



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 AM GMT

PDB ID : 2BKT  
Title : CRYSTAL STRUCTURE OF RENIN-PF00257567 COMPLEX  
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Deposited on : 2005-02-18  
Resolution : 2.30 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](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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

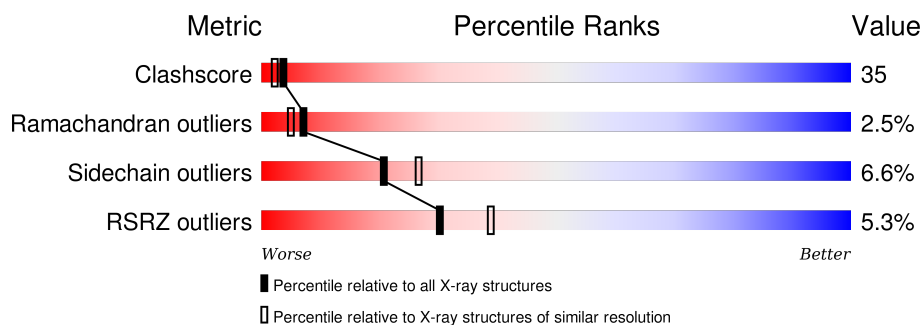
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	340	<div> <div>7%</div> <div>45%</div> <div>46%</div> <div>6%</div> <div>.</div> </div>
1	B	340	<div> <div>4%</div> <div>47%</div> <div>44%</div> <div>5%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

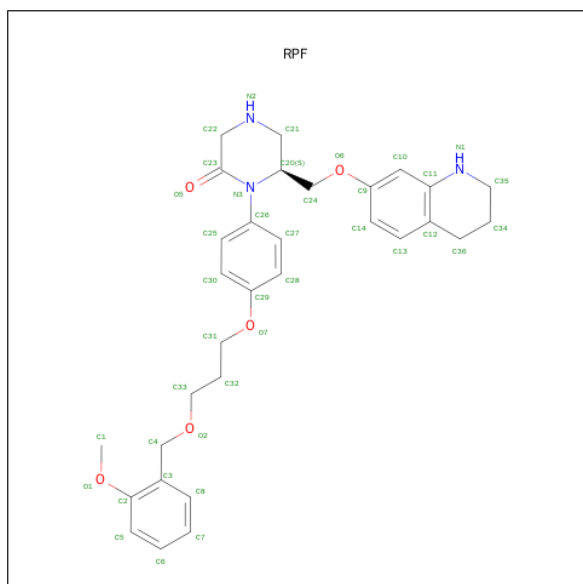
There are 3 unique types of molecules in this entry. The entry contains 5278 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	1
			2542	1626	411	491	14			
1	B	330	Total	C	N	O	S	0	0	1
			2542	1626	411	491	14			

- Molecule 2 is 1-{4-[3-(2-METHOXY-BENZYLOXY)-PROPOXY]-PHENYL}-6-(1,2,3,4-TETRAHYDRO-QUINOLIN-7-YLOXYMETHYL)-PIPERAZIN-2-ONE (three-letter code: RPF) (formula: C<sub>31</sub>H<sub>37</sub>N<sub>3</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			39	31	3	5		
2	B	1	Total	C	N	O	0	0
			39	31	3	5		

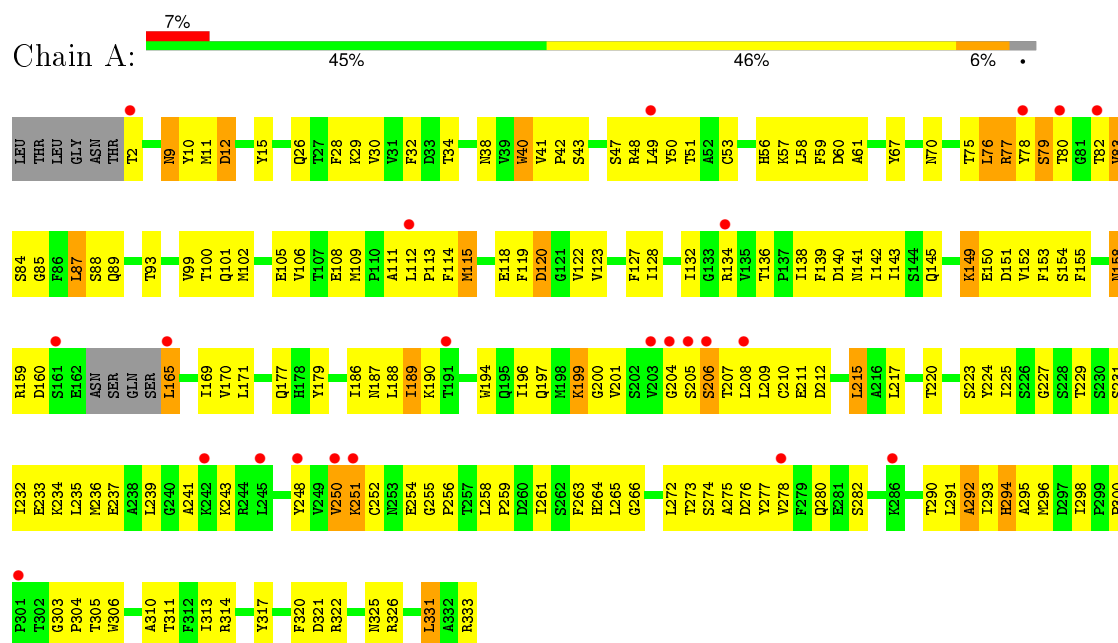
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total 47	O 47	0	0
3	B	69	Total 69	O 69	0	0

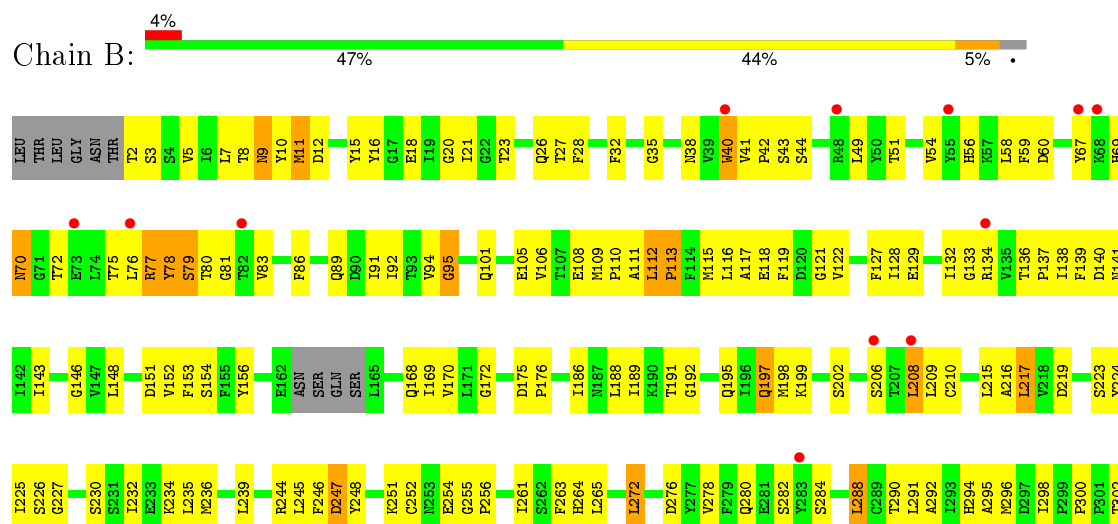
### 3 Residue-property plots

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



#### • Molecule 1: RENIN



G303	F304	T305	W306	A307
A310	T311	F312	Y317	D321
R322	R323	W324	W325	R326
F329	A330	L331	A332	R333

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.90Å 138.90Å 138.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 46.30 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.3 (50.00-2.30) 93.3 (46.30-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.244 , 0.291 0.248 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 25.7	EDS
Estimated twinning fraction	0.074 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 38613 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: RPF

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	0.40	0/2601	0.71	0/3526
1	B	0.42	0/2601	0.74	0/3526
All	All	0.41	0/5202	0.72	0/7052

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	2542	0	2477	193	0
1	B	2542	0	2477	167	0
2	A	39	0	37	5	0
2	B	39	0	37	11	0
3	A	47	0	0	3	0
3	B	69	0	0	3	0
All	All	5278	0	5028	360	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 35.

All (360) 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:B:198:MET:HG3	1:B:216:ALA:HB2	1.43	0.96
1:A:158:ASN:ND2	1:A:159:ARG:H	1.65	0.95
1:A:158:ASN:HD22	1:A:159:ARG:H	1.06	0.94
1:A:26:GLN:HE22	1:A:60:ASP:H	1.10	0.91
1:A:273:THR:HG23	1:A:275:ALA:H	1.36	0.90
1:A:87:LEU:HD21	1:A:102:MET:HB3	1.56	0.88
1:B:217:LEU:HD13	1:B:219:ASP:HB2	1.58	0.86
1:B:215:LEU:HB2	1:B:305:THR:HG23	1.60	0.83
1:B:255:GLY:HA3	1:B:280:GLN:HE22	1.45	0.82
1:A:250:VAL:HG11	1:A:258:LEU:HD11	1.61	0.81
1:B:43:SER:HB2	1:B:105:GLU:HB3	1.62	0.81
1:A:251:LYS:NZ	1:A:254:GLU:HB3	1.96	0.81
1:A:158:ASN:HD22	1:A:159:ARG:N	1.79	0.80
1:A:77:ARG:H	1:A:77:ARG:HD2	1.46	0.80
1:A:149:LYS:HA	1:A:149:LYS:HE3	1.64	0.79
1:A:199:LYS:NZ	1:A:264:HIS:HB3	1.97	0.79
1:B:232:ILE:HG13	1:B:295:ALA:HA	1.65	0.79
1:B:195:GLN:HE21	1:B:305:THR:HG21	1.47	0.77
1:B:217:LEU:CD1	1:B:219:ASP:HB2	2.15	0.77
1:A:101:GLN:NE2	1:A:138:ILE:HA	2.00	0.77
1:A:40:TRP:HH2	1:A:132:ILE:HD12	1.50	0.77
1:A:298:ILE:HG22	1:A:303:GLY:HA3	1.68	0.76
1:B:76:LEU:HB2	1:B:83:VAL:CG1	2.16	0.75
1:B:75:THR:C	1:B:76:LEU:HD22	2.06	0.75
1:B:26:GLN:HE22	1:B:60:ASP:H	1.33	0.74
1:A:158:ASN:ND2	1:A:159:ARG:N	2.34	0.74
1:A:274:SER:O	1:A:278:VAL:HG12	1.86	0.74
1:A:211:GLU:O	1:A:212:ASP:HB2	1.88	0.74
1:B:78:TYR:O	1:B:81:GLY:N	2.20	0.74
1:B:215:LEU:CB	1:B:305:THR:HG23	2.19	0.73
1:A:76:LEU:HB3	1:A:132:ILE:CD1	2.19	0.73
1:B:9:ASN:HD21	1:B:12:ASP:H	1.36	0.72
1:B:208:LEU:HD13	1:B:208:LEU:H	1.55	0.72
1:A:234:LYS:O	1:A:237:GLU:HG3	1.89	0.72
1:B:224:TYR:HB3	1:B:292:ALA:O	1.89	0.71
1:B:40:TRP:CZ2	1:B:76:LEU:HD21	2.25	0.71
1:A:76:LEU:HB3	1:A:132:ILE:HD11	1.73	0.70
1:A:99:VAL:HG21	1:A:142:ILE:HG12	1.73	0.70
1:B:176:PRO:HG3	3:B:2038:HOH:O	1.90	0.69
1:B:246:PHE:O	1:B:247:ASP:O	2.11	0.69
1:B:40:TRP:HH2	1:B:132:ILE:HG13	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ASP:OD1	1:B:326:ARG:NH1	2.26	0.69
1:A:239:LEU:HD21	1:A:261:ILE:HD11	1.74	0.68
1:A:50:TYR:CZ	1:A:108:GLU:HG3	2.27	0.68
1:A:61:ALA:HB1	1:A:67:TYR:CE1	2.29	0.68
1:B:198:MET:HG2	1:B:265:LEU:CD2	2.24	0.68
1:A:99:VAL:HG11	1:A:141:ASN:HB3	1.77	0.67
1:A:251:LYS:HB2	1:A:251:LYS:HZ3	1.60	0.67
1:B:255:GLY:HA3	1:B:280:GLN:NE2	2.09	0.67
1:B:331:LEU:HD11	3:B:2067:HOH:O	1.94	0.67
1:A:188:LEU:HG	1:A:325:ASN:O	1.96	0.66
1:B:81:GLY:HA2	1:B:110:PRO:HG2	1.78	0.66
1:A:77:ARG:HA	1:A:82:THR:HA	1.79	0.65
1:B:151:ASP:HB2	1:B:323:ARG:HB2	1.77	0.65
1:A:48:ARG:HH12	1:A:58:LEU:HD11	1.61	0.65
1:A:250:VAL:HG22	1:A:251:LYS:HZ2	1.62	0.64
1:A:75:THR:O	1:A:132:ILE:HD13	1.98	0.64
1:B:42:PRO:HG3	2:B:567:RPF:H8	1.79	0.63
1:B:225:ILE:HG13	1:B:311:THR:HB	1.80	0.63
1:B:153:PHE:HA	1:B:170:VAL:O	1.97	0.63
1:B:198:MET:HG2	1:B:265:LEU:HD21	1.80	0.63
1:A:292:ALA:HB1	1:A:311:THR:OG1	1.99	0.63
1:A:199:LYS:HZ3	1:A:264:HIS:HB3	1.62	0.63
1:B:195:GLN:HE21	1:B:305:THR:CG2	2.12	0.62
1:B:236:MET:HG3	1:B:248:TYR:CG	2.35	0.62
1:B:208:LEU:O	1:B:209:LEU:HD23	1.99	0.62
1:A:250:VAL:HG22	1:A:251:LYS:NZ	2.15	0.62
1:B:83:VAL:HA	1:B:108:GLU:O	2.00	0.62
1:A:232:ILE:HG13	1:A:295:ALA:HA	1.80	0.62
1:B:78:TYR:HB3	1:B:81:GLY:HA3	1.81	0.62
1:B:9:ASN:C	1:B:9:ASN:HD22	2.03	0.61
1:A:83:VAL:HG21	2:A:567:RPF:H321	1.82	0.61
1:B:76:LEU:HD11	1:B:132:ILE:HG13	1.83	0.60
1:A:251:LYS:H	1:A:251:LYS:HE3	1.65	0.60
1:B:42:PRO:HB2	1:B:58:LEU:HD23	1.83	0.60
1:B:76:LEU:HB2	1:B:83:VAL:HG13	1.84	0.60
1:A:128:ILE:HD12	1:A:136:THR:HA	1.83	0.60
1:A:189:ILE:HD12	1:A:215:LEU:HG	1.83	0.60
1:A:251:LYS:HZ1	1:A:254:GLU:HB3	1.65	0.60
1:A:106:VAL:HG21	2:A:567:RPF:O2	2.01	0.60
1:B:244:ARG:C	1:B:245:LEU:HD12	2.22	0.59
1:A:200:GLY:HA2	1:A:210:CYS:SG	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LEU:HG	1:B:239:LEU:CD2	2.32	0.59
1:A:251:LYS:HZ2	1:A:251:LYS:N	2.01	0.59
1:A:243:LYS:HB2	1:A:248:TYR:CE2	2.38	0.59
1:A:42:PRO:HG2	1:A:57:LYS:O	2.03	0.59
1:A:236:MET:SD	1:A:291:LEU:HD12	2.43	0.58
1:A:47:SER:OG	1:A:49:LEU:HD23	2.03	0.58
1:A:236:MET:O	1:A:241:ALA:HB3	2.04	0.58
1:A:106:VAL:HG11	1:A:109:MET:HB3	1.84	0.58
1:B:9:ASN:ND2	1:B:12:ASP:H	2.02	0.58
1:B:236:MET:HG3	1:B:248:TYR:CD2	2.39	0.58
1:A:303:GLY:HA2	1:A:305:THR:HG22	1.86	0.58
1:A:209:LEU:HD21	1:A:234:LYS:HD3	1.86	0.58
1:A:140:ASP:CG	1:A:322:ARG:HH22	2.07	0.58
1:A:78:TYR:O	1:A:79:SER:C	2.43	0.57
1:A:273:THR:HG23	1:A:275:ALA:N	2.14	0.57
1:B:226:SER:OG	1:B:307:ALA:HB3	2.03	0.57
1:B:78:TYR:O	1:B:80:THR:N	2.38	0.57
1:A:188:LEU:HG	1:A:325:ASN:C	2.25	0.57
1:A:251:LYS:HZ3	1:A:254:GLU:HB3	1.69	0.57
1:A:153:PHE:HA	1:A:170:VAL:O	2.05	0.57
1:B:199:LYS:HB2	1:B:264:HIS:ND1	2.20	0.57
1:A:186:ILE:HG21	1:A:196:ILE:HB	1.87	0.56
1:B:244:ARG:HG3	1:B:245:LEU:H	1.68	0.56
1:A:199:LYS:O	1:A:264:HIS:HB2	2.06	0.56
1:A:208:LEU:O	1:A:209:LEU:HG	2.05	0.56
1:B:77:ARG:H	1:B:77:ARG:HD2	1.70	0.56
1:B:10:TYR:CD2	1:B:118:GLU:HG3	2.40	0.56
1:B:77:ARG:N	1:B:77:ARG:HD2	2.21	0.56
1:B:9:ASN:HD21	1:B:12:ASP:N	2.02	0.55
1:B:133:GLY:O	1:B:134:ARG:CG	2.54	0.55
1:B:202:SER:HB3	1:B:206:SER:O	2.05	0.55
1:A:224:TYR:HB3	1:A:292:ALA:O	2.07	0.55
1:B:76:LEU:N	1:B:76:LEU:HD22	2.20	0.55
1:A:251:LYS:NZ	1:A:251:LYS:HB2	2.22	0.55
1:B:10:TYR:CG	1:B:118:GLU:HG3	2.42	0.55
1:A:251:LYS:H	1:A:251:LYS:CE	2.20	0.54
1:B:226:SER:HA	1:B:294:HIS:O	2.07	0.54
1:B:101:GLN:NE2	1:B:138:ILE:HA	2.23	0.54
1:B:305:THR:HG22	1:B:306:TRP:O	2.08	0.54
1:B:235:LEU:HG	1:B:239:LEU:HD21	1.90	0.54
1:B:32:PHE:CD1	1:B:169:ILE:HD12	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:TYR:OH	1:A:314:ARG:HD3	2.08	0.54
1:B:188:LEU:HG	1:B:325:ASN:O	2.08	0.54
1:A:76:LEU:HD22	1:A:76:LEU:O	2.07	0.54
1:A:61:ALA:HB1	1:A:67:TYR:CD1	2.44	0.53
1:A:155:PHE:CD1	1:A:220:THR:HG21	2.43	0.53
1:A:10:TYR:CD2	1:A:118:GLU:HG3	2.42	0.53
1:A:89:GLN:HE21	1:A:100:THR:HG22	1.73	0.53
1:B:154:SER:HB3	1:B:317:TYR:CE1	2.43	0.53
1:B:112:LEU:HD23	1:B:113:PRO:CA	2.39	0.53
1:B:198:MET:HG3	1:B:216:ALA:CB	2.28	0.53
1:A:48:ARG:NH1	1:A:58:LEU:HD11	2.23	0.53
1:B:298:ILE:O	1:B:303:GLY:HA3	2.08	0.53
1:B:112:LEU:HD23	1:B:113:PRO:HB3	1.90	0.53
1:A:199:LYS:HZ1	1:A:264:HIS:HB3	1.73	0.53
1:A:76:LEU:CD1	1:A:83:VAL:HG13	2.39	0.53
1:A:209:LEU:CD2	1:A:234:LYS:HD3	2.39	0.53
1:A:290:THR:CG2	1:A:291:LEU:N	2.72	0.53
1:B:252:CYS:HB3	1:B:282:SER:O	2.09	0.53
1:B:32:PHE:CD1	1:B:169:ILE:CD1	2.92	0.53
1:B:208:LEU:CD2	1:B:209:LEU:HG	2.39	0.52
1:A:111:ALA:O	1:A:115:MET:HB2	2.10	0.52
1:B:75:THR:O	1:B:76:LEU:HD13	2.10	0.52
1:A:292:ALA:HB1	1:A:311:THR:HG1	1.73	0.52
1:A:42:PRO:HD3	1:A:120:ASP:O	2.10	0.52
1:B:23:THR:OG1	1:B:91:ILE:HD11	2.09	0.52
1:A:43:SER:HB2	1:A:105:GLU:HB3	1.92	0.52
1:A:151:ASP:CG	1:A:322:ARG:HB2	2.30	0.52
1:B:312:PHE:HE2	1:B:329:PHE:CE2	2.27	0.52
1:B:226:SER:HB2	1:B:296:MET:HB3	1.91	0.52
1:B:199:LYS:HD3	1:B:264:HIS:CE1	2.45	0.51
1:B:122:VAL:HG23	2:B:567:RPF:C1	2.40	0.51
1:A:76:LEU:HD13	1:A:83:VAL:HG13	1.91	0.51
1:B:223:SER:O	1:B:310:ALA:HB3	2.10	0.51
1:A:138:ILE:HG23	1:A:139:PHE:N	2.26	0.51
1:B:3:SER:OG	1:B:95:GLY:O	2.29	0.51
1:A:101:GLN:HE22	1:A:138:ILE:HA	1.75	0.51
1:A:152:VAL:HG12	1:A:321:ASP:HA	1.93	0.51
1:A:273:THR:HG22	1:A:276:ASP:OD1	2.11	0.51
1:A:77:ARG:CD	1:A:77:ARG:H	2.17	0.51
1:A:229:THR:O	1:A:233:GLU:HG3	2.10	0.51
1:A:151:ASP:OD1	1:A:322:ARG:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ASN:HB2	1:B:40:TRP:CZ3	2.46	0.51
1:A:290:THR:HG22	1:A:291:LEU:N	2.25	0.51
1:B:210:CYS:SG	1:B:210:CYS:O	2.69	0.51
1:B:40:TRP:CH2	1:B:76:LEU:HD11	2.46	0.51
1:B:122:VAL:HG23	2:B:567:RPF:H1C1	1.92	0.51
1:B:272:LEU:HD13	1:B:276:ASP:HB3	1.91	0.51
1:B:56:HIS:CD2	1:B:119:PHE:O	2.64	0.50
1:A:298:ILE:O	1:A:303:GLY:HA3	2.11	0.50
1:B:232:ILE:HG13	1:B:295:ALA:CA	2.40	0.50
1:B:251:LYS:HB2	1:B:254:GLU:HB2	1.93	0.50
1:B:133:GLY:O	1:B:134:ARG:HG3	2.11	0.50
1:B:324:ASN:HB2	1:B:326:ARG:HH11	1.76	0.50
1:A:40:TRP:CH2	1:A:132:ILE:HD12	2.39	0.50
1:A:9:ASN:HD22	1:A:10:TYR:N	2.10	0.50
1:B:89:GLN:NE2	3:B:2017:HOH:O	2.45	0.50
1:B:113:PRO:O	1:B:116:LEU:HB2	2.11	0.50
1:A:272:LEU:HD22	1:A:276:ASP:HB3	1.93	0.49
1:B:7:LEU:HD11	1:B:169:ILE:HG13	1.94	0.49
1:B:9:ASN:ND2	1:B:9:ASN:C	2.64	0.49
1:B:8:THR:O	1:B:15:TYR:HA	2.13	0.49
1:B:168:GLN:HE22	1:B:175:ASP:CB	2.25	0.49
1:B:11:MET:O	1:B:12:ASP:HB2	2.12	0.49
1:B:72:THR:O	1:B:86:PHE:HA	2.12	0.49
1:B:139:PHE:CE1	1:B:143:ILE:HD11	2.48	0.49
1:B:20:GLY:O	1:B:92:ILE:HA	2.12	0.49
1:A:9:ASN:HD21	1:A:12:ASP:HA	1.78	0.49
1:A:99:VAL:CG1	1:A:141:ASN:HB3	2.41	0.49
1:A:10:TYR:CE1	1:A:11:MET:HE3	2.48	0.49
1:A:154:SER:HB3	1:A:317:TYR:CE1	2.48	0.49
1:A:210:CYS:SG	1:A:210:CYS:O	2.71	0.49
1:A:85:GLY:HA3	1:A:105:GLU:O	2.13	0.49
1:B:42:PRO:HG3	2:B:567:RPF:C8	2.43	0.48
1:B:5:VAL:HG13	1:B:169:ILE:HB	1.95	0.48
1:A:177:GLN:O	1:A:333:ARG:HD2	2.13	0.48
1:B:5:VAL:CG1	1:B:169:ILE:HB	2.43	0.48
1:A:99:VAL:HG22	1:A:145:GLN:OE1	2.13	0.48
1:A:236:MET:HB3	1:A:241:ALA:HB3	1.94	0.48
1:B:136:THR:HG21	1:B:141:ASN:ND2	2.29	0.48
1:A:186:ILE:HG12	1:A:265:LEU:HB3	1.94	0.48
1:B:83:VAL:HG21	2:B:567:RPF:H321	1.96	0.48
1:B:208:LEU:HD23	1:B:209:LEU:HG	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:TYR:CZ	1:B:69:HIS:HA	2.48	0.48
1:B:256:PRO:HD3	1:B:280:GLN:NE2	2.29	0.48
1:B:305:THR:HG22	1:B:306:TRP:N	2.29	0.48
1:B:148:LEU:HB3	1:B:172:GLY:HA2	1.96	0.48
1:A:250:VAL:HG21	1:A:258:LEU:HD21	1.96	0.47
1:B:331:LEU:HD13	1:B:332:ALA:O	2.13	0.47
1:A:9:ASN:HD21	1:A:12:ASP:H	1.62	0.47
1:A:200:GLY:HA2	1:A:210:CYS:CB	2.43	0.47
1:B:137:PRO:HD2	1:B:140:ASP:OD2	2.14	0.47
1:A:200:GLY:HA2	1:A:210:CYS:HB3	1.95	0.47
1:B:156:TYR:HB2	1:B:317:TYR:CE2	2.49	0.47
1:B:191:THR:HG23	1:B:325:ASN:OD1	2.14	0.47
1:B:278:VAL:HG22	1:B:291:LEU:CD2	2.44	0.47
1:B:232:ILE:O	1:B:236:MET:HG2	2.15	0.47
1:A:179:TYR:HA	1:A:331:LEU:O	2.14	0.47
1:A:70:ASN:HB3	1:A:87:LEU:O	2.15	0.47
1:A:122:VAL:HG23	2:A:567:RPF:C1	2.45	0.46
1:B:292:ALA:HB1	1:B:311:THR:OG1	2.15	0.46
1:A:229:THR:HG22	1:A:233:GLU:HG3	1.97	0.46
1:A:41:VAL:O	1:A:105:GLU:HA	2.15	0.46
1:A:50:TYR:O	1:A:53:CYS:HB2	2.15	0.46
1:A:201:VAL:HG22	1:A:263:PHE:CD2	2.51	0.46
1:A:48:ARG:HH12	1:A:58:LEU:CD1	2.27	0.46
1:B:51:THR:HA	1:B:54:VAL:HG23	1.98	0.46
1:B:9:ASN:HD22	1:B:10:TYR:N	2.14	0.46
1:B:198:MET:CE	1:B:263:PHE:HB3	2.46	0.46
1:B:77:ARG:O	1:B:79:SER:N	2.49	0.46
1:A:43:SER:CB	1:A:105:GLU:HB3	2.46	0.46
1:B:119:PHE:CE2	2:B:567:RPF:H1C2	2.50	0.45
1:A:223:SER:O	1:A:310:ALA:HB3	2.16	0.45
1:A:87:LEU:HD23	1:A:88:SER:H	1.81	0.45
1:A:291:LEU:C	1:A:293:ILE:H	2.20	0.45
1:B:302:THR:O	1:B:305:THR:OG1	2.34	0.45
1:A:209:LEU:C	1:A:211:GLU:H	2.19	0.45
1:B:189:ILE:HD11	1:B:197:GLN:CB	2.46	0.45
1:B:40:TRP:HH2	1:B:76:LEU:HD11	1.81	0.45
1:B:7:LEU:HD11	1:B:169:ILE:CG1	2.46	0.45
1:B:127:PHE:HB2	1:B:192:GLY:HA2	1.99	0.45
1:A:274:SER:HA	1:A:277:TYR:CE2	2.52	0.45
1:A:10:TYR:CG	1:A:118:GLU:HG3	2.52	0.45
1:B:333:ARG:HH11	1:B:333:ARG:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:CG1	1:A:109:MET:HB3	2.47	0.45
1:B:256:PRO:HD3	1:B:280:GLN:HE22	1.81	0.44
1:A:139:PHE:O	1:A:143:ILE:HG13	2.17	0.44
1:A:278:VAL:HG13	1:A:278:VAL:O	2.17	0.44
1:A:186:ILE:N	1:A:186:ILE:HD12	2.33	0.44
1:A:189:ILE:HD11	1:A:196:ILE:C	2.37	0.44
1:B:278:VAL:HG22	1:B:291:LEU:HD22	1.98	0.44
1:A:303:GLY:HA2	1:A:304:PRO:C	2.37	0.44
1:A:278:VAL:HG11	1:A:280:GLN:NE2	2.33	0.44
1:B:78:TYR:C	1:B:81:GLY:H	2.17	0.44
1:A:28:PHE:HZ	1:A:59:PHE:HA	1.83	0.44
1:A:84:SER:OG	1:A:108:GLU:HB3	2.18	0.44
1:A:187:ASN:O	1:A:196:ILE:HG22	2.17	0.44
1:A:235:LEU:C	1:A:235:LEU:HD23	2.37	0.44
1:A:165:LEU:N	1:A:165:LEU:HD23	2.32	0.44
1:B:28:PHE:HZ	1:B:59:PHE:HA	1.82	0.44
1:B:227:GLY:N	1:B:232:ILE:HD11	2.32	0.44
1:A:30:VAL:HG21	1:A:123:VAL:CG2	2.48	0.44
1:A:150:GLU:HG2	1:A:152:VAL:HG13	1.99	0.44
1:A:229:THR:O	1:A:233:GLU:CG	2.66	0.43
1:A:9:ASN:C	1:A:9:ASN:HD22	2.19	0.43
1:B:111:ALA:HB1	1:B:115:MET:HE2	2.00	0.43
1:A:165:LEU:N	1:A:165:LEU:CD2	2.81	0.43
1:B:49:LEU:HA	1:B:49:LEU:HD13	1.86	0.43
1:B:43:SER:CB	1:B:105:GLU:HB3	2.40	0.43
1:A:236:MET:HE3	1:A:248:TYR:HB2	2.00	0.43
1:A:112:LEU:HA	1:A:113:PRO:HA	1.77	0.43
1:B:112:LEU:HD23	1:B:113:PRO:CB	2.48	0.43
1:B:91:ILE:O	1:B:91:ILE:HG13	2.19	0.43
1:B:69:HIS:ND1	1:B:70:ASN:N	2.66	0.43
1:B:18:GLU:HB3	1:B:27:THR:HG23	1.99	0.43
1:B:106:VAL:HG21	2:B:567:RPF:O2	2.19	0.43
1:B:76:LEU:HB2	1:B:83:VAL:HG11	1.97	0.43
1:A:251:LYS:NZ	1:A:251:LYS:CB	2.82	0.43
1:A:186:ILE:CG2	1:A:196:ILE:HB	2.48	0.43
1:B:112:LEU:HA	1:B:113:PRO:HA	1.73	0.43
1:A:32:PHE:HB2	1:A:169:ILE:HD11	2.01	0.43
1:A:255:GLY:N	1:A:256:PRO:CD	2.81	0.43
1:A:189:ILE:HB	1:A:190:LYS:H	1.52	0.43
1:A:155:PHE:CG	1:A:220:THR:HG21	2.54	0.43
1:A:119:PHE:CE2	2:A:567:RPF:H1C2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ILE:N	3:A:2021:HOH:O	2.16	0.43
1:A:78:TYR:HE2	1:A:113:PRO:CD	2.32	0.43
1:B:128:ILE:HG13	1:B:137:PRO:HD3	2.01	0.43
1:A:87:LEU:HD23	1:A:88:SER:N	2.34	0.43
1:B:117:ALA:HA	2:B:567:RPF:H341	2.01	0.43
1:B:122:VAL:CG2	2:B:567:RPF:H1C1	2.48	0.43
1:A:40:TRP:CD1	1:A:106:VAL:HG22	2.54	0.43
1:B:129:GLU:OE1	1:B:129:GLU:N	2.51	0.43
1:B:219:ASP:CG	2:B:567:RPF:H2	2.21	0.43
1:B:209:LEU:HD11	1:B:235:LEU:HB2	2.01	0.43
1:A:34:THR:HG23	1:A:220:THR:OG1	2.18	0.43
1:A:30:VAL:HG21	1:A:123:VAL:HG23	2.00	0.43
1:A:231:SER:HB3	1:A:306:TRP:CZ2	2.54	0.42
1:A:189:ILE:CD1	1:A:215:LEU:HG	2.47	0.42
1:A:220:THR:HA	1:A:313:ILE:CD1	2.49	0.42
1:A:9:ASN:ND2	1:A:9:ASN:C	2.73	0.42
1:A:252:CYS:HB3	1:A:282:SER:O	2.20	0.42
1:B:245:LEU:N	1:B:245:LEU:HD12	2.34	0.42
1:B:290:THR:CG2	1:B:291:LEU:N	2.82	0.42
1:B:152:VAL:HG12	1:B:321:ASP:HA	2.02	0.42
1:A:127:PHE:HA	3:A:2021:HOH:O	2.19	0.42
1:B:154:SER:O	1:B:169:ILE:HA	2.19	0.42
1:B:127:PHE:CB	1:B:192:GLY:HA2	2.50	0.42
1:B:40:TRP:O	1:B:121:GLY:HA3	2.20	0.42
1:A:229:THR:HA	1:A:295:ALA:HB1	2.01	0.42
1:B:230:SER:O	1:B:234:LYS:HG3	2.18	0.42
1:B:239:LEU:HD11	1:B:261:ILE:HD11	2.01	0.42
1:A:298:ILE:HG22	1:A:303:GLY:CA	2.45	0.42
1:A:239:LEU:CD2	1:A:259:PRO:HG2	2.49	0.42
1:A:261:ILE:HG12	1:A:277:TYR:CE2	2.55	0.42
1:A:227:GLY:HA2	1:A:306:TRP:HA	2.02	0.42
1:A:300:PRO:HG3	1:A:303:GLY:O	2.20	0.42
1:B:111:ALA:HB1	1:B:115:MET:CE	2.50	0.42
1:A:207:THR:O	1:A:207:THR:HG22	2.19	0.42
1:A:56:HIS:HE1	1:A:114:PHE:O	2.03	0.42
1:A:70:ASN:OD1	1:A:87:LEU:HB3	2.20	0.41
1:B:252:CYS:HB2	1:B:284:SER:O	2.20	0.41
1:A:76:LEU:HD11	1:A:83:VAL:HG22	2.03	0.41
1:A:209:LEU:C	1:A:211:GLU:N	2.72	0.41
1:B:21:ILE:CD1	1:B:41:VAL:HG11	2.50	0.41
1:A:132:ILE:C	1:A:134:ARG:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:O	1:A:119:PHE:HB2	2.21	0.41
1:A:38:ASN:HB2	1:A:40:TRP:CZ3	2.55	0.41
1:A:265:LEU:HA	3:A:2040:HOH:O	2.20	0.41
1:B:35:GLY:HA3	2:B:567:RPF:H222	2.03	0.41
1:B:109:MET:HA	1:B:110:PRO:HD3	1.81	0.41
1:B:78:TYR:CD2	1:B:78:TYR:O	2.73	0.41
1:B:198:MET:HE1	1:B:263:PHE:HA	2.02	0.41
1:A:225:ILE:HG13	1:A:311:THR:HB	2.02	0.41
1:B:288:LEU:HA	1:B:288:LEU:HD12	1.81	0.41
1:A:243:LYS:HB2	1:A:248:TYR:CD2	2.55	0.41
1:A:236:MET:CE	1:A:291:LEU:HD12	2.51	0.41
1:A:89:GLN:NE2	1:A:100:THR:HG22	2.35	0.41
1:A:154:SER:O	1:A:169:ILE:HA	2.21	0.41
1:A:28:PHE:HZ	1:A:59:PHE:CA	2.34	0.41
1:A:83:VAL:HG21	2:A:567:RPF:C32	2.50	0.41
1:A:9:ASN:HD21	1:A:12:ASP:N	2.17	0.41
1:B:186:ILE:N	1:B:186:ILE:HD12	2.36	0.41
1:A:294:HIS:CE1	1:A:296:MET:HE1	2.56	0.41
1:A:132:ILE:C	1:A:134:ARG:N	2.74	0.40
1:A:50:TYR:OH	1:A:108:GLU:HG3	2.21	0.40
1:B:326:ARG:HH11	1:B:326:ARG:HG2	1.87	0.40
1:A:77:ARG:N	1:A:77:ARG:HD2	2.25	0.40
1:A:76:LEU:HD13	1:A:76:LEU:O	2.21	0.40
1:A:78:TYR:CG	1:A:78:TYR:O	2.73	0.40
1:A:294:HIS:C	1:A:294:HIS:CD2	2.95	0.40
1:A:205:SER:O	1:A:206:SER:HB3	2.21	0.40
1:B:44:SER:OG	1:B:60:ASP:HA	2.21	0.40
1:A:186:ILE:HG13	1:A:266:GLY:HA3	2.02	0.40
1:B:94:VAL:O	1:B:95:GLY:C	2.60	0.40
1:B:16:TYR:CD1	1:B:16:TYR:N	2.89	0.40
1:A:194:TRP:CH2	1:A:320:PHE:HB3	2.57	0.40
1:A:47:SER:HG	1:A:49:LEU:HD23	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	326/340 (96%)	289 (89%)	28 (9%)	9 (3%)	6	4
1	B	326/340 (96%)	298 (91%)	21 (6%)	7 (2%)	9	7
All	All	652/680 (96%)	587 (90%)	49 (8%)	16 (2%)	7	5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	THR
1	A	189	ILE
1	B	78	TYR
1	B	247	ASP
1	A	204	GLY
1	B	79	SER
1	A	206	SER
1	A	12	ASP
1	A	160	ASP
1	A	292	ALA
1	B	70	ASN
1	A	79	SER
1	B	95	GLY
1	B	146	GLY
1	B	300	PRO
1	A	250	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	280/290 (97%)	257 (92%)	23 (8%)	14	17
1	B	280/290 (97%)	266 (95%)	14 (5%)	30	41
All	All	560/580 (97%)	523 (93%)	37 (7%)	21	27

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	9	ASN
1	A	40	TRP
1	A	51	THR
1	A	76	LEU
1	A	77	ARG
1	A	83	VAL
1	A	87	LEU
1	A	93	THR
1	A	115	MET
1	A	120	ASP
1	A	149	LYS
1	A	158	ASN
1	A	165	LEU
1	A	171	LEU
1	A	197	GLN
1	A	199	LYS
1	A	215	LEU
1	A	217	LEU
1	A	251	LYS
1	A	294	HIS
1	A	326	ARG
1	A	331	LEU
1	B	2	THR
1	B	9	ASN
1	B	11	MET
1	B	40	TRP
1	B	77	ARG
1	B	112	LEU
1	B	113	PRO
1	B	197	GLN
1	B	208	LEU
1	B	217	LEU
1	B	272	LEU
1	B	288	LEU
1	B	325	ASN
1	B	333	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	26	GLN
1	A	89	GLN
1	A	101	GLN
1	A	141	ASN
1	A	145	GLN
1	A	158	ASN
1	A	168	GLN
1	A	187	ASN
1	A	195	GLN
1	A	197	GLN
1	A	280	GLN
1	A	324	ASN
1	B	9	ASN
1	B	26	GLN
1	B	101	GLN
1	B	141	ASN
1	B	145	GLN
1	B	168	GLN
1	B	178	HIS
1	B	187	ASN
1	B	195	GLN
1	B	197	GLN
1	B	280	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

2 ligands 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	RPF	A	567	-	42,43,43	1.49	7 (16%)	47,57,57	1.28	4 (8%)
2	RPF	B	567	-	42,43,43	1.41	6 (14%)	47,57,57	1.28	4 (8%)

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	RPF	A	567	-	-	0/20/41/41	0/5/5/5
2	RPF	B	567	-	-	0/20/41/41	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	567	RPF	C26-N3	-2.17	1.39	1.43
2	A	567	RPF	C35-N1	2.07	1.48	1.45
2	A	567	RPF	C30-C25	2.20	1.42	1.38
2	A	567	RPF	C11-C12	2.20	1.43	1.40
2	A	567	RPF	C24-C20	2.22	1.57	1.52
2	B	567	RPF	C28-C29	2.26	1.43	1.38
2	A	567	RPF	C27-C26	2.31	1.43	1.39
2	B	567	RPF	C24-C20	2.42	1.57	1.52
2	A	567	RPF	C14-C9	2.63	1.44	1.38
2	B	567	RPF	C14-C9	2.84	1.44	1.38
2	B	567	RPF	C11-C12	3.05	1.44	1.40
2	B	567	RPF	C22-C23	3.14	1.53	1.51
2	A	567	RPF	C22-C23	3.51	1.54	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	567	RPF	C1-O1-C2	-4.36	110.93	117.54
2	A	567	RPF	C1-O1-C2	-3.87	111.67	117.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	567	RPF	O1-C2-C5	-3.20	118.97	124.35
2	B	567	RPF	O1-C2-C5	-2.92	119.44	124.35
2	B	567	RPF	O5-C23-N3	2.01	124.28	122.61
2	A	567	RPF	C11-C10-C9	2.24	121.89	117.68
2	B	567	RPF	O1-C2-C3	3.66	120.52	115.83
2	A	567	RPF	O1-C2-C3	3.90	120.83	115.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	567	RPF	5	0
2	B	567	RPF	11	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, 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	330/340 (97%)	0.60	23 (6%) 19 27	29, 51, 80, 91	0
1	B	330/340 (97%)	0.45	12 (3%) 46 55	26, 47, 71, 80	0
All	All	660/680 (97%)	0.53	35 (5%) 30 39	26, 49, 75, 91	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	SER	5.5
1	A	161	SER	5.1
1	B	55	TYR	4.9
1	A	204	GLY	4.2
1	A	286	LYS	3.6
1	B	208	LEU	3.4
1	B	82	THR	3.3
1	A	242	LYS	3.3
1	A	206	SER	3.1
1	A	250	VAL	3.0
1	B	134	ARG	2.9
1	A	245	LEU	2.8
1	A	112	LEU	2.7
1	A	2	THR	2.7
1	A	208	LEU	2.7
1	B	206	SER	2.6
1	A	82	THR	2.5
1	A	278	VAL	2.5
1	B	68	LYS	2.4
1	B	283	TYR	2.3
1	A	165	LEU	2.3
1	B	48	ARG	2.2
1	A	203	VAL	2.2
1	A	301	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	191	THR	2.2
1	B	67	TYR	2.2
1	B	76	LEU	2.2
1	A	78	TYR	2.2
1	A	251	LYS	2.2
1	A	49	LEU	2.1
1	A	80	THR	2.1
1	B	40	TRP	2.1
1	A	248	TYR	2.1
1	B	73	GLU	2.0
1	A	134	ARG	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 carbohydrates 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. 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	RPF	A	567	39/39	0.91	0.18	0.61	39,44,51,57	0
2	RPF	B	567	39/39	0.92	0.17	0.38	40,47,56,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.