



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 10, 2026 – 12:04 PM EDT

PDB ID : 9YW4 / pdb\_00009yw4  
Title : T cell receptor N17.2 complexed w/ HLA.A1 and NRAS peptide  
Authors : Gallagher, D.T.; Mariuzza, R.A.  
Deposited on : 2025-10-23  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

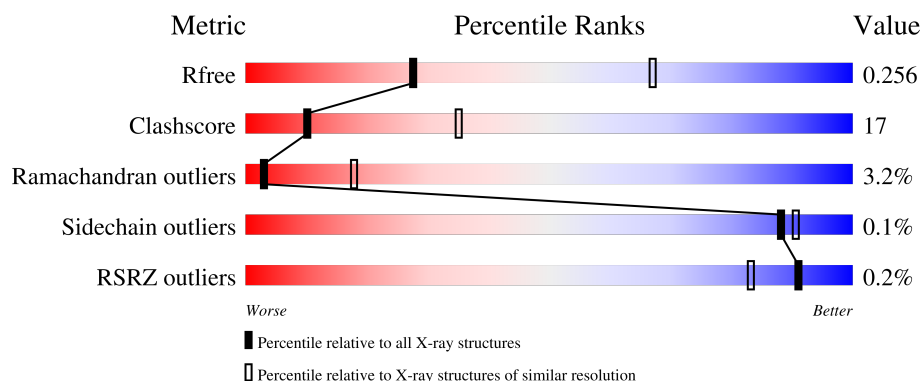
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	206	 61% 32% • 6%
2	B	244	 61% 37% ..
3	P	10	 60% 30% 10%
4	D	276	 70% 28% ..
5	E	100	 53% 45% •

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6508 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 TCR Alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1504	945	243	307	9			

- Molecule 2 is a protein called TCR Beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1903	1205	327	362	9			

- Molecule 3 is a protein called NRAS neopeptide with oncogenic mutation Q61K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	0	0	0
			80	50	11	19			

- Molecule 4 is a protein called HLA class I histocompatibility antigen, A-1 alpha chain variant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	274	Total	C	N	O	S	0	0	0
			2189	1363	396	420	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP Q59GJ2

- Molecule 5 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	100	Total	C	N	O	S	0	0	0
			832	530	140	158	4			

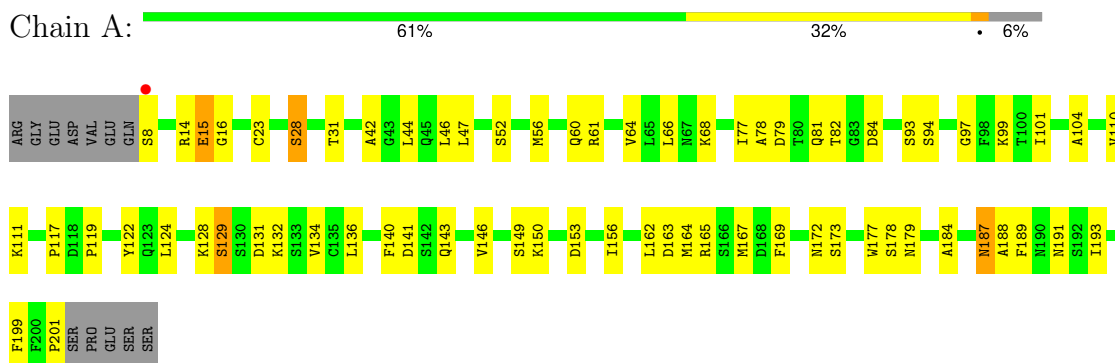
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	initiating methionine	UNP P61769

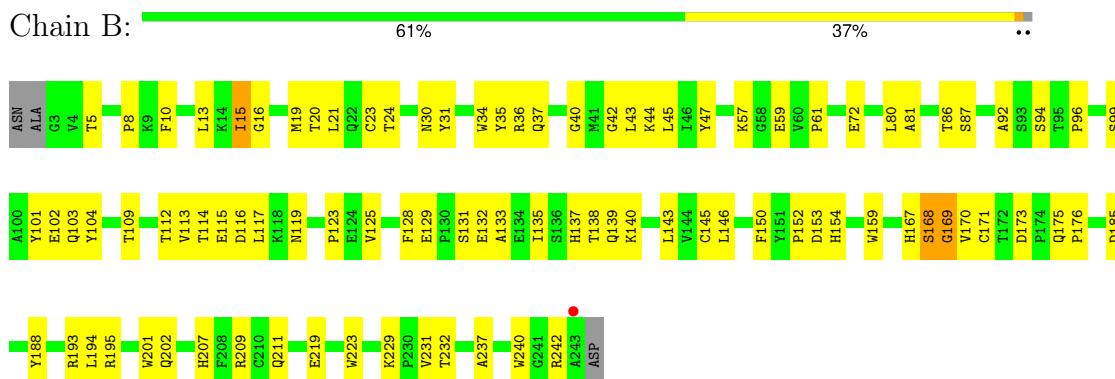
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: TCR Alpha chain



#### • Molecule 2: TCR Beta chain



#### • Molecule 3: NRAS neopeptide with oncogenic mutation Q61K

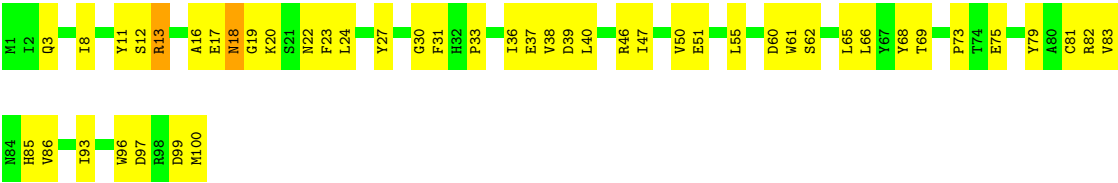


#### • Molecule 4: HLA class I histocompatibility antigen, A-1 alpha chain variant





● Molecule 5: Beta-2-microglobulin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.45Å 126.45Å 174.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.99 – 3.10 39.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.2 (39.99-3.10) 91.1 (39.99-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487+SVN	Depositor
R, $R_{free}$	0.203 , 0.257 0.203 , 0.256	Depositor DCC
$R_{free}$ test set	1220 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.4	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 70.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6508	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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](#)

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	0.36	0/1533	0.65	0/2074
2	B	0.40	0/1957	0.63	0/2668
3	P	0.42	0/80	0.61	0/105
4	D	0.37	0/2249	0.57	0/3057
5	E	0.33	0/855	0.56	0/1158
All	All	0.37	0/6674	0.61	0/9062

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	1504	0	1430	61	0
2	B	1903	0	1802	75	0
3	P	80	0	77	5	0
4	D	2189	0	2015	58	0
5	E	832	0	792	37	0
All	All	6508	0	6116	217	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 17.

All (217) 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)
4:D:194:ILE:HB	4:D:198:GLU:HB3	1.56	0.86
4:D:235:PRO:HG2	5:E:66:LEU:HD22	1.67	0.77
4:D:99:TYR:HB3	4:D:114:ARG:HG2	1.66	0.75
1:A:134:VAL:HG12	1:A:177:TRP:HB3	1.66	0.75
1:A:162:LEU:HD11	2:B:195:ARG:HB2	1.72	0.72
4:D:111:ARG:NH1	4:D:113:TYR:HD2	1.90	0.70
2:B:5:THR:HG23	2:B:24:THR:HG23	1.73	0.68
4:D:35:ARG:HE	4:D:46:GLU:HG3	1.58	0.68
2:B:138:THR:HG22	2:B:140:LYS:HG2	1.75	0.67
2:B:170:VAL:HG22	2:B:194:LEU:HD13	1.77	0.67
4:D:13:SER:HB3	4:D:78:LEU:HD13	1.75	0.66
5:E:60:ASP:OD2	5:E:62:SER:HB3	1.95	0.66
1:A:149:SER:HA	1:A:191:ASN:HD22	1.61	0.65
4:D:33:PHE:CD1	4:D:34:VAL:HG13	2.32	0.65
2:B:21:LEU:HD11	2:B:109:THR:HG21	1.79	0.65
4:D:35:ARG:HG2	4:D:46:GLU:HB2	1.77	0.65
4:D:269:PRO:O	4:D:270:LEU:HB2	1.97	0.64
1:A:66:LEU:HD21	1:A:68:LYS:HG3	1.80	0.64
4:D:216:THR:HB	4:D:260:HIS:HB3	1.80	0.64
2:B:209:ARG:HH12	2:B:211:GLN:HG3	1.63	0.64
2:B:176:PRO:HB2	2:B:188:TYR:HB3	1.79	0.63
5:E:18:ASN:OD1	5:E:75:GLU:N	2.31	0.63
1:A:184:ALA:O	1:A:187:ASN:HB2	1.98	0.63
4:D:194:ILE:HD11	4:D:200:THR:OG1	1.99	0.63
5:E:8:ILE:HG12	5:E:83:VAL:HG21	1.81	0.63
4:D:6:ARG:HD2	4:D:8:PHE:HZ	1.63	0.62
5:E:40:LEU:HB3	5:E:47:ILE:HD12	1.80	0.62
4:D:117:ALA:HB2	5:E:61:TRP:CE2	2.34	0.62
1:A:132:LYS:HE3	1:A:179:ASN:HB3	1.81	0.62
4:D:111:ARG:NH1	4:D:113:TYR:CD2	2.68	0.62
2:B:116:ASP:O	2:B:119:ASN:ND2	2.33	0.61
4:D:138:MET:O	4:D:141:GLN:HB2	2.01	0.60
1:A:14:ARG:O	1:A:16:GLY:N	2.33	0.60
2:B:86:THR:HG23	2:B:112:THR:HA	1.82	0.60
2:B:173:ASP:OD1	2:B:193:ARG:NH2	2.35	0.60
5:E:38:VAL:HG22	5:E:83:VAL:HG22	1.84	0.59
2:B:145:CYS:HB2	2:B:159:TRP:CZ2	2.37	0.59
4:D:44:LYS:HA	4:D:64:THR:HG21	1.83	0.59
1:A:149:SER:HA	1:A:191:ASN:ND2	2.19	0.58
2:B:16:GLY:H	2:B:81:ALA:HB3	1.68	0.58
5:E:12:SER:HB2	5:E:22:ASN:HD22	1.68	0.58
2:B:72:GLU:CD	2:B:72:GLU:H	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:SER:HB2	1:A:97:GLY:HA2	1.85	0.57
2:B:129:GLU:OE2	2:B:201:TRP:HH2	1.88	0.57
5:E:24:LEU:HD23	5:E:40:LEU:HD13	1.86	0.57
1:A:140:PHE:CE1	1:A:172:ASN:HB3	2.40	0.56
2:B:35:TYR:HB3	2:B:43:LEU:HD12	1.87	0.56
5:E:55:LEU:HD13	5:E:65:LEU:HD23	1.86	0.56
2:B:170:VAL:HG12	2:B:171:CYS:N	2.22	0.55
2:B:37:GLN:HB2	2:B:43:LEU:HD13	1.88	0.55
2:B:102:GLU:HG2	2:B:104:TYR:CE1	2.42	0.55
1:A:189:PHE:C	1:A:191:ASN:H	2.13	0.55
4:D:259:CYS:HB3	4:D:272:LEU:HB2	1.89	0.55
3:P:4:THR:HG22	3:P:5:ALA:H	1.73	0.54
1:A:149:SER:HB2	1:A:156:ILE:HD11	1.88	0.54
4:D:189:MET:HE3	4:D:274:TRP:HB2	1.90	0.54
5:E:27:TYR:HB2	5:E:66:LEU:HD13	1.89	0.54
4:D:6:ARG:HD2	4:D:8:PHE:CZ	2.41	0.54
5:E:16:ALA:HB3	5:E:22:ASN:HB2	1.91	0.53
2:B:15:ILE:HD12	2:B:115:GLU:HA	1.91	0.53
1:A:14:ARG:HD3	1:A:143:GLN:HE22	1.72	0.53
1:A:111:LYS:HD3	1:A:143:GLN:HG2	1.91	0.53
5:E:12:SER:HB2	5:E:22:ASN:ND2	2.24	0.53
1:A:52:SER:HB2	1:A:68:LYS:HD2	1.91	0.52
1:A:93:SER:HA	1:A:99:LYS:O	2.10	0.52
1:A:94:SER:O	1:A:99:LYS:HB3	2.10	0.52
1:A:164:MET:HB2	1:A:169:PHE:HB3	1.92	0.52
2:B:96:PRO:HB3	2:B:101:TYR:CE1	2.45	0.52
1:A:131:ASP:OD1	1:A:132:LYS:NZ	2.43	0.52
5:E:17:GLU:O	5:E:73:PRO:HG2	2.10	0.52
2:B:47:TYR:CE1	2:B:57:LYS:HG2	2.45	0.51
4:D:259:CYS:SG	4:D:260:HIS:N	2.81	0.51
3:P:10:TYR:HA	4:D:143:THR:HG23	1.93	0.51
1:A:128:LYS:NZ	1:A:129:SER:HB2	2.24	0.51
1:A:117:PRO:C	1:A:119:PRO:HD3	2.37	0.50
2:B:19:MET:HG2	2:B:20:THR:N	2.26	0.50
5:E:36:ILE:HG12	5:E:37:GLU:H	1.75	0.50
4:D:64:THR:HG22	4:D:68:LYS:HE3	1.92	0.50
1:A:164:MET:HE3	2:B:195:ARG:HB3	1.93	0.50
2:B:143:LEU:N	2:B:194:LEU:O	2.38	0.50
4:D:127:ASN:OD1	4:D:134:THR:OG1	2.25	0.50
1:A:122:TYR:HB3	2:B:131:SER:CB	2.41	0.50
1:A:167:MET:HE1	2:B:140:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:97:ASP:C	5:E:99:ASP:H	2.19	0.50
2:B:92:ALA:HA	2:B:104:TYR:O	2.11	0.50
1:A:28:SER:HB3	4:D:62:GLN:HE22	1.77	0.49
1:A:117:PRO:HB3	1:A:141:ASP:HA	1.95	0.49
1:A:150:LYS:H	1:A:191:ASN:HD21	1.61	0.49
3:P:10:TYR:HE2	4:D:95:ILE:HD13	1.78	0.49
1:A:61:ARG:HB3	1:A:78:ALA:O	2.12	0.49
1:A:132:LYS:HD2	1:A:178:SER:O	2.12	0.49
2:B:23:CYS:HB2	2:B:34:TRP:CZ2	2.48	0.49
2:B:131:SER:O	2:B:135:ILE:HD12	2.13	0.49
5:E:85:HIS:ND1	5:E:86:VAL:N	2.61	0.49
4:D:61:ASP:O	4:D:65:ARG:HG3	2.12	0.48
1:A:132:LYS:HE3	1:A:179:ASN:CB	2.43	0.48
4:D:33:PHE:HD1	4:D:34:VAL:HG13	1.78	0.48
1:A:187:ASN:O	1:A:189:PHE:N	2.47	0.48
4:D:114:ARG:NH1	4:D:116:ASP:OD1	2.47	0.48
1:A:15:GLU:HG3	1:A:82:THR:HG23	1.95	0.48
1:A:124:LEU:HD13	1:A:134:VAL:HG23	1.95	0.48
1:A:136:LEU:HD11	1:A:173:SER:HB3	1.95	0.48
1:A:163:ASP:O	2:B:169:GLY:HA2	2.13	0.48
5:E:51:GLU:HG3	5:E:68:TYR:CE1	2.49	0.48
4:D:141:GLN:O	4:D:145:ARG:HG3	2.14	0.48
5:E:50:VAL:HG13	5:E:69:THR:HB	1.96	0.47
5:E:51:GLU:OE2	5:E:68:TYR:HE1	1.96	0.47
2:B:219:GLU:H	2:B:219:GLU:CD	2.18	0.47
5:E:30:GLY:HA2	5:E:62:SER:HB2	1.95	0.47
1:A:15:GLU:O	1:A:15:GLU:HG2	2.14	0.47
4:D:8:PHE:HB2	4:D:25:VAL:HG23	1.97	0.47
2:B:167:HIS:C	2:B:169:GLY:H	2.22	0.47
2:B:96:PRO:HB3	2:B:101:TYR:HE1	1.78	0.47
4:D:49:ALA:O	4:D:52:ILE:HG22	2.15	0.47
5:E:3:GLN:HG2	5:E:33:PRO:HD3	1.97	0.47
1:A:47:LEU:HA	1:A:47:LEU:HD12	1.65	0.47
1:A:132:LYS:HA	1:A:132:LYS:HD3	1.64	0.47
1:A:165:ARG:HD3	2:B:168:SER:HB3	1.96	0.47
2:B:150:PHE:CE1	2:B:188:TYR:HB2	2.50	0.47
2:B:152:PRO:HG2	2:B:154:HIS:CD2	2.50	0.47
4:D:100:GLY:O	4:D:160:LEU:HD22	2.14	0.47
2:B:42:GLY:O	2:B:44:LYS:HE2	2.15	0.47
4:D:208:PHE:CE1	4:D:241:PHE:HB2	2.50	0.47
1:A:101:ILE:O	1:A:101:ILE:HG13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:GLY:HA2	5:E:62:SER:CB	2.45	0.46
1:A:199:PHE:CZ	1:A:201:PRO:HB3	2.51	0.46
5:E:46:ARG:HE	5:E:46:ARG:HB3	1.51	0.46
2:B:8:PRO:O	2:B:109:THR:HG23	2.14	0.46
5:E:39:ASP:HB2	5:E:82:ARG:HB3	1.97	0.46
4:D:242:GLN:NE2	5:E:13:ARG:O	2.49	0.46
1:A:46:LEU:HD23	1:A:47:LEU:N	2.30	0.46
2:B:145:CYS:O	2:B:146:LEU:HD23	2.16	0.46
2:B:36:ARG:NH2	2:B:87:SER:HB2	2.30	0.46
1:A:122:TYR:HB3	2:B:131:SER:OG	2.15	0.45
2:B:175:GLN:N	2:B:175:GLN:OE1	2.50	0.45
2:B:223:TRP:CG	2:B:229:LYS:HG3	2.51	0.45
4:D:14:ARG:NH1	4:D:17:ARG:HH21	2.15	0.45
5:E:81:CYS:O	5:E:93:ILE:HA	2.16	0.45
1:A:81:GLN:O	1:A:110:VAL:HG21	2.16	0.45
2:B:145:CYS:HB2	2:B:159:TRP:CH2	2.51	0.45
4:D:249:VAL:HG12	4:D:257:TYR:CE2	2.51	0.45
1:A:94:SER:HB3	1:A:101:ILE:HG12	1.99	0.45
4:D:82:ARG:HG2	4:D:87:GLN:HB2	1.99	0.45
1:A:15:GLU:HB2	1:A:111:LYS:O	2.17	0.44
1:A:77:ILE:HG21	1:A:84:ASP:OD2	2.17	0.44
1:A:153:ASP:O	1:A:178:SER:OG	2.26	0.44
2:B:231:VAL:HG23	2:B:232:THR:O	2.18	0.44
4:D:230:LEU:HD21	4:D:243:LYS:HE3	1.99	0.44
5:E:33:PRO:HD2	5:E:85:HIS:HE1	1.80	0.44
1:A:117:PRO:O	1:A:119:PRO:HD3	2.18	0.44
2:B:125:VAL:HG12	2:B:237:ALA:CB	2.48	0.44
2:B:72:GLU:OE2	2:B:72:GLU:N	2.39	0.44
4:D:43:GLN:OE1	4:D:43:GLN:HA	2.16	0.44
4:D:235:PRO:HA	4:D:241:PHE:HD1	1.82	0.44
1:A:14:ARG:HD3	1:A:143:GLN:NE2	2.31	0.44
2:B:16:GLY:O	2:B:80:LEU:HD12	2.18	0.44
2:B:45:LEU:O	2:B:59:GLU:N	2.50	0.44
2:B:185:ASP:OD1	2:B:185:ASP:N	2.40	0.44
4:D:35:ARG:O	4:D:45:MET:HG3	2.18	0.44
4:D:189:MET:HE1	4:D:272:LEU:O	2.18	0.44
5:E:16:ALA:HB1	5:E:20:LYS:HG2	1.98	0.44
1:A:132:LYS:HE3	1:A:179:ASN:HA	2.00	0.43
2:B:207:HIS:HB2	2:B:240:TRP:CZ3	2.53	0.43
1:A:149:SER:HB2	1:A:156:ILE:CD1	2.47	0.43
5:E:13:ARG:HB2	5:E:23:PHE:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:TYR:HB2	2:B:94:SER:O	2.19	0.43
4:D:81:LEU:HD23	4:D:84:TYR:HD2	1.82	0.43
5:E:12:SER:HA	5:E:23:PHE:O	2.18	0.43
4:D:121:LYS:HE2	4:D:121:LYS:HB3	1.59	0.43
5:E:79:TYR:O	5:E:96:TRP:N	2.38	0.43
1:A:189:PHE:C	1:A:191:ASN:N	2.75	0.43
1:A:111:LYS:HD3	1:A:143:GLN:OE1	2.19	0.43
2:B:15:ILE:HG13	2:B:114:THR:O	2.18	0.43
5:E:17:GLU:O	5:E:19:GLY:N	2.52	0.43
2:B:133:ALA:O	2:B:137:HIS:N	2.26	0.42
2:B:194:LEU:HD12	2:B:195:ARG:H	1.83	0.42
4:D:201:LEU:HD12	4:D:249:VAL:HG11	2.01	0.42
4:D:234:ARG:HB2	5:E:11:TYR:OH	2.20	0.42
1:A:128:LYS:HZ3	1:A:129:SER:HB2	1.83	0.42
2:B:57:LYS:HB3	2:B:61:PRO:HG3	2.01	0.42
4:D:21:ARG:NH1	4:D:39:ASP:HB2	2.34	0.42
4:D:42:SER:C	4:D:44:LYS:H	2.27	0.42
4:D:225:THR:HA	4:D:228:THR:HG23	2.02	0.42
4:D:133:TRP:HH2	4:D:156:ARG:HG3	1.84	0.42
2:B:116:ASP:C	2:B:116:ASP:OD1	2.62	0.42
2:B:167:HIS:O	2:B:169:GLY:N	2.52	0.42
4:D:104:GLY:HA2	4:D:110:LEU:HD11	2.02	0.42
2:B:125:VAL:HG12	2:B:237:ALA:HB2	2.02	0.42
4:D:189:MET:HB2	4:D:189:MET:HE2	1.72	0.42
2:B:21:LEU:HD13	2:B:21:LEU:HA	1.86	0.41
1:A:14:ARG:C	1:A:16:GLY:H	2.26	0.41
2:B:13:LEU:O	2:B:113:VAL:HA	2.20	0.41
5:E:40:LEU:HD23	5:E:40:LEU:HA	1.80	0.41
5:E:99:ASP:O	5:E:100:MET:HB2	2.20	0.41
2:B:154:HIS:CD2	2:B:154:HIS:N	2.88	0.41
2:B:202:GLN:HG2	2:B:242:ARG:O	2.19	0.41
2:B:47:TYR:CZ	2:B:57:LYS:HG2	2.56	0.41
2:B:128:PHE:CD1	2:B:128:PHE:N	2.88	0.41
4:D:14:ARG:NH1	4:D:17:ARG:NH2	2.68	0.41
4:D:191:HIS:HA	4:D:200:THR:O	2.19	0.41
2:B:8:PRO:HB2	2:B:10:PHE:O	2.20	0.41
2:B:30:ASN:OD1	2:B:30:ASN:N	2.53	0.41
2:B:117:LEU:C	2:B:119:ASN:H	2.29	0.41
4:D:187:THR:HA	4:D:204:TRP:O	2.21	0.41
4:D:220:ASP:OD2	4:D:256:ARG:NH1	2.53	0.41
1:A:44:LEU:HD11	2:B:43:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:PRO:HB3	2:B:150:PHE:HB3	2.03	0.41
2:B:92:ALA:HB1	2:B:103:GLN:HG2	2.01	0.41
1:A:8:SER:HB3	2:B:40:GLY:O	2.21	0.40
3:P:1:ILE:HG21	4:D:163:ARG:HG2	2.03	0.40
5:E:31:PHE:CD1	5:E:31:PHE:N	2.88	0.40
1:A:31:THR:OG1	3:P:4:THR:HB	2.21	0.40
1:A:46:LEU:HD12	2:B:102:GLU:HB2	2.04	0.40
2:B:139:GLN:C	2:B:140:LYS:HD3	2.47	0.40
2:B:35:TYR:CB	2:B:43:LEU:HD12	2.49	0.40
1:A:56:MET:HA	1:A:64:VAL:O	2.21	0.40
4:D:204:TRP:HE3	4:D:206:LEU:HD11	1.87	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	192/206 (93%)	157 (82%)	24 (12%)	11 (6%)	1	8
2	B	239/244 (98%)	214 (90%)	19 (8%)	6 (2%)	4	21
3	P	8/10 (80%)	6 (75%)	1 (12%)	1 (12%)	0	1
4	D	272/276 (99%)	244 (90%)	22 (8%)	6 (2%)	5	24
5	E	98/100 (98%)	83 (85%)	13 (13%)	2 (2%)	6	25
All	All	809/836 (97%)	704 (87%)	79 (10%)	26 (3%)	3	18

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	60	GLN
1	A	104	ALA

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Mol	Chain	Res	Type
2	B	99	SER
2	B	153	ASP
4	D	267	PRO
4	D	269	PRO
5	E	18	ASN
1	A	28	SER
2	B	15	ILE
2	B	132	GLU
3	P	4	THR
4	D	270	LEU
1	A	129	SER
1	A	187	ASN
1	A	188	ALA
2	B	168	SER
4	D	260	HIS
1	A	79	ASP
5	E	13	ARG
1	A	42	ALA
2	B	169	GLY
4	D	14	ARG
1	A	193	ILE
4	D	229	GLU
1	A	146	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	170/184 (92%)	169 (99%)	1 (1%)	78	83
2	B	205/211 (97%)	205 (100%)	0	100	100
3	P	8/8 (100%)	8 (100%)	0	100	100
4	D	221/233 (95%)	221 (100%)	0	100	100
5	E	94/95 (99%)	94 (100%)	0	100	100
All	All	698/731 (96%)	697 (100%)	1 (0%)	88	90

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

Mol	Chain	Res	Type
1	A	23	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	191	ASN
4	D	62	GLN
4	D	224	GLN
4	D	226	GLN
5	E	22	ASN
5	E	52	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

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	194/206 (94%)	-0.26	1 (0%) 87 73	68, 106, 145, 160	0
2	B	241/244 (98%)	-0.49	1 (0%) 88 76	56, 84, 125, 142	0
3	P	10/10 (100%)	-0.46	0 100 100	65, 76, 81, 86	0
4	D	274/276 (99%)	-0.53	0 100 100	60, 95, 120, 138	0
5	E	100/100 (100%)	-0.47	0 100 100	71, 102, 139, 152	0
All	All	819/836 (97%)	-0.45	2 (0%) 91 83	56, 94, 137, 160	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	SER	2.5
2	B	243	ALA	2.4

### 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 oligosaccharides 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.