:MET:CE	2.14	0.78
2:D:662:ARG:HH11	2:D:665:ILE:CD1	1.96	0.78
1:B:66:GLU:OE2	1:B:80:ARG:CA	2.32	0.78
2:C:625:ILE:HD13	2:C:669:VAL:CG2	2.14	0.78
2:D:462:ARG:CB	2:D:472:TYR:CE1	2.67	0.76
2:C:659:ILE:HD11	2:C:668:MET:HE1	1.68	0.75
1:B:122:LYS:HE3	1:B:126:TYR:HE2	1.50	0.74
2:C:463:ILE:HD11	2:C:473:LYS:HB2	1.70	0.74
1:A:160:MET:HE3	1:A:167:ARG:HB2	1.69	0.74
1:B:214:SER:HA	1:B:217:ILE:HG22	1.71	0.73
1:A:227:LEU:HG	2:D:723:LYS:HD2	1.69	0.72
2:D:662:ARG:NH1	2:D:665:ILE:HD13	2.03	0.72
1:B:223:ASP:OD2	2:C:723:LYS:CG	2.36	0.71
2:D:672:GLY:O	2:D:699:LYS:NZ	2.23	0.71
2:C:724:ILE:N	2:C:724:ILE:HD12	2.07	0.70
2:D:733:LEU:HD12	2:D:733:LEU:N	2.06	0.70
2:C:625:ILE:CD1	2:C:669:VAL:CG2	2.69	0.70
2:C:623:GLU:HG2	2:C:701:ARG:HD2	1.73	0.69
2:C:724:ILE:H	2:C:724:ILE:HD12	1.58	0.68
1:B:167:ARG:HD2	1:B:167:ARG:C	2.13	0.68
2:C:717:LEU:HD23	2:C:717:LEU:C	2.13	0.68
1:B:102:GLU:OE2	1:B:122:LYS:NZ	2.26	0.68
1:B:157:LYS:HG2	1:B:157:LYS:O	1.94	0.68
2:D:662:ARG:HH11	2:D:665:ILE:HD13	1.55	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ARG:HD2	1:B:167:ARG:O	1.94	0.68
2:C:721:LEU:C	2:C:721:LEU:HD12	2.15	0.67
1:A:205:THR:O	1:A:205:THR:CG2	2.44	0.66
2:D:662:ARG:HD2	2:D:665:ILE:HD12	1.77	0.66
2:D:700:LYS:O	2:D:703:GLU:HG2	1.95	0.66
2:C:717:LEU:HD23	2:C:717:LEU:O	1.95	0.66
2:D:462:ARG:CA	2:D:472:TYR:CD1	2.79	0.65
1:A:127:ARG:NH1	2:D:729:SEP:O1P	2.23	0.65
2:D:733:LEU:H	2:D:733:LEU:HD12	1.61	0.64
2:D:470:THR:HG21	2:D:486:ASN:ND2	2.12	0.64
2:D:620:MET:HE3	2:D:624:VAL:HG12	1.78	0.64
2:D:470:THR:OG1	2:D:472:TYR:CE2	2.51	0.63
1:B:127:ARG:NH2	2:C:729:SEP:O3P	2.33	0.62
2:D:661:ASN:OD1	2:D:664:GLN:HB2	1.99	0.62
2:C:622:PRO:O	2:C:626:ARG:HG3	2.00	0.62
1:A:173:ASN:HD21	2:D:729:SEP:HB3	1.64	0.62
2:C:659:ILE:HD13	2:C:668:MET:HE3	1.80	0.62
2:C:625:ILE:CG2	2:C:666:ILE:HG23	2.30	0.61
2:C:659:ILE:HD13	2:C:668:MET:HE1	1.78	0.61
2:C:659:ILE:CD1	2:C:668:MET:CE	2.74	0.61
1:B:153:PHE:O	1:B:156:SER:OG	2.20	0.60
1:B:116:VAL:HG11	1:B:160:MET:HE1	1.80	0.60
2:D:701:ARG:HA	2:D:704:ARG:HH21	1.65	0.60
1:A:27:LYS:HG3	1:A:100:LEU:HD11	1.83	0.60
2:D:642:PHE:O	2:D:646:LEU:HD13	2.02	0.60
2:D:623:GLU:CB	2:D:626:ARG:HH21	2.12	0.59
2:D:642:PHE:HA	2:D:645:VAL:HG12	1.84	0.59
1:B:22:MET:HG2	1:B:47:ALA:HB2	1.83	0.59
2:D:463:ILE:HD11	2:D:473:LYS:HB2	1.85	0.58
2:C:644:ILE:O	2:C:648:GLU:HG3	2.04	0.58
2:C:672:GLY:O	2:C:699:LYS:NZ	2.34	0.58
1:B:112:ALA:O	1:B:116:VAL:HG12	2.04	0.57
2:C:642:PHE:HA	2:C:645:VAL:HG12	1.86	0.57
1:B:56:ARG:HH12	2:C:729:SEP:P	2.27	0.57
2:C:724:ILE:CD1	2:C:724:ILE:H	2.16	0.57
1:A:153:PHE:CZ	1:A:157:LYS:HD2	2.39	0.57
2:C:509:ARG:HD3	2:D:516:PHE:O	2.05	0.57
2:C:687:LYS:HG2	2:C:691:ARG:HE	1.70	0.56
1:A:70:GLU:HG2	1:A:71:GLY:H	1.71	0.56
2:D:618:LEU:HD21	2:D:662:ARG:HH22	1.70	0.56
2:D:733:LEU:H	2:D:733:LEU:CD1	2.18	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:MET:HG2	1:A:47:ALA:HB2	1.87	0.56
1:A:30:THR:HG21	1:A:100:LEU:HD13	1.88	0.55
2:D:623:GLU:HB3	2:D:626:ARG:NH2	2.17	0.55
1:A:77:GLN:O	1:A:81:GLU:HG3	2.06	0.55
1:A:26:MET:O	1:A:30:THR:HG22	2.07	0.55
1:B:126:TYR:HB3	1:B:145:SER:HB2	1.89	0.55
1:B:87:GLU:HG2	1:B:91:ARG:CZ	2.38	0.54
1:A:112:ALA:O	1:A:116:VAL:HG12	2.08	0.54
2:D:506:ARG:HD2	3:D:801:EDO:O2	2.08	0.54
1:B:9:LYS:HD3	1:B:25:CYS:SG	2.48	0.54
2:C:573:ILE:HG22	2:C:575:ARG:HG2	1.90	0.54
1:B:223:ASP:CB	2:C:724:ILE:HG13	2.32	0.54
2:D:662:ARG:NH1	2:D:665:ILE:CD1	2.66	0.53
1:B:162:PRO:HA	1:B:167:ARG:HH21	1.73	0.53
2:C:506:ARG:HD2	3:D:801:EDO:H11	1.90	0.53
1:B:181:ILE:HG22	1:B:182:LEU:HD12	1.90	0.53
1:A:56:ARG:O	1:A:60:ARG:HG3	2.08	0.53
2:C:623:GLU:HA	2:C:626:ARG:CZ	2.39	0.53
1:A:173:ASN:ND2	2:D:729:SEP:HB3	2.22	0.53
2:C:477:HIS:ND1	2:D:565:ASP:OD2	2.30	0.53
2:D:624:VAL:HA	2:D:632:PRO:HB2	1.90	0.53
2:C:516:PHE:O	2:D:509:ARG:HD3	2.08	0.52
1:A:60:ARG:HD3	2:D:726:ARG:CZ	2.39	0.52
2:C:482:VAL:HG12	2:C:528:VAL:HG12	1.90	0.52
2:C:724:ILE:O	2:C:724:ILE:HD13	2.09	0.52
2:D:733:LEU:CD1	2:D:733:LEU:N	2.73	0.52
2:D:701:ARG:CA	2:D:704:ARG:NH2	2.60	0.52
1:A:74:LYS:O	1:A:78:MET:HG3	2.10	0.52
1:B:64:SER:HA	1:B:67:GLN:HG2	1.92	0.51
2:C:688:ARG:HH22	2:C:716:GLU:HB3	1.75	0.51
2:C:578:LYS:HE3	2:C:580:ASN:HB3	1.93	0.51
1:B:223:ASP:HB3	2:C:724:ILE:HG12	1.93	0.51
1:B:172:LEU:O	1:B:176:VAL:HG13	2.11	0.51
2:C:625:ILE:HG23	2:C:666:ILE:HG23	1.93	0.51
1:B:146:GLN:HB2	1:B:177:PHE:CE2	2.46	0.51
1:B:172:LEU:HD23	2:C:730:GLU:CB	2.38	0.51
2:D:522:LYS:HB3	2:D:523:PRO:HD3	1.93	0.51
2:D:625:ILE:HD12	2:D:666:ILE:HG23	1.92	0.51
1:A:14:GLU:HB2	1:A:22:MET:SD	2.51	0.51
2:C:642:PHE:CZ	2:C:646:LEU:HD11	2.46	0.51
2:D:463:ILE:HD13	2:D:531:TRP:HH2	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:O	1:A:56:ARG:HG3	2.10	0.50
2:D:470:THR:O	2:D:470:THR:OG1	2.30	0.50
2:C:579:SER:HB3	2:C:648:GLU:OE1	2.11	0.50
2:D:664:GLN:O	2:D:667:GLU:N	2.45	0.50
2:C:522:LYS:HB3	2:C:523:PRO:HD3	1.93	0.50
2:D:470:THR:OG1	2:D:472:TYR:HE2	1.94	0.50
2:D:550:MET:O	2:D:554:ILE:HG12	2.12	0.50
1:B:3:LYS:HB2	1:B:32:GLN:OE1	2.11	0.50
2:C:700:LYS:O	2:C:703:GLU:HG2	2.11	0.49
2:C:626:ARG:HE	2:C:628:GLN:CD	2.16	0.49
1:B:162:PRO:O	1:B:167:ARG:NH2	2.46	0.49
1:B:27:LYS:HG3	1:B:100:LEU:HD21	1.93	0.49
2:D:692:LEU:HD21	2:D:710:ILE:HG23	1.95	0.49
1:B:116:VAL:HG11	1:B:160:MET:CE	2.43	0.49
1:B:116:VAL:HG23	1:B:152:ALA:HB1	1.93	0.49
1:A:216:LEU:HB2	2:C:543:ALA:O	2.13	0.49
2:C:550:MET:O	2:C:554:ILE:HG12	2.12	0.49
1:B:150:GLN:O	1:B:154:GLU:HG2	2.12	0.49
2:C:659:ILE:HD12	2:C:674:LEU:CD2	2.43	0.49
1:B:30:THR:HG22	1:B:36:LEU:HD11	1.95	0.48
2:C:642:PHE:O	2:C:646:LEU:HD13	2.12	0.48
1:A:219:GLN:HE22	1:A:222:ARG:NH2	2.11	0.48
2:D:607:SER:O	2:D:607:SER:OG	2.26	0.48
2:D:587:ASP:N	2:D:587:ASP:OD1	2.47	0.47
1:A:80:ARG:HG3	1:A:83:ARG:HH21	1.80	0.47
2:C:565:ASP:OD2	2:D:477:HIS:ND1	2.32	0.47
1:B:14:GLU:HB2	1:B:22:MET:SD	2.54	0.47
1:B:77:GLN:OE1	1:B:80:ARG:NH2	2.47	0.47
1:B:164:HIS:CE1	1:B:166:ILE:HB	2.50	0.47
2:C:661:ASN:OD1	2:C:664:GLN:HB3	2.14	0.47
2:C:573:ILE:HD11	2:C:601:LYS:HB2	1.96	0.47
2:C:623:GLU:CD	2:C:701:ARG:HG2	2.36	0.47
2:D:662:ARG:HH11	2:D:665:ILE:HD12	1.76	0.46
1:B:119:LEU:O	1:B:122:LYS:HB3	2.16	0.46
1:B:214:SER:HB3	1:B:218:MET:CE	2.45	0.46
1:A:124:ASP:OD1	1:A:149:TYR:OH	2.25	0.46
2:D:482:VAL:HG12	2:D:528:VAL:HG12	1.97	0.46
2:C:688:ARG:HB2	2:C:717:LEU:HD12	1.97	0.46
1:B:42:ASN:O	1:B:46:VAL:HG23	2.16	0.45
2:D:687:LYS:HG2	2:D:691:ARG:HE	1.81	0.45
2:D:468:PHE:HB3	2:D:483:LYS:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:665:ILE:O	2:C:669:VAL:HG13	2.16	0.45
1:A:156:SER:HB2	1:A:167:ARG:HG3	1.98	0.45
2:C:483:LYS:NZ	2:C:501:GLU:OE1	2.41	0.45
2:C:625:ILE:HD12	2:C:669:VAL:CG2	2.44	0.45
1:A:163:THR:HB	1:A:206:LEU:HD11	1.98	0.45
1:B:210:SER:HA	1:B:213:ASP:HB2	1.98	0.45
2:D:463:ILE:HD13	2:D:531:TRP:CH2	2.52	0.45
2:D:644:ILE:O	2:D:648:GLU:HG3	2.17	0.45
1:B:77:GLN:O	1:B:81:GLU:HG3	2.16	0.45
1:A:87:GLU:HG2	1:A:91:ARG:NH1	2.32	0.45
2:C:620:MET:HE2	2:C:620:MET:HB3	1.83	0.45
1:B:101:LEU:HA	1:B:105:LEU:HD12	1.98	0.44
2:C:530:GLN:HE22	2:C:591:LYS:HE3	1.82	0.44
2:D:623:GLU:HA	2:D:626:ARG:NE	2.24	0.44
1:B:124:ASP:OD1	1:B:173:ASN:ND2	2.50	0.44
2:D:449:ASP:OD1	2:D:450:TRP:N	2.49	0.44
1:A:208:GLU:O	1:A:212:LYS:HG3	2.18	0.44
1:B:66:GLU:O	1:B:69:THR:HG23	2.18	0.44
2:D:698:LYS:HB2	2:D:703:GLU:HG3	1.99	0.44
1:B:218:MET:HA	1:B:221:LEU:HD12	2.00	0.44
1:B:83:ARG:NH1	1:B:87:GLU:OE1	2.52	0.43
2:C:449:ASP:N	2:C:449:ASP:OD1	2.51	0.43
1:A:9:LYS:HE2	1:A:25:CYS:SG	2.58	0.43
1:B:77:GLN:NE2	1:B:80:ARG:HH12	2.17	0.43
2:C:615:GLY:O	2:C:617:ILE:HG23	2.19	0.43
2:C:706:SER:O	2:C:710:ILE:HG13	2.18	0.43
2:D:647:TYR:CZ	2:D:651:THR:HG21	2.54	0.43
1:A:212:LYS:HD3	2:C:542:HIS:O	2.18	0.43
2:C:499:LYS:HD3	2:C:499:LYS:HA	1.78	0.43
1:A:126:TYR:HB3	1:A:145:SER:HB2	2.00	0.43
2:D:462:ARG:CA	2:D:472:TYR:CE1	3.01	0.43
1:A:68:LYS:NZ	1:A:68:LYS:HB3	2.34	0.42
2:D:698:LYS:HB3	2:D:703:GLU:OE2	2.19	0.42
2:D:698:LYS:CB	2:D:703:GLU:HG3	2.49	0.42
2:C:512:ASN:ND2	2:C:559:GLN:HB3	2.34	0.42
2:D:623:GLU:CA	2:D:626:ARG:HH21	2.31	0.42
2:D:578:LYS:O	2:D:582:ILE:HG13	2.20	0.42
1:A:173:ASN:HD21	2:D:730:GLU:H	1.67	0.42
1:A:211:TYR:CZ	1:A:215:THR:HG21	2.55	0.42
2:C:504:VAL:HG13	2:C:572:ILE:HD13	2.02	0.42
2:C:667:GLU:HG3	2:C:667:GLU:H	1.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TRP:CE2	1:A:132:VAL:HG12	2.54	0.42
2:C:647:TYR:O	2:C:651:THR:HG23	2.20	0.41
1:B:7:VAL:HG12	1:B:11:LYS:HE3	2.03	0.41
2:D:538:TYR:HE1	2:D:654:LEU:HD21	1.86	0.41
1:A:211:TYR:CE1	1:A:215:THR:HG21	2.55	0.41
2:C:650:MET:CE	2:C:689:MET:HG2	2.50	0.41
2:D:550:MET:HA	2:D:553:LEU:HD12	2.01	0.41
1:A:58:SER:O	1:A:62:VAL:HG13	2.20	0.41
1:B:66:GLU:OE2	1:B:80:ARG:N	2.53	0.41
2:D:468:PHE:HB3	2:D:469:GLY:H	1.55	0.41
1:A:70:GLU:HG2	1:A:71:GLY:N	2.34	0.41
1:B:158:LYS:HG2	1:B:159:GLU:CD	2.41	0.41
2:C:659:ILE:HD12	2:C:674:LEU:HD21	2.02	0.41
1:A:46:VAL:HG22	2:D:732:SER:HB2	2.02	0.41
1:B:170:LEU:HD12	1:B:170:LEU:O	2.20	0.41
1:A:80:ARG:O	1:A:84:GLU:HG3	2.20	0.41
1:A:218:MET:HA	1:A:221:LEU:HD12	2.03	0.41
2:C:558:ARG:NH1	2:C:718:ALA:HB1	2.36	0.41
1:B:167:ARG:NH1	1:B:195:ALA:HB1	2.36	0.40
1:B:29:VAL:O	1:B:32:GLN:HB2	2.21	0.40
1:B:146:GLN:HB2	1:B:177:PHE:HE2	1.85	0.40
2:C:601:LYS:NZ	2:C:603:ARG:HA	2.36	0.40
2:D:540:HIS:CD2	2:D:584:LEU:HD22	2.56	0.40
1:B:67:GLN:CA	1:B:67:GLN:OE1	2.69	0.40
1:A:97:VAL:HG11	1:A:125:TYR:CE2	2.57	0.40
2:D:620:MET:HE2	2:D:625:ILE:HD13	2.02	0.40

There are no symmetry-related clashes.

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	228/232 (98%)	224 (98%)	4 (2%)	0	100	100
1	B	219/232 (94%)	208 (95%)	11 (5%)	0	100	100
2	C	269/290 (93%)	256 (95%)	13 (5%)	0	100	100
2	D	271/290 (93%)	257 (95%)	13 (5%)	1 (0%)	34	66
All	All	987/1044 (94%)	945 (96%)	41 (4%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	470	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	200/201 (100%)	198 (99%)	2 (1%)	76	86
1	B	193/201 (96%)	189 (98%)	4 (2%)	53	75
2	C	241/254 (95%)	237 (98%)	4 (2%)	60	78
2	D	244/254 (96%)	238 (98%)	6 (2%)	47	72
All	All	878/910 (96%)	862 (98%)	16 (2%)	59	78

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	PHE
1	A	174	PHE
1	B	65	ILE
1	B	170	LEU
1	B	181	ILE
1	B	186	GLU
2	C	623	GLU
2	C	721	LEU
2	C	724	ILE
2	C	725	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	470	THR
2	D	587	ASP
2	D	607	SER
2	D	629	ASP
2	D	721	LEU
2	D	727	SER

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

Mol	Chain	Res	Type
2	D	486	ASN
2	D	524	GLN
2	D	725	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	SEP	C	729	2	8,9,10	0.88	0	8,12,14	1.43	1 (12%)
2	SEP	D	729	2	8,9,10	1.29	2 (25%)	8,12,14	2.36	1 (12%)

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	SEP	C	729	2	-	1/5/8/10	-
2	SEP	D	729	2	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	729	SEP	P-O2P	-2.21	1.46	1.54
2	D	729	SEP	P-O3P	-2.13	1.46	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	729	SEP	OG-CB-CA	6.05	114.04	108.14
2	C	729	SEP	OG-CB-CA	2.57	110.64	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	729	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	729	SEP	2	0
2	D	729	SEP	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	EDO	D	801	-	3,3,3	0.18	0	2,2,2	1.08	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	EDO	D	801	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	801	EDO	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	230/232 (99%)	0.05	1 (0%) 92 93	69, 111, 168, 244	0
1	B	223/232 (96%)	0.41	16 (7%) 15 15	97, 157, 219, 288	0
2	C	275/290 (94%)	0.20	4 (1%) 73 72	76, 115, 191, 256	0
2	D	277/290 (95%)	0.27	8 (2%) 51 50	76, 128, 199, 266	0
All	All	1005/1044 (96%)	0.23	29 (2%) 51 50	69, 126, 204, 288	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	467	SER	6.2
1	A	230	SER	5.2
1	B	162	PRO	5.0
1	B	0	SER	4.2
1	B	71	GLY	4.2
2	D	662	ARG	3.9
2	D	488	THR	3.7
1	B	163	THR	3.5
2	C	628	GLN	2.9
1	B	227	LEU	2.9
1	B	181	ILE	2.8
1	B	200	ILE	2.8
2	D	663	ASP	2.7
2	D	532	CYS	2.6
1	B	167	ARG	2.6
2	C	466	GLY	2.6
1	B	196	PHE	2.5
2	D	604	TRP	2.5
1	B	22	MET	2.4
1	B	119	LEU	2.3
2	C	604	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	106	ILE	2.1
2	D	689	MET	2.1
1	B	168	LEU	2.1
1	B	126	TYR	2.1
2	D	655	PRO	2.1
2	D	607	SER	2.1
1	B	224	ASN	2.0
1	B	70	GLU	2.0

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, 95th 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 ²)	Q<0.9
2	SEP	C	729	10/11	0.89	0.17	136,144,156,158	0
2	SEP	D	729	10/11	0.95	0.15	85,88,90,91	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, 95th 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 ²)	Q<0.9
3	EDO	D	801	4/4	0.94	0.39	74,75,76,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.