



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:16 pm GMT

PDB ID : 1A37  
Title : 14-3-3 PROTEIN ZETA BOUND TO PS-RAF259 PEPTIDE  
Authors : Petosa, C.; Masters, S.C.; Pohl, J.; Wang, B.; Fu, H.; Liddington, R.C.  
Deposited on : 1998-01-28  
Resolution : 3.60 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:

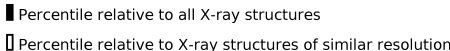
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

**i**

## X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.



<b>Metric</b>	<b>Whole archive (#Entries)</b>	<b>Similar resolution (#Entries, resolution range(Å))</b>
R <sub>free</sub>	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	245	
1	B	245	
2	P	15	
2	Q	15	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3194 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1563	984	265	305	9			
1	B	195	Total	C	N	O	S	0	0	0
			1563	984	265	305	9			

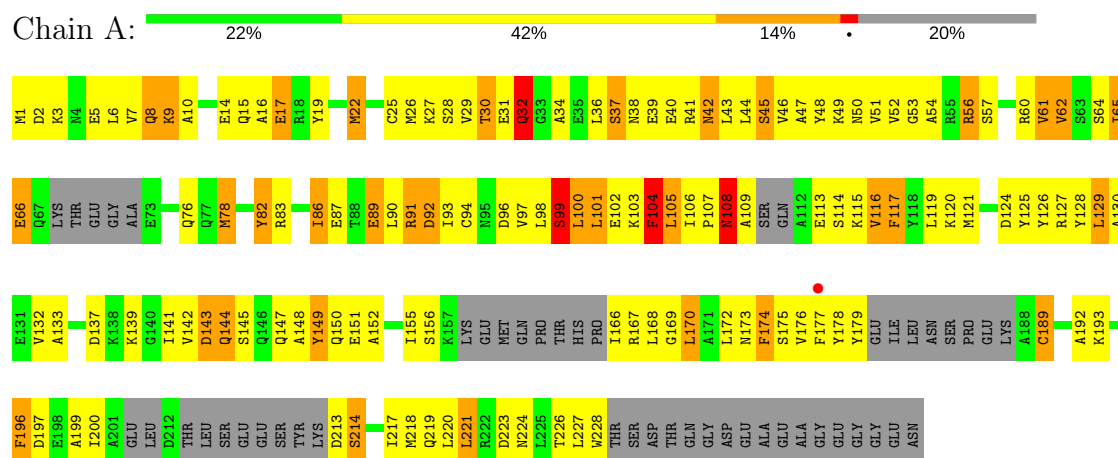
- Molecule 2 is a protein called PS-RAF259 PEPTIDE LSQRQRST(SEP)TPNVHM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	P	4	0	0
			34	15	7	11	1			
2	Q	7	Total	C	N	O	P	4	0	0
			34	15	7	11	1			

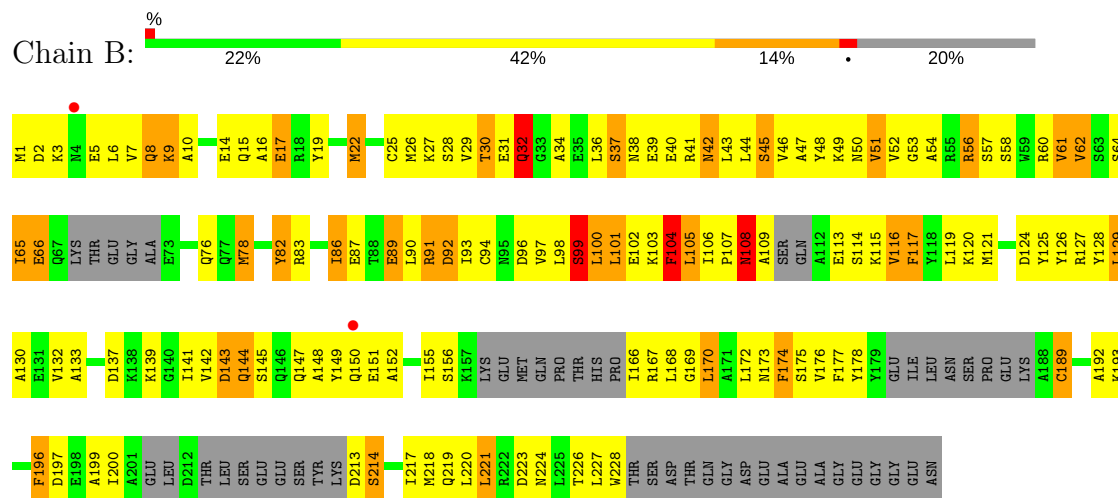
### 3 Residue-property plots

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



#### • Molecule 1: 14-3-3 PROTEIN ZETA



#### • Molecule 2: PS-RAF259 PEPTIDE LSQRQRST(SEP)TPNVHM



● Molecule 2: PS-RAF259 PEPTIDE LSQRQRST(SEP)TPNVHM

Chain Q:  13% 33% 53%

LYS	SER	GLN	ARG	GLN	R256	S257	T258	S259	T260	P261	N262	VAL	HIS	MET
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.73Å 94.73Å 250.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.60 38.99 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.60) 93.1 (38.99-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 3.32Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.320 , 0.360 0.316 , 0.341	Depositor DCC
$R_{free}$ test set	1462 reflections (11.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.5	Xtriage
Anisotropy	0.904	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.115 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	3194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.56% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.65	0/1578	0.91	1/2111 (0.0%)
1	B	0.65	0/1578	0.91	1/2111 (0.0%)
2	P	0.77	0/22	1.24	0/24
2	Q	0.77	0/22	1.24	0/24
All	All	0.66	0/3200	0.91	2/4270 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	GLN	N-CA-C	-6.05	94.66	111.00
1	B	32	GLN	N-CA-C	-6.05	94.66	111.00

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	1563	0	1558	151	0
1	B	1563	0	1558	149	0
2	P	34	0	7	1	0
2	Q	34	0	7	1	0
All	All	3194	0	3130	296	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 47.

All (296) 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:22:MET:SD	1:A:47:ALA:HB2	2.09	0.93
1:B:22:MET:SD	1:B:47:ALA:HB2	2.09	0.93
1:A:46:VAL:HA	1:A:49:LYS:HG2	1.63	0.79
1:B:46:VAL:HA	1:B:49:LYS:HG2	1.63	0.78
1:A:15:GLN:O	1:B:61:VAL:HG21	1.83	0.78
1:A:94:CYS:SG	1:A:129:LEU:HD11	2.24	0.78
1:B:94:CYS:SG	1:B:129:LEU:HD11	2.24	0.77
1:A:92:ASP:O	1:A:96:ASP:HB2	1.84	0.77
1:B:94:CYS:SG	1:B:129:LEU:CD1	2.73	0.77
1:B:92:ASP:O	1:B:96:ASP:HB2	1.85	0.77
1:B:101:LEU:HA	1:B:105:LEU:HB2	1.66	0.76
1:A:101:LEU:HA	1:A:105:LEU:HB2	1.66	0.76
1:A:94:CYS:SG	1:A:129:LEU:CD1	2.73	0.76
1:A:48:TYR:O	1:A:52:VAL:HG12	1.86	0.75
1:B:48:TYR:O	1:B:52:VAL:HG12	1.86	0.74
1:B:172:LEU:O	1:B:175:SER:HB3	1.87	0.73
1:A:223:ASP:O	1:A:226:THR:HB	1.89	0.73
1:A:172:LEU:O	1:A:175:SER:HB3	1.87	0.73
1:B:223:ASP:O	1:B:226:THR:HB	1.89	0.73
1:B:30:THR:HG21	1:B:100:LEU:HD23	1.71	0.72
1:A:87:GLU:HG3	1:A:132:VAL:CG1	2.20	0.71
1:A:30:THR:HG21	1:A:100:LEU:HD23	1.71	0.71
1:B:87:GLU:HG3	1:B:132:VAL:CG1	2.20	0.70
1:A:61:VAL:HG21	1:B:15:GLN:O	1.91	0.70
1:B:214:SER:O	1:B:218:MET:HG3	1.92	0.70
1:A:89:GLU:O	1:A:93:ILE:HG12	1.92	0.70
1:A:214:SER:O	1:A:218:MET:HG3	1.92	0.69
1:B:89:GLU:O	1:B:93:ILE:HG12	1.92	0.69
1:B:223:ASP:O	1:B:227:LEU:HG	1.93	0.68
1:A:221:LEU:H	1:A:221:LEU:HD23	1.59	0.68
1:B:221:LEU:HD23	1:B:221:LEU:H	1.59	0.68
1:A:124:ASP:O	1:A:127:ARG:HB3	1.94	0.67
1:A:223:ASP:O	1:A:227:LEU:HG	1.93	0.67
1:B:38:ASN:OD1	1:B:41:ARG:HD3	1.94	0.67
1:B:124:ASP:O	1:B:127:ARG:HB3	1.94	0.67
1:B:166:ILE:HG23	1:B:167:ARG:H	1.60	0.66
1:A:38:ASN:OD1	1:A:41:ARG:HD3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:SER:HB2	1:B:167:ARG:HG3	1.77	0.66
1:B:22:MET:SD	1:B:47:ALA:CB	2.83	0.66
1:A:48:TYR:CE2	1:A:97:VAL:HB	2.31	0.66
1:B:48:TYR:CE2	1:B:97:VAL:HB	2.31	0.66
1:A:93:ILE:O	1:A:97:VAL:HG12	1.97	0.65
1:A:87:GLU:HG2	1:A:91:ARG:NH2	2.12	0.65
1:A:121:MET:O	1:A:124:ASP:HB2	1.97	0.65
1:A:166:ILE:HG23	1:A:167:ARG:H	1.60	0.65
1:A:22:MET:SD	1:A:47:ALA:CB	2.84	0.65
1:B:87:GLU:HG2	1:B:91:ARG:NH2	2.12	0.65
1:B:93:ILE:O	1:B:97:VAL:HG12	1.97	0.64
1:A:156:SER:HB2	1:A:167:ARG:HG3	1.77	0.64
1:A:114:SER:O	1:A:117:PHE:HB3	1.97	0.64
1:B:114:SER:O	1:B:117:PHE:HB3	1.97	0.64
1:B:121:MET:O	1:B:124:ASP:HB2	1.97	0.64
1:A:139:LYS:O	1:A:142:VAL:HG12	1.97	0.64
1:B:217:ILE:O	1:B:221:LEU:HD23	1.98	0.64
1:A:217:ILE:O	1:A:221:LEU:HD23	1.98	0.64
1:A:31:GLU:HA	1:A:104:PHE:CZ	2.33	0.64
1:B:139:LYS:O	1:B:142:VAL:HG12	1.97	0.63
1:B:31:GLU:HA	1:B:104:PHE:CZ	2.33	0.62
1:A:217:ILE:O	1:A:220:LEU:HB2	2.00	0.62
1:A:39:GLU:O	1:A:43:LEU:HD13	2.00	0.62
1:B:39:GLU:O	1:B:43:LEU:HD13	2.00	0.62
1:B:217:ILE:O	1:B:220:LEU:HB2	2.00	0.61
1:B:98:LEU:O	1:B:102:GLU:HG3	2.01	0.61
1:B:174:PHE:CD1	1:B:178:TYR:HE1	2.19	0.61
1:B:46:VAL:HG23	1:B:49:LYS:CE	2.31	0.61
1:A:98:LEU:O	1:A:102:GLU:HG3	2.01	0.61
1:B:52:VAL:HG11	1:B:125:TYR:HE1	1.66	0.61
1:A:46:VAL:HG23	1:A:49:LYS:CE	2.31	0.60
1:A:174:PHE:CD1	1:A:178:TYR:HE1	2.19	0.60
1:A:119:LEU:HB3	1:A:152:ALA:HB2	1.82	0.60
1:A:52:VAL:HG11	1:A:125:TYR:HE1	1.66	0.60
1:B:90:LEU:HD21	1:B:132:VAL:HG21	1.83	0.60
1:B:46:VAL:HG23	1:B:49:LYS:HE2	1.84	0.60
1:A:94:CYS:SG	1:A:129:LEU:HD13	2.42	0.60
1:A:90:LEU:HD21	1:A:132:VAL:HG21	1.83	0.60
1:B:119:LEU:HB3	1:B:152:ALA:HB2	1.82	0.59
1:A:46:VAL:HG23	1:A:49:LYS:HE2	1.84	0.59
1:A:87:GLU:O	1:A:90:LEU:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:GLY:O	1:B:172:LEU:HB3	2.03	0.59
1:A:147:GLN:O	1:A:151:GLU:HB2	2.02	0.59
1:B:147:GLN:O	1:B:151:GLU:HB2	2.02	0.59
1:B:87:GLU:O	1:B:90:LEU:HB3	2.02	0.59
1:A:127:ARG:HH22	2:P:259:SEP:P	2.25	0.59
1:A:169:GLY:O	1:A:172:LEU:HB3	2.03	0.59
1:A:27:LYS:O	1:A:31:GLU:HG2	2.03	0.58
1:B:100:LEU:O	1:B:104:PHE:HB2	2.03	0.58
1:B:27:LYS:O	1:B:31:GLU:HG2	2.03	0.58
1:A:126:TYR:CE2	1:A:144:GLN:HB3	2.38	0.58
1:B:127:ARG:HH22	2:Q:259:SEP:P	2.26	0.58
1:A:100:LEU:O	1:A:104:PHE:HB2	2.03	0.58
1:B:126:TYR:CE2	1:B:144:GLN:HB3	2.38	0.58
1:B:94:CYS:SG	1:B:129:LEU:HD13	2.42	0.58
1:B:14:GLU:C	1:B:16:ALA:H	2.08	0.57
1:A:14:GLU:C	1:A:16:ALA:H	2.08	0.57
1:B:106:ILE:HG13	1:B:107:PRO:HD3	1.86	0.57
1:B:128:TYR:O	1:B:132:VAL:HG23	2.04	0.57
1:A:196:PHE:CZ	1:A:200:ILE:HD11	2.40	0.56
1:B:98:LEU:HD11	1:B:126:TYR:CE1	2.40	0.56
1:B:150:GLN:HA	1:B:174:PHE:CE2	2.41	0.56
1:A:106:ILE:HG13	1:A:107:PRO:HD3	1.86	0.56
1:A:109:ALA:CB	1:A:115:LYS:HG3	2.36	0.56
1:A:128:TYR:O	1:A:132:VAL:HG23	2.04	0.56
1:B:196:PHE:CZ	1:B:200:ILE:HD11	2.40	0.56
1:A:98:LEU:HD11	1:A:126:TYR:CE1	2.40	0.56
1:B:109:ALA:CB	1:B:115:LYS:HG3	2.36	0.56
1:A:26:MET:HB3	1:A:44:LEU:CD1	2.36	0.55
1:B:57:SER:O	1:B:60:ARG:HB2	2.07	0.55
1:A:9:LYS:HG2	1:B:78:MET:SD	2.47	0.55
1:A:193:LYS:HA	1:A:196:PHE:HD2	1.71	0.55
1:A:150:GLN:HA	1:A:174:PHE:CE2	2.41	0.55
1:A:174:PHE:O	1:A:177:PHE:HB3	2.07	0.55
1:B:193:LYS:HA	1:B:196:PHE:HD2	1.71	0.55
1:B:26:MET:HB3	1:B:44:LEU:CD1	2.36	0.55
1:B:196:PHE:HB2	1:B:221:LEU:HD12	1.89	0.55
1:A:57:SER:O	1:A:60:ARG:HB2	2.07	0.55
1:A:196:PHE:HB2	1:A:221:LEU:HD12	1.89	0.55
1:A:196:PHE:CG	1:A:197:ASP:N	2.76	0.54
1:B:174:PHE:O	1:B:177:PHE:HB3	2.07	0.54
1:B:196:PHE:CG	1:B:197:ASP:N	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:MET:SD	1:B:9:LYS:HG2	2.49	0.53
1:A:150:GLN:HA	1:A:174:PHE:HE2	1.74	0.53
1:B:127:ARG:O	1:B:130:ALA:HB3	2.09	0.53
1:B:150:GLN:HA	1:B:174:PHE:HE2	1.73	0.53
1:B:117:PHE:O	1:B:120:LYS:HB3	2.09	0.52
1:A:196:PHE:CE1	1:A:200:ILE:HD11	2.45	0.52
1:B:41:ARG:HG2	1:B:117:PHE:HE2	1.75	0.52
1:A:117:PHE:O	1:A:120:LYS:HB3	2.09	0.52
1:A:127:ARG:O	1:A:130:ALA:HB3	2.09	0.52
1:B:174:PHE:CE1	1:B:178:TYR:CE1	2.98	0.51
1:A:174:PHE:CE1	1:A:178:TYR:CE1	2.98	0.51
1:B:196:PHE:CE1	1:B:200:ILE:HD11	2.45	0.51
1:A:41:ARG:HG2	1:A:117:PHE:HE2	1.75	0.51
1:B:113:GLU:O	1:B:116:VAL:HG23	2.11	0.51
1:A:26:MET:HB3	1:A:44:LEU:HD13	1.93	0.51
1:B:109:ALA:HB1	1:B:115:LYS:HG3	1.94	0.50
1:B:224:ASN:HB3	1:B:228:TRP:CZ3	2.47	0.50
1:A:98:LEU:HD11	1:A:126:TYR:CD1	2.46	0.50
1:A:113:GLU:O	1:A:116:VAL:HG23	2.11	0.50
1:A:167:ARG:O	1:A:170:LEU:HB3	2.12	0.50
1:A:224:ASN:HB3	1:A:228:TRP:CZ3	2.47	0.50
1:B:167:ARG:O	1:B:170:LEU:HB3	2.12	0.50
1:B:10:ALA:HB2	1:B:25:CYS:HB3	1.94	0.50
1:B:26:MET:HB3	1:B:44:LEU:HD13	1.93	0.50
1:A:109:ALA:HB1	1:A:115:LYS:HG3	1.94	0.50
1:A:192:ALA:O	1:A:196:PHE:HB3	2.12	0.50
1:A:126:TYR:CD2	1:A:144:GLN:HB3	2.46	0.50
1:A:10:ALA:HB2	1:A:25:CYS:HB3	1.94	0.50
1:B:98:LEU:HD11	1:B:126:TYR:CD1	2.46	0.50
1:A:32:GLN:O	1:A:104:PHE:HE1	1.95	0.49
1:A:17:GLU:O	1:A:17:GLU:HG2	2.12	0.49
1:A:3:LYS:O	1:A:7:VAL:HG23	2.12	0.49
1:B:126:TYR:CD2	1:B:144:GLN:HB3	2.46	0.49
1:B:98:LEU:HD21	1:B:126:TYR:CD1	2.48	0.49
1:A:174:PHE:CD1	1:A:178:TYR:CE1	3.00	0.49
1:B:32:GLN:O	1:B:104:PHE:HE1	1.95	0.49
1:A:156:SER:HB2	1:A:167:ARG:CG	2.43	0.49
1:B:3:LYS:O	1:B:7:VAL:HG23	2.12	0.49
1:A:126:TYR:O	1:A:130:ALA:N	2.46	0.49
1:A:90:LEU:CD2	1:A:132:VAL:HG21	2.42	0.49
1:B:192:ALA:O	1:B:196:PHE:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:CD2	1:B:132:VAL:HG21	2.42	0.49
1:A:193:LYS:HA	1:A:196:PHE:CD2	2.48	0.48
1:B:53:GLY:O	1:B:56:ARG:N	2.46	0.48
1:A:193:LYS:O	1:A:197:ASP:HB2	2.14	0.48
1:A:48:TYR:CD2	1:A:97:VAL:HB	2.48	0.48
1:A:53:GLY:O	1:A:56:ARG:N	2.46	0.48
1:A:197:ASP:HA	1:A:200:ILE:CD1	2.44	0.48
1:B:156:SER:HB2	1:B:167:ARG:CG	2.43	0.48
1:B:48:TYR:CD2	1:B:97:VAL:HB	2.48	0.48
1:B:173:ASN:HA	1:B:176:VAL:HG12	1.95	0.48
1:B:17:GLU:HG2	1:B:17:GLU:O	2.12	0.48
1:A:173:ASN:HA	1:A:176:VAL:HG12	1.95	0.48
1:B:193:LYS:O	1:B:197:ASP:HB2	2.14	0.48
1:A:98:LEU:HD21	1:A:126:TYR:CD1	2.48	0.47
1:B:193:LYS:HA	1:B:196:PHE:CD2	2.48	0.47
1:B:151:GLU:O	1:B:155:ILE:HG13	2.14	0.47
1:A:9:LYS:HD2	1:A:25:CYS:SG	2.55	0.47
1:A:145:SER:O	1:A:148:ALA:HB3	2.15	0.47
1:B:174:PHE:CD1	1:B:178:TYR:CE1	3.00	0.47
1:A:103:LYS:O	1:A:104:PHE:CD2	2.67	0.47
1:A:151:GLU:O	1:A:155:ILE:HG13	2.14	0.47
1:A:26:MET:CB	1:A:44:LEU:HD12	2.44	0.47
1:B:221:LEU:HD23	1:B:221:LEU:N	2.28	0.47
1:B:26:MET:CB	1:B:44:LEU:HD12	2.44	0.47
1:B:145:SER:O	1:B:148:ALA:HB3	2.15	0.47
1:B:103:LYS:O	1:B:104:PHE:CD2	2.67	0.47
1:B:61:VAL:HG22	1:B:62:VAL:N	2.29	0.47
1:A:189:CYS:O	1:A:192:ALA:HB3	2.15	0.47
1:B:19:TYR:CD2	1:B:50:ASN:ND2	2.83	0.47
1:A:19:TYR:CD2	1:A:50:ASN:ND2	2.83	0.47
1:A:137:ASP:O	1:A:141:ILE:HG13	2.15	0.47
1:A:61:VAL:HG22	1:A:62:VAL:N	2.29	0.47
1:B:197:ASP:HA	1:B:200:ILE:CD1	2.44	0.46
1:B:9:LYS:HD2	1:B:25:CYS:SG	2.55	0.46
1:A:46:VAL:HG23	1:A:49:LYS:HE3	1.97	0.46
1:A:166:ILE:HG12	1:A:167:ARG:N	2.31	0.46
1:B:137:ASP:O	1:B:141:ILE:HG13	2.15	0.46
1:B:46:VAL:HG23	1:B:49:LYS:HE3	1.97	0.46
1:B:189:CYS:O	1:B:192:ALA:HB3	2.15	0.46
1:A:64:SER:O	1:A:66:GLU:N	2.50	0.45
1:B:43:LEU:CD1	1:B:43:LEU:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PHE:O	1:A:199:ALA:HB3	2.16	0.45
1:A:64:SER:O	1:A:65:ILE:C	2.55	0.45
1:B:143:ASP:O	1:B:147:GLN:HG3	2.16	0.45
1:A:52:VAL:HG11	1:A:125:TYR:CE1	2.50	0.45
1:B:196:PHE:O	1:B:199:ALA:HB3	2.16	0.45
1:B:43:LEU:CD1	1:B:43:LEU:N	2.80	0.45
1:B:90:LEU:HD21	1:B:132:VAL:CG2	2.47	0.45
1:A:43:LEU:CD1	1:A:43:LEU:H	2.29	0.45
1:B:126:TYR:O	1:B:130:ALA:N	2.46	0.45
1:A:54:ALA:O	1:A:57:SER:HB3	2.17	0.44
1:B:142:VAL:HG13	1:B:143:ASP:N	2.32	0.44
1:B:166:ILE:HG12	1:B:167:ARG:N	2.31	0.44
1:A:119:LEU:HD23	1:A:151:GLU:HB3	2.00	0.44
1:A:142:VAL:HG13	1:A:143:ASP:N	2.32	0.44
1:A:6:LEU:HD13	1:A:28:SER:OG	2.18	0.44
1:B:14:GLU:C	1:B:16:ALA:N	2.71	0.44
1:A:101:LEU:HA	1:A:101:LEU:HD12	1.87	0.44
1:B:64:SER:O	1:B:65:ILE:C	2.55	0.44
1:A:42:ASN:O	1:A:45:SER:OG	2.36	0.44
1:A:90:LEU:HD21	1:A:132:VAL:CG2	2.47	0.44
1:A:43:LEU:CD1	1:A:43:LEU:N	2.80	0.44
1:B:119:LEU:HD22	1:B:155:ILE:HD12	1.99	0.44
1:B:64:SER:O	1:B:66:GLU:N	2.50	0.44
1:B:42:ASN:O	1:B:45:SER:OG	2.36	0.44
1:A:143:ASP:O	1:A:147:GLN:HG3	2.16	0.43
1:A:196:PHE:CD2	1:A:197:ASP:N	2.86	0.43
1:B:196:PHE:CD2	1:B:197:ASP:N	2.86	0.43
1:B:6:LEU:HD13	1:B:28:SER:OG	2.18	0.43
1:B:87:GLU:HG3	1:B:132:VAL:HG11	1.99	0.43
1:A:119:LEU:HD22	1:A:155:ILE:HD12	1.99	0.43
1:A:38:ASN:HA	1:A:41:ARG:HB3	2.00	0.43
1:A:89:GLU:HG2	1:A:89:GLU:H	1.66	0.43
1:B:52:VAL:HG11	1:B:125:TYR:CE1	2.50	0.43
1:A:14:GLU:C	1:A:16:ALA:N	2.71	0.43
1:A:221:LEU:N	1:A:221:LEU:HD23	2.28	0.43
1:B:142:VAL:CG1	1:B:143:ASP:N	2.82	0.43
1:B:107:PRO:O	1:B:108:ASN:HB2	2.19	0.43
1:B:54:ALA:O	1:B:57:SER:HB3	2.17	0.43
1:B:41:ARG:HE	1:B:117:PHE:HD2	1.67	0.43
1:B:119:LEU:HD23	1:B:151:GLU:HB3	1.99	0.43
1:A:8:GLN:OE1	1:A:8:GLN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:SER:HB3	1:B:40:GLU:HG3	2.01	0.43
1:B:86:ILE:HA	1:B:89:GLU:HG2	2.01	0.42
1:B:96:ASP:O	1:B:100:LEU:HD13	2.19	0.42
1:A:142:VAL:CG1	1:A:143:ASP:N	2.82	0.42
1:A:37:SER:HB3	1:A:40:GLU:HG3	2.01	0.42
1:A:41:ARG:HE	1:A:117:PHE:HD2	1.67	0.42
1:A:53:GLY:O	1:A:54:ALA:C	2.57	0.42
1:B:109:ALA:HB3	1:B:115:LYS:CG	2.49	0.42
1:B:38:ASN:HA	1:B:41:ARG:HB3	2.00	0.42
1:B:8:GLN:N	1:B:8:GLN:OE1	2.52	0.42
1:A:107:PRO:O	1:A:108:ASN:HB2	2.19	0.42
1:A:117:PHE:CD1	1:A:117:PHE:C	2.90	0.42
1:A:170:LEU:C	1:A:170:LEU:HD12	2.40	0.42
1:A:179:TYR:HD2	1:A:228:TRP:HE1	1.62	0.42
1:A:43:LEU:H	1:A:43:LEU:HD13	1.85	0.42
1:A:83:ARG:O	1:A:86:ILE:HG13	2.20	0.42
1:A:156:SER:CB	1:A:167:ARG:HG3	2.49	0.42
1:A:87:GLU:HG2	1:A:91:ARG:HH21	1.83	0.42
1:A:87:GLU:HG3	1:A:132:VAL:HG11	1.99	0.42
1:A:86:ILE:HA	1:A:89:GLU:HG2	2.01	0.42
1:B:37:SER:HB3	1:B:40:GLU:CD	2.40	0.42
1:B:43:LEU:H	1:B:43:LEU:HD13	1.85	0.42
1:B:83:ARG:O	1:B:86:ILE:HG13	2.20	0.42
1:B:99:SER:O	1:B:100:LEU:C	2.58	0.42
1:A:129:LEU:HA	1:A:129:LEU:HD12	1.78	0.42
1:B:89:GLU:H	1:B:89:GLU:HG2	1.66	0.42
1:B:46:VAL:O	1:B:49:LYS:N	2.53	0.41
1:B:82:TYR:O	1:B:86:ILE:HG12	2.20	0.41
1:A:82:TYR:O	1:A:86:ILE:HG12	2.20	0.41
1:A:99:SER:O	1:A:100:LEU:C	2.58	0.41
1:B:117:PHE:CD1	1:B:117:PHE:C	2.90	0.41
1:A:52:VAL:HG23	1:A:90:LEU:HD12	2.02	0.41
1:B:26:MET:O	1:B:29:VAL:N	2.54	0.41
1:A:96:ASP:O	1:A:100:LEU:HD13	2.19	0.41
1:A:26:MET:O	1:A:29:VAL:N	2.54	0.41
1:A:37:SER:HB3	1:A:40:GLU:CD	2.40	0.41
1:B:170:LEU:C	1:B:170:LEU:HD12	2.40	0.41
1:B:53:GLY:O	1:B:54:ALA:C	2.57	0.41
1:A:109:ALA:HB3	1:A:115:LYS:CG	2.50	0.41
1:A:149:TYR:O	1:A:152:ALA:N	2.54	0.41
1:A:32:GLN:HE21	1:A:32:GLN:CA	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:O	1:A:49:LYS:N	2.53	0.41
1:B:52:VAL:HG23	1:B:90:LEU:HD12	2.02	0.41
1:A:26:MET:HB3	1:A:44:LEU:HD12	2.02	0.41
1:B:30:THR:HG21	1:B:100:LEU:CD2	2.47	0.41
1:B:32:GLN:HE21	1:B:32:GLN:CA	2.33	0.41
1:B:51:VAL:HG12	1:B:93:ILE:HG21	2.03	0.41
1:A:46:VAL:O	1:A:47:ALA:C	2.59	0.40
1:A:179:TYR:CD2	1:A:228:TRP:NE1	2.83	0.40
1:B:26:MET:HB3	1:B:44:LEU:HD12	2.02	0.40
1:B:46:VAL:O	1:B:47:ALA:C	2.59	0.40
1:B:87:GLU:HG2	1:B:91:ARG:HH21	1.83	0.40
1:B:156:SER:CB	1:B:167:ARG:HG3	2.49	0.40
1:B:58:SER:O	1:B:62:VAL:HG12	2.21	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	183/245 (75%)	131 (72%)	41 (22%)	11 (6%)	2	22
1	B	183/245 (75%)	131 (72%)	41 (22%)	11 (6%)	2	22
2	P	4/15 (27%)	0	0	4 (100%)	0	0
2	Q	4/15 (27%)	0	0	4 (100%)	0	0
All	All	374/520 (72%)	262 (70%)	82 (22%)	30 (8%)	1	14

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ALA
1	A	108	ASN

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Mol	Chain	Res	Type
2	P	257	SER
2	P	260	THR
2	P	261	PRO
1	B	34	ALA
1	B	108	ASN
2	Q	257	SER
2	Q	260	THR
2	Q	261	PRO
1	A	5	GLU
1	A	51	VAL
1	A	66	GLU
1	A	104	PHE
1	B	5	GLU
1	B	51	VAL
1	B	66	GLU
1	B	104	PHE
1	A	133	ALA
2	P	258	THR
1	B	133	ALA
2	Q	258	THR
1	A	100	LEU
1	B	100	LEU
1	A	2	ASP
1	A	65	ILE
1	A	99	SER
1	B	2	ASP
1	B	65	ILE
1	B	99	SER

### 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	166/209 (79%)	125 (75%)	41 (25%)	1	5
1	B	166/209 (79%)	125 (75%)	41 (25%)	1	5
All	All	332/418 (79%)	250 (75%)	82 (25%)	1	5



All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	GLN
1	A	9	LYS
1	A	17	GLU
1	A	22	MET
1	A	30	THR
1	A	32	GLN
1	A	36	LEU
1	A	37	SER
1	A	42	ASN
1	A	45	SER
1	A	56	ARG
1	A	61	VAL
1	A	62	VAL
1	A	76	GLN
1	A	78	MET
1	A	82	TYR
1	A	86	ILE
1	A	89	GLU
1	A	91	ARG
1	A	92	ASP
1	A	99	SER
1	A	101	LEU
1	A	104	PHE
1	A	105	LEU
1	A	108	ASN
1	A	116	VAL
1	A	117	PHE
1	A	129	LEU
1	A	143	ASP
1	A	144	GLN
1	A	149	TYR
1	A	168	LEU
1	A	170	LEU
1	A	174	PHE
1	A	189	CYS
1	A	196	PHE
1	A	213	ASP
1	A	214	SER
1	A	219	GLN
1	A	221	LEU
1	B	1	MET

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Mol	Chain	Res	Type
1	B	8	GLN
1	B	9	LYS
1	B	17	GLU
1	B	22	MET
1	B	30	THR
1	B	32	GLN
1	B	36	LEU
1	B	37	SER
1	B	42	ASN
1	B	45	SER
1	B	56	ARG
1	B	61	VAL
1	B	62	VAL
1	B	76	GLN
1	B	78	MET
1	B	82	TYR
1	B	86	ILE
1	B	89	GLU
1	B	91	ARG
1	B	92	ASP
1	B	99	SER
1	B	101	LEU
1	B	104	PHE
1	B	105	LEU
1	B	108	ASN
1	B	116	VAL
1	B	117	PHE
1	B	129	LEU
1	B	143	ASP
1	B	144	GLN
1	B	149	TYR
1	B	168	LEU
1	B	170	LEU
1	B	174	PHE
1	B	189	CYS
1	B	196	PHE
1	B	213	ASP
1	B	214	SER
1	B	219	GLN
1	B	221	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	42	ASN
1	A	67	GLN
1	A	144	GLN
1	B	32	GLN
1	B	42	ASN
1	B	67	GLN
1	B	144	GLN

### 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	P	259	2	9,9,10	2.98	3 (33%)	9,12,14	7.97	3 (33%)
2	SEP	Q	259	2	9,9,10	2.97	3 (33%)	9,12,14	7.98	3 (33%)

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	P	259	2	-	0/5/8/10	0/0/0/0
2	SEP	Q	259	2	-	0/5/8/10	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	259	SEP	OG-CB	-5.01	1.24	1.44
2	Q	259	SEP	OG-CB	-4.99	1.25	1.44
2	Q	259	SEP	P-OG	4.53	1.74	1.60
2	P	259	SEP	P-OG	4.54	1.74	1.60
2	Q	259	SEP	CA-C	5.37	1.57	1.50
2	P	259	SEP	CA-C	5.38	1.57	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	259	SEP	P-OG-CB	-4.17	106.82	118.30
2	Q	259	SEP	P-OG-CB	-4.16	106.82	118.30
2	Q	259	SEP	O2P-P-OG	-2.20	100.87	106.73
2	P	259	SEP	O2P-P-OG	-2.20	100.88	106.73
2	P	259	SEP	OG-CB-CA	23.28	131.13	108.17
2	Q	259	SEP	OG-CB-CA	23.30	131.15	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	259	SEP	1	0
2	Q	259	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	195/245 (79%)	-0.05	1 (0%) 90 84	32, 77, 99, 100	0
1	B	195/245 (79%)	-0.00	2 (1%) 82 70	32, 77, 99, 100	0
2	P	5/15 (33%)	-0.70	0 100 100	45, 57, 62, 65	0
2	Q	5/15 (33%)	-0.39	0 100 100	45, 57, 62, 65	0
All	All	400/520 (76%)	-0.04	3 (0%) 86 75	32, 77, 99, 100	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	ASN	2.4
1	A	177	PHE	2.2
1	B	150	GLN	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. 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(Å <sup>2</sup> )	Q<0.9
2	SEP	P	259	10/11	0.82	0.19	-	46,66,66,66	0
2	SEP	Q	259	10/11	0.83	0.19	-	46,66,66,66	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.