



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 10, 2026 – 12:04 PM EDT

PDB ID : 9ZKI / pdb\_00009zki  
Title : Human NRAS specific T cell receptor N17.2  
Authors : Gallagher, D.T.; Mariuzza, R.A.  
Deposited on : 2025-12-07  
Resolution : 2.91 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>.

---

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

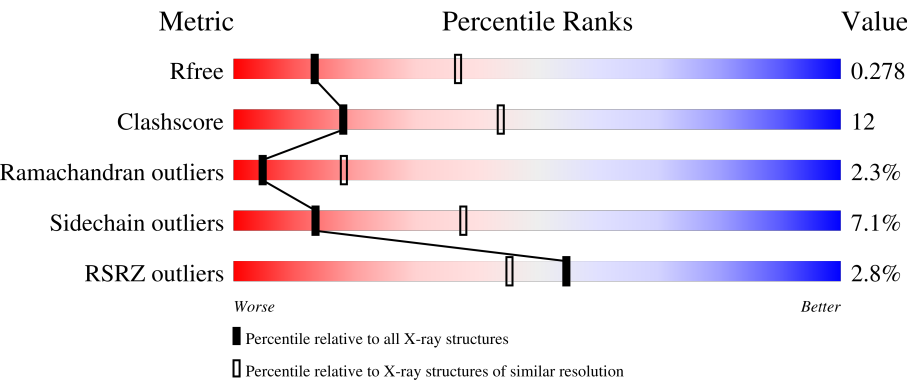
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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 <sub>free</sub>	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>65%25%7%</div></div>
1	D	206	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>55%33%10%</div></div>
1	F	206	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>64%23%10%</div></div>
2	B	244	<div><div>0%</div><div><div></div><div></div><div></div><div></div></div><div>75%23%</div></div>
2	E	244	<div><div>0%</div><div><div></div><div></div><div></div><div></div></div><div>69%29%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	244	<div><div></div><div>2%</div><div>64%</div><div>34%</div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10023 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	192	Total	C	N	O	S	0	0	0
			1485	936	238	302	9			
1	D	185	Total	C	N	O	S	0	0	0
			1417	894	227	287	9			
1	F	185	Total	C	N	O	S	0	0	0
			1431	905	229	289	8			

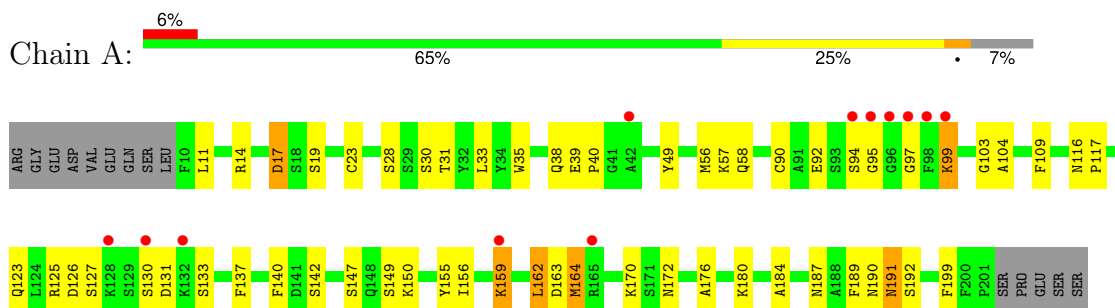
- Molecule 2 is a protein called TCR Beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1900	1202	327	363	8			
2	E	243	Total	C	N	O	S	0	0	0
			1893	1198	326	361	8			
2	G	243	Total	C	N	O	S	0	0	0
			1897	1203	326	359	9			

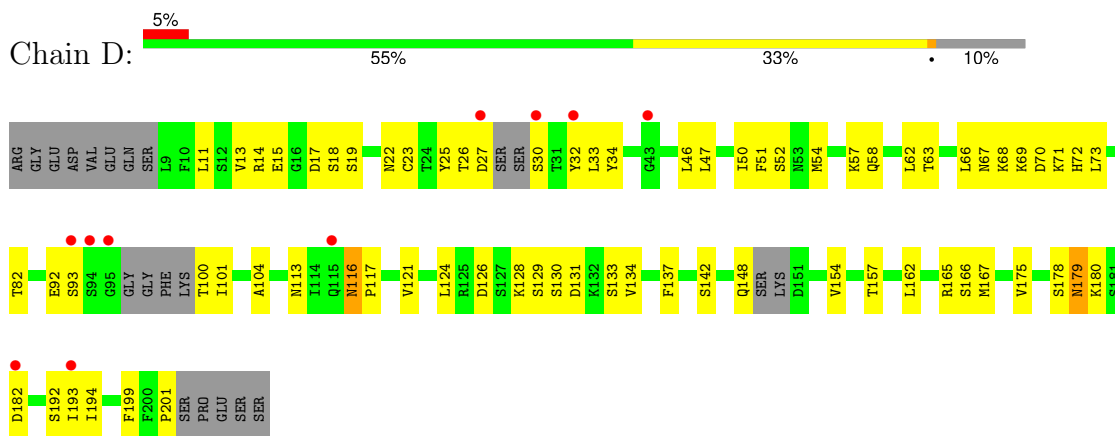
### 3 Residue-property plots [i](#)

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.

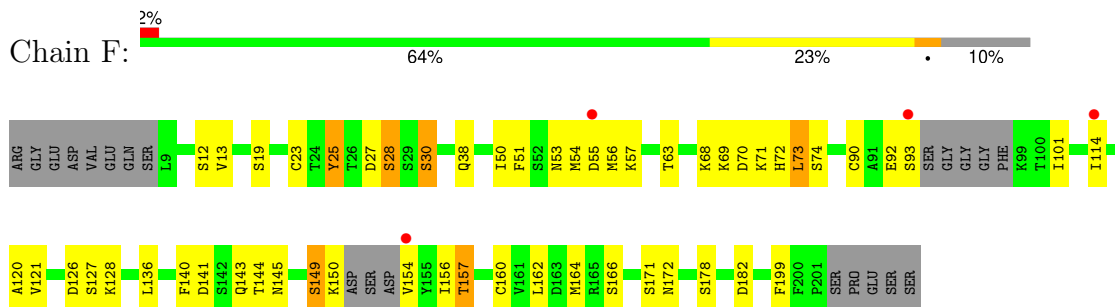
- Molecule 1: TCR Alpha chain



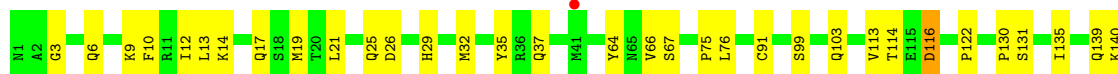
- Molecule 1: TCR Alpha chain



- Molecule 1: TCR Alpha chain



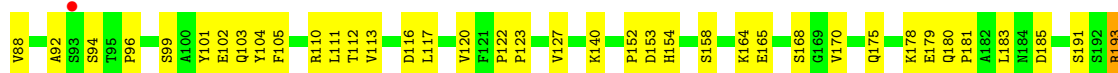
- Molecule 2: TCR Beta chain



• Molecule 2: TCR Beta chain



• Molecule 2: TCR Beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	286.40Å 286.40Å 103.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.80 – 2.91 34.80 – 2.91	Depositor EDS
% Data completeness (in resolution range)	88.1 (34.80-2.91) 88.0 (34.80-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487+SVN	Depositor
R, $R_{free}$	0.249 , 0.279 0.249 , 0.278	Depositor DCC
$R_{free}$ test set	2360 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.7	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 17.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10023	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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	0.41	0/1515	0.67	1/2050 (0.0%)
1	D	0.38	0/1442	0.65	0/1952
1	F	0.36	0/1458	0.58	0/1974
2	B	0.40	0/1954	0.58	0/2668
2	E	0.36	0/1947	0.57	0/2661
2	G	0.43	1/1951 (0.1%)	0.66	2/2664 (0.1%)
All	All	0.39	1/10267 (0.0%)	0.62	3/13969 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	61	PRO	CG-CD	-6.38	1.29	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	61	PRO	CA-CB-CG	-9.68	86.10	104.50
2	G	61	PRO	N-CD-CG	-9.02	89.67	103.20
1	A	191	ASN	N-CA-C	-5.83	106.79	112.97

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	1485	0	1402	33	0
1	D	1417	0	1309	38	0
1	F	1431	0	1343	29	0
2	B	1900	0	1781	40	0
2	E	1893	0	1773	46	0
2	G	1897	0	1789	63	0
All	All	10023	0	9397	236	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 12.

All (236) 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:F:38:GLN:HE22	2:G:37:GLN:HE22	1.25	0.85
2:E:11:ARG:HG2	2:E:19:MET:HE3	1.63	0.80
1:A:39:GLU:HB3	1:A:40:PRO:HD3	1.64	0.78
1:D:93:SER:HA	1:D:100:THR:HG22	1.69	0.75
2:E:64:TYR:HB3	2:E:76:LEU:HD11	1.69	0.75
1:A:56:MET:HE1	1:A:58:GLN:HE21	1.53	0.73
2:G:68:ARG:HH21	2:G:71:THR:HA	1.55	0.72
2:B:25:GLN:NE2	2:B:29:HIS:H	1.89	0.70
2:E:52:ALA:HB2	2:E:71:THR:HG23	1.75	0.69
1:D:22:ASN:HD22	1:D:72:HIS:HE1	1.41	0.69
1:A:164:MET:HE1	2:B:140:LYS:HD3	1.74	0.68
2:G:25:GLN:NE2	2:G:29:HIS:HB2	2.10	0.66
2:G:19:MET:HE1	2:G:111:LEU:HD12	1.75	0.66
2:G:64:TYR:HB3	2:G:76:LEU:HD11	1.78	0.66
2:G:241:GLY:O	2:G:242:ARG:HG2	1.96	0.65
1:A:56:MET:HE3	1:A:58:GLN:HG3	1.77	0.65
2:B:6:GLN:OE1	2:B:91:CYS:HB3	1.96	0.65
2:G:111:LEU:HD21	2:G:113:VAL:HG23	1.79	0.64
2:E:26:ASP:OD2	1:F:54:MET:HE1	1.97	0.64
2:B:130:PRO:HD3	2:B:143:LEU:HG	1.80	0.63
2:B:25:GLN:HE22	2:B:29:HIS:H	1.46	0.63
2:G:20:THR:HG22	2:G:77:ARG:HB2	1.81	0.62
2:B:14:LYS:N	2:B:17:GLN:OE1	2.26	0.62
1:D:126:ASP:HB3	1:D:130:SER:HB2	1.82	0.61
2:B:131:SER:O	2:B:135:ILE:HD12	1.99	0.61
2:B:25:GLN:HE22	2:B:29:HIS:N	1.98	0.61
1:F:25:TYR:HD1	1:F:25:TYR:H	1.48	0.61
2:B:14:LYS:HE3	2:B:116:ASP:HA	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:SER:HB2	1:F:71:LYS:NZ	2.16	0.61
1:F:114:ILE:HD12	1:F:171:SER:HA	1.81	0.61
2:G:11:ARG:HG2	2:G:19:MET:HE2	1.81	0.61
2:E:94:SER:HB3	2:E:96:PRO:HD3	1.84	0.60
2:G:86:THR:HG23	2:G:112:THR:HA	1.83	0.60
2:G:94:SER:HB2	2:G:96:PRO:HD3	1.82	0.60
1:A:109:PHE:CZ	1:A:159:LYS:HB3	2.37	0.59
2:G:27:MET:HE1	2:G:104:TYR:CG	2.38	0.59
1:D:124:LEU:HB2	1:D:134:VAL:HG23	1.85	0.59
1:F:144:THR:HG22	1:F:145:ASN:H	1.68	0.58
2:G:122:PRO:HD3	2:G:230:PRO:HB3	1.86	0.58
2:E:122:PRO:HD3	2:E:230:PRO:HB3	1.86	0.58
2:G:25:GLN:HE22	2:G:29:HIS:HB2	1.69	0.58
1:D:32:TYR:HB3	1:D:51:PHE:CE1	2.39	0.57
2:E:18:SER:HB2	2:E:78:LEU:O	2.04	0.57
2:E:78:LEU:HD23	2:E:85:GLN:OE1	2.05	0.57
1:D:25:TYR:HB2	1:D:92:GLU:OE2	2.04	0.57
1:D:26:THR:HB	1:D:92:GLU:OE1	2.06	0.56
1:D:27:ASP:O	1:D:68:LYS:NZ	2.38	0.56
1:F:50:ILE:HD12	1:F:57:LYS:HB3	1.86	0.56
1:D:180:LYS:HG2	1:D:182:ASP:H	1.71	0.56
2:G:85:GLN:O	2:G:111:LEU:HD22	2.06	0.56
2:B:202:GLN:O	2:B:243:ALA:HB2	2.06	0.55
2:G:123:PRO:HD3	2:G:214:PHE:CD2	2.41	0.55
2:E:38:ASP:OD1	2:E:87:SER:OG	2.16	0.55
2:E:19:MET:HE1	2:E:21:LEU:HD21	1.88	0.55
2:G:116:ASP:OD1	2:G:117:LEU:N	2.40	0.55
2:G:18:SER:OG	2:G:79:GLU:O	2.25	0.55
2:E:130:PRO:HD3	2:E:143:LEU:HG	1.88	0.55
2:E:205:ARG:HH11	2:E:205:ARG:HB2	1.71	0.54
2:G:12:ILE:HD11	2:G:152:PRO:HD3	1.89	0.54
2:G:94:SER:OG	2:G:103:GLN:HG3	2.06	0.54
1:D:15:GLU:OE1	1:D:113:ASN:N	2.39	0.54
2:B:9:LYS:HG2	2:B:10:PHE:CE2	2.42	0.54
1:F:164:MET:HE1	2:G:140:LYS:HD3	1.88	0.54
1:A:162:LEU:HD21	2:B:195:ARG:HB3	1.89	0.54
2:B:122:PRO:HD3	2:B:230:PRO:HB3	1.91	0.53
2:G:32:MET:HE1	2:G:72:GLU:O	2.08	0.53
2:G:19:MET:HE1	2:G:111:LEU:CD1	2.37	0.53
2:B:218:SER:O	2:B:221:ASP:HB2	2.08	0.53
1:A:38:GLN:HE22	2:B:37:GLN:HE22	1.57	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:MET:HE3	1:D:57:LYS:HB2	1.91	0.52
2:G:36:ARG:NH1	2:G:64:TYR:OH	2.42	0.52
2:E:9:LYS:HE2	2:E:156:GLU:OE2	2.08	0.52
2:B:197:SER:HB2	2:B:200:PHE:H	1.72	0.52
1:D:92:GLU:HG2	1:D:101:ILE:HG12	1.91	0.52
2:G:92:ALA:HB2	2:G:105:PHE:CD1	2.44	0.52
2:E:13:LEU:HD22	2:E:111:LEU:HD21	1.91	0.52
1:D:126:ASP:CB	1:D:130:SER:HB2	2.40	0.51
2:G:29:HIS:HB3	2:G:94:SER:O	2.10	0.51
1:F:141:ASP:OD2	1:F:143:GLN:HG2	2.11	0.51
2:G:47:TYR:HD2	2:G:66:VAL:HG12	1.76	0.51
1:F:51:PHE:H	1:F:54:MET:HE2	1.76	0.51
2:E:27:MET:HB2	2:E:29:HIS:ND1	2.26	0.51
2:G:20:THR:HA	2:G:77:ARG:HA	1.93	0.51
1:D:27:ASP:HB2	1:D:30:SER:HB3	1.93	0.51
1:F:120:ALA:HB2	1:F:199:PHE:HB3	1.93	0.51
2:G:47:TYR:HD2	2:G:66:VAL:CG1	2.24	0.51
2:E:29:HIS:HB3	2:E:94:SER:O	2.12	0.50
2:G:164:LYS:HE3	2:G:165:GLU:O	2.10	0.50
2:E:87:SER:HB3	2:E:89:TYR:CE1	2.46	0.50
1:F:162:LEU:HD11	2:G:195:ARG:HB2	1.93	0.50
2:G:120:VAL:HG11	2:G:217:LEU:HD11	1.94	0.50
1:A:33:LEU:HD23	1:A:92:GLU:HB3	1.93	0.50
2:B:161:VAL:HB	2:B:166:VAL:HG21	1.94	0.50
1:A:31:THR:H	1:A:94:SER:HB3	1.76	0.49
1:F:30:SER:HB3	1:F:93:SER:C	2.37	0.49
2:G:27:MET:HE1	2:G:104:TYR:CD1	2.47	0.49
2:B:145:CYS:O	2:B:146:LEU:HD23	2.11	0.49
2:E:27:MET:HB2	2:E:29:HIS:CE1	2.47	0.49
2:G:68:ARG:HH21	2:G:71:THR:CA	2.24	0.49
1:D:26:THR:O	1:D:71:LYS:HE3	2.12	0.49
1:F:73:LEU:HD23	1:F:74:SER:N	2.28	0.49
2:B:13:LEU:O	2:B:113:VAL:HA	2.13	0.49
1:F:149:SER:OG	1:F:150:LYS:N	2.45	0.49
2:B:19:MET:HE2	2:B:21:LEU:HG	1.95	0.48
2:G:96:PRO:HB3	2:G:101:TYR:CE2	2.48	0.48
2:G:223:TRP:CD1	2:G:229:LYS:HA	2.48	0.48
1:F:69:LYS:HE3	1:F:70:ASP:OD1	2.14	0.48
2:E:145:CYS:HB2	2:E:159:TRP:CZ2	2.49	0.48
2:B:154:HIS:N	2:B:154:HIS:CD2	2.82	0.47
1:A:163:ASP:HB2	1:A:170:LYS:HD3	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:231:VAL:O	2:B:233:GLN:HG2	2.14	0.47
2:B:67:SER:O	2:B:75:PRO:HD2	2.15	0.47
2:B:13:LEU:HB2	2:B:113:VAL:HG22	1.97	0.47
2:B:64:TYR:HB3	2:B:76:LEU:HD11	1.97	0.47
2:E:43:LEU:O	2:E:44:LYS:HG2	2.15	0.47
2:E:204:PRO:HA	2:E:241:GLY:O	2.14	0.47
1:A:49:TYR:CZ	1:A:57:LYS:HE2	2.50	0.47
2:E:12:ILE:HD11	2:E:152:PRO:HD3	1.97	0.47
1:F:51:PHE:HD1	1:F:53:ASN:H	1.62	0.47
2:G:168:SER:O	2:G:170:VAL:HG23	2.14	0.47
2:E:68:ARG:HD2	2:E:73:ASP:O	2.15	0.47
2:E:197:SER:OG	2:E:199:THR:HB	2.15	0.47
1:F:126:ASP:OD1	1:F:127:SER:N	2.48	0.47
2:G:38:ASP:OD2	2:G:87:SER:OG	2.29	0.47
2:B:12:ILE:HD11	2:B:216:GLY:HA2	1.97	0.46
1:A:94:SER:OG	1:A:97:GLY:HA3	2.15	0.46
2:B:3:GLY:HA3	2:B:26:ASP:OD1	2.16	0.46
2:B:130:PRO:HB2	2:B:135:ILE:HD11	1.97	0.46
2:E:49:SER:OG	2:E:68:ARG:NH1	2.48	0.46
1:A:155:TYR:O	1:A:176:ALA:HA	2.15	0.46
1:D:13:VAL:HG21	1:D:19:SER:HB2	1.97	0.46
1:D:14:ARG:HB2	1:D:17:ASP:OD1	2.16	0.46
2:G:217:LEU:HD12	2:G:230:PRO:O	2.16	0.46
2:E:3:GLY:HA3	2:E:26:ASP:OD1	2.15	0.46
1:F:140:PHE:CE1	1:F:172:ASN:HB3	2.50	0.45
2:G:102:GLU:HB3	2:G:104:TYR:CE1	2.51	0.45
1:D:116:ASN:H	1:D:117:PRO:HD3	1.80	0.45
1:A:184:ALA:H	1:A:187:ASN:ND2	2.14	0.45
1:D:33:LEU:HB3	1:D:73:LEU:HD22	1.98	0.45
2:B:9:LYS:HG2	2:B:10:PHE:CD2	2.51	0.45
2:B:35:TYR:OH	2:B:103:GLN:NE2	2.49	0.45
2:G:153:ASP:C	2:G:154:HIS:HD2	2.24	0.45
2:B:25:GLN:NE2	2:B:29:HIS:HB2	2.32	0.45
1:A:199:PHE:CD1	1:A:199:PHE:C	2.95	0.45
1:D:54:MET:CE	1:D:57:LYS:HB2	2.46	0.45
1:D:121:VAL:HG22	1:D:137:PHE:HB2	1.99	0.45
2:G:10:PHE:CD1	2:G:110:ARG:HB3	2.52	0.45
1:F:154:VAL:N	1:F:178:SER:HG	2.14	0.45
1:D:32:TYR:HB3	1:D:51:PHE:CD1	2.51	0.45
2:G:21:LEU:HD22	2:G:76:LEU:HD23	1.98	0.45
2:G:72:GLU:H	2:G:72:GLU:CD	2.24	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:164:LYS:HE2	2:G:164:LYS:HB3	1.72	0.45
1:A:137:PHE:HB2	1:A:189:PHE:CE2	2.52	0.44
2:G:183:LEU:HD12	2:G:185:ASP:OD1	2.18	0.44
1:F:126:ASP:OD2	1:F:128:LYS:HG2	2.17	0.44
1:D:199:PHE:CZ	1:D:201:PRO:HB3	2.52	0.44
1:F:13:VAL:HG11	1:F:19:SER:HB3	1.98	0.44
2:G:178:LYS:HD3	2:G:181:PRO:HA	2.00	0.44
2:B:161:VAL:HG22	2:B:208:PHE:CD1	2.52	0.44
2:E:172:THR:HG23	2:E:192:SER:HB2	1.99	0.44
1:F:156:ILE:HG22	1:F:157:THR:O	2.18	0.44
1:A:35:TRP:CZ3	1:A:90:CYS:HB3	2.53	0.44
2:B:183:LEU:HD12	2:B:184:ASN:H	1.82	0.44
2:G:33:TYR:HB3	2:G:35:TYR:CE2	2.52	0.44
2:E:35:TYR:CD2	2:E:43:LEU:HD12	2.52	0.44
2:G:47:TYR:HE1	2:G:61:PRO:HA	1.82	0.44
2:G:153:ASP:C	2:G:154:HIS:CD2	2.96	0.44
2:E:14:LYS:O	2:E:17:GLN:HG3	2.18	0.44
2:E:14:LYS:N	2:E:17:GLN:OE1	2.43	0.44
2:B:204:PRO:HA	2:B:241:GLY:O	2.17	0.44
1:D:66:LEU:HD12	1:D:67:ASN:N	2.32	0.44
2:E:205:ARG:HB2	2:E:205:ARG:NH1	2.32	0.44
2:G:52:ALA:HA	2:G:68:ARG:HG3	1.99	0.44
1:A:126:ASP:OD1	1:A:127:SER:N	2.51	0.43
1:D:179:ASN:OD1	1:D:179:ASN:N	2.51	0.43
2:E:199:THR:HG22	2:E:200:PHE:N	2.33	0.43
1:A:56:MET:CE	1:A:58:GLN:HE21	2.28	0.43
1:D:51:PHE:HE2	2:G:28:ASN:HB3	1.83	0.43
1:D:50:ILE:HG13	1:D:54:MET:HE2	2.00	0.43
1:F:114:ILE:HG21	1:F:140:PHE:O	2.18	0.43
2:G:26:ASP:OD2	2:G:26:ASP:C	2.62	0.43
2:E:25:GLN:NE2	2:E:93:SER:OG	2.52	0.43
2:E:169:GLY:O	2:E:194:LEU:HA	2.18	0.43
2:E:11:ARG:CG	2:E:19:MET:HE3	2.42	0.43
1:D:66:LEU:HD12	1:D:67:ASN:H	1.83	0.43
1:A:150:LYS:HD3	1:A:191:ASN:HB2	2.00	0.43
2:G:11:ARG:HG2	2:G:19:MET:CE	2.48	0.43
2:G:12:ILE:HD11	2:G:152:PRO:CD	2.48	0.43
1:A:162:LEU:HD11	2:B:195:ARG:HB2	2.00	0.43
1:D:154:VAL:HG22	1:D:178:SER:CB	2.49	0.43
1:A:109:PHE:HZ	1:A:159:LYS:HB3	1.83	0.42
1:A:123:GLN:O	2:B:131:SER:HB2	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ARG:NH2	1:A:131:ASP:HB2	2.33	0.42
1:D:67:ASN:OD1	1:D:69:LYS:HB3	2.19	0.42
1:A:39:GLU:HB3	1:A:40:PRO:CD	2.44	0.42
1:D:46:LEU:HD12	1:D:47:LEU:N	2.34	0.42
2:E:154:HIS:N	2:E:154:HIS:CD2	2.86	0.42
1:A:140:PHE:CE1	1:A:172:ASN:HB3	2.53	0.42
1:A:190:ASN:HD22	1:A:190:ASN:HA	1.69	0.42
1:D:58:GLN:HG3	1:D:62:LEU:O	2.19	0.42
2:E:130:PRO:HG3	2:E:141:ALA:HB1	2.01	0.42
2:B:203:ASN:HA	2:B:204:PRO:HD3	1.85	0.42
1:F:92:GLU:HG2	1:F:101:ILE:HD11	2.02	0.42
1:A:99:LYS:HD3	1:A:99:LYS:HA	1.69	0.42
2:G:223:TRP:HB2	2:G:229:LYS:HE3	2.01	0.42
1:D:175:VAL:HG11	2:E:144:VAL:HG11	2.02	0.42
1:A:14:ARG:O	1:A:17:ASP:HB2	2.20	0.42
1:F:28:SER:HB2	1:F:71:LYS:HZ2	1.85	0.42
1:F:121:VAL:HA	1:F:136:LEU:O	2.20	0.42
2:G:33:TYR:N	2:G:92:ALA:O	2.53	0.42
2:B:32:MET:HE2	2:B:32:MET:HB3	1.85	0.42
1:D:27:ASP:HB2	1:D:30:SER:CB	2.49	0.41
2:E:59:GLU:O	2:E:60:VAL:C	2.62	0.41
1:A:117:PRO:HD2	2:E:205:ARG:NE	2.35	0.41
2:E:13:LEU:HD11	2:E:19:MET:HG2	2.02	0.41
1:D:70:ASP:OD1	1:D:70:ASP:N	2.54	0.41
2:E:11:ARG:HA	2:E:11:ARG:HD2	1.70	0.41
1:D:52:SER:HA	1:D:66:LEU:CD2	2.51	0.41
2:G:179:GLU:O	2:G:180:GLN:HG3	2.21	0.41
2:E:120:VAL:HG12	2:E:230:PRO:HB2	2.02	0.41
1:F:51:PHE:HB3	1:F:54:MET:HB2	2.02	0.41
1:A:190:ASN:C	1:A:192:SER:H	2.29	0.41
2:G:96:PRO:HA	2:G:101:TYR:CD2	2.55	0.41
2:E:196:VAL:HG23	2:E:197:SER:O	2.20	0.40
2:G:14:LYS:HB2	2:G:117:LEU:CD1	2.50	0.40
1:A:126:ASP:HB3	1:A:130:SER:N	2.36	0.40
2:B:130:PRO:HD2	2:B:201:TRP:CZ2	2.56	0.40
1:D:32:TYR:HB2	1:D:34:TYR:CE1	2.57	0.40
2:E:82:ALA:C	2:E:113:VAL:HG11	2.46	0.40
1:A:117:PRO:HD2	2:E:205:ARG:HE	1.87	0.40
1:D:180:LYS:HD3	1:D:182:ASP:OD1	2.21	0.40
1:F:101:ILE:O	1:F:101:ILE:HD12	2.22	0.40
2:G:60:VAL:HG13	2:G:60:VAL:O	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:84:SER:C	2:G:86:THR:H	2.30	0.40
2:B:139:GLN:OE1	2:B:139:GLN:HA	2.21	0.40
2:G:170:VAL:HA	2:G:193:ARG:O	2.22	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	190/206 (92%)	163 (86%)	19 (10%)	8 (4%)	2	7
1	D	177/206 (86%)	141 (80%)	28 (16%)	8 (4%)	2	7
1	F	179/206 (87%)	146 (82%)	31 (17%)	2 (1%)	11	35
2	B	241/244 (99%)	221 (92%)	18 (8%)	2 (1%)	16	43
2	E	241/244 (99%)	212 (88%)	24 (10%)	5 (2%)	5	20
2	G	241/244 (99%)	213 (88%)	24 (10%)	4 (2%)	7	24
All	All	1269/1350 (94%)	1096 (86%)	144 (11%)	29 (2%)	5	18

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ALA
1	A	159	LYS
1	D	104	ALA
1	D	116	ASN
2	E	39	PRO
1	D	131	ASP
2	E	2	ALA
1	F	56	MET
1	A	17	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	180	LYS
2	B	225	GLN
1	D	133	SER
1	D	167	MET
2	E	99	SER
2	G	30	ASN
2	G	69	SER
1	A	133	SER
1	D	194	ILE
2	E	32	MET
2	G	242	ARG
1	A	164	MET
1	D	129	SER
2	E	69	SER
1	F	27	ASP
2	B	241	GLY
2	G	199	THR
1	D	193	ILE
1	A	103	GLY
1	A	95	GLY

### 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	166/184 (90%)	154 (93%)	12 (7%)	13	37
1	D	153/184 (83%)	139 (91%)	14 (9%)	8	26
1	F	158/184 (86%)	142 (90%)	16 (10%)	7	23
2	B	201/211 (95%)	193 (96%)	8 (4%)	28	61
2	E	201/211 (95%)	188 (94%)	13 (6%)	15	42
2	G	202/211 (96%)	188 (93%)	14 (7%)	14	39
All	All	1081/1185 (91%)	1004 (93%)	77 (7%)	13	38

All (77) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	11	LEU
1	A	19	SER
1	A	23	CYS
1	A	28	SER
1	A	30	SER
1	A	99	LYS
1	A	116	ASN
1	A	142	SER
1	A	147	SER
1	A	149	SER
1	A	156	ILE
1	A	162	LEU
2	B	66	VAL
2	B	99	SER
2	B	114	THR
2	B	116	ASP
2	B	161	VAL
2	B	168	SER
2	B	186	SER
2	B	233	GLN
1	D	11	LEU
1	D	18	SER
1	D	23	CYS
1	D	63	THR
1	D	82	THR
1	D	128	LYS
1	D	142	SER
1	D	148	GLN
1	D	157	THR
1	D	162	LEU
1	D	165	ARG
1	D	166	SER
1	D	179	ASN
1	D	192	SER
2	E	5	THR
2	E	7	THR
2	E	13	LEU
2	E	25	GLN
2	E	49	SER
2	E	67	SER
2	E	80	LEU
2	E	114	THR
2	E	127	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	153	ASP
2	E	158	SER
2	E	175	GLN
2	E	199	THR
1	F	12	SER
1	F	23	CYS
1	F	25	TYR
1	F	28	SER
1	F	30	SER
1	F	55	ASP
1	F	63	THR
1	F	68	LYS
1	F	72	HIS
1	F	73	LEU
1	F	90	CYS
1	F	149	SER
1	F	157	THR
1	F	160	CYS
1	F	166	SER
1	F	182	ASP
2	G	5	THR
2	G	7	THR
2	G	49	SER
2	G	61	PRO
2	G	67	SER
2	G	69	SER
2	G	71	THR
2	G	88	VAL
2	G	99	SER
2	G	127	VAL
2	G	158	SER
2	G	175	GLN
2	G	191	SER
2	G	193	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	38	GLN
1	A	58	GLN
1	A	72	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	123	GLN
1	A	187	ASN
1	A	190	ASN
1	A	191	ASN
2	B	25	GLN
2	B	28	ASN
2	B	29	HIS
2	B	65	ASN
2	B	103	GLN
2	B	175	GLN
2	B	233	GLN
1	D	22	ASN
1	D	45	GLN
1	D	58	GLN
1	D	190	ASN
2	E	29	HIS
2	E	103	GLN
2	E	119	ASN
2	E	206	ASN
2	E	225	GLN
2	E	233	GLN
1	F	22	ASN
1	F	38	GLN
1	F	53	ASN
1	F	113	ASN
1	F	115	GLN
1	F	123	GLN
2	G	22	GLN
2	G	25	GLN
2	G	202	GLN
2	G	203	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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

### 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	192/206 (93%)	0.18	12 (6%) 26 20	11, 29, 79, 126	0
1	D	185/206 (89%)	0.49	10 (5%) 31 24	25, 46, 75, 91	0
1	F	185/206 (89%)	0.23	4 (2%) 62 53	23, 41, 70, 103	0
2	B	243/244 (99%)	-0.14	2 (0%) 82 76	8, 24, 50, 74	0
2	E	243/244 (99%)	0.21	3 (1%) 76 69	17, 42, 59, 68	0
2	G	243/244 (99%)	0.17	5 (2%) 63 54	21, 40, 61, 73	0
All	All	1291/1350 (95%)	0.17	36 (2%) 55 45	8, 37, 67, 126	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	PHE	8.2
1	D	95	GLY	7.0
1	A	97	GLY	5.5
1	D	94	SER	5.3
1	F	154	VAL	5.2
1	D	30	SER	3.6
1	A	99	LYS	3.6
1	D	27	ASP	3.6
1	D	93	SER	3.5
1	F	93	SER	3.5
1	A	132	LYS	3.5
2	G	47	TYR	3.4
2	B	243	ALA	3.3
1	A	95	GLY	3.3
1	A	96	GLY	3.1
2	G	243	ALA	3.0
1	D	32	TYR	2.9
2	E	101	TYR	2.6
1	F	55	ASP	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	G	60	VAL	2.5
2	G	31	TYR	2.4
1	A	159	LYS	2.4
1	D	43	GLY	2.3
1	D	115	GLN	2.3
1	D	182	ASP	2.3
1	A	130	SER	2.3
1	F	114	ILE	2.3
1	A	94	SER	2.2
1	A	42	ALA	2.2
1	A	128	LYS	2.1
1	A	165	ARG	2.1
1	D	193	ILE	2.1
2	E	103	GLN	2.1
2	B	41	MET	2.1
2	G	93	SER	2.0
2	E	243	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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.