



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:57 AM GMT

PDB ID : 1D0G  
Title : CRYSTAL STRUCTURE OF DEATH RECEPTOR 5 (DR5) BOUND TO APO2L/TRAIL  
Authors : Hymowitz, S.G.; Christinger, H.W.; Fuh, G.; O'Connell, M.P.; Kelley, R.F.; Ashkenazi, A.; de Vos, A.M.  
Deposited on : 1999-09-09  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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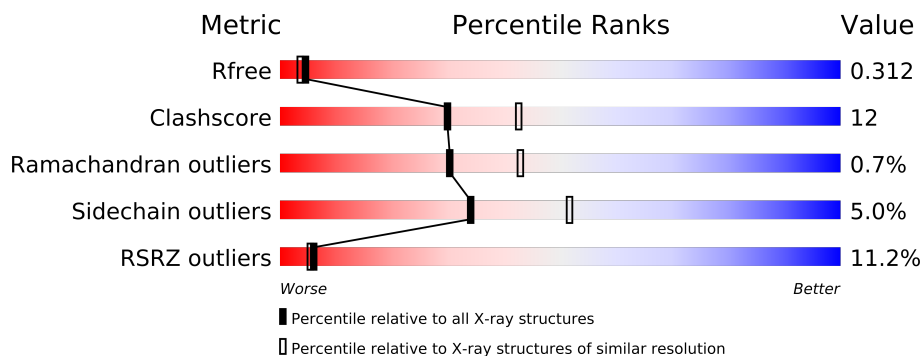
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	R	130	
1	S	130	
1	T	130	
2	A	168	
2	B	168	
2	D	168	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ZN	A	300	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6576 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DEATH RECEPTOR-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	108	Total	C	N	O	S	0	0	0
			833	498	150	169	16			
1	S	110	Total	C	N	O	S	0	0	0
			849	506	152	175	16			
1	T	110	Total	C	N	O	S	0	0	0
			849	506	152	175	16			

- Molecule 2 is a protein called APOPTOSIS-2 LIGAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	151	Total	C	N	O	S	8	1	0
			1253	800	216	233	4			
2	B	151	Total	C	N	O	S	16	1	0
			1253	800	216	233	4			
2	D	151	Total	C	N	O	S	16	1	0
			1253	800	216	233	4			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

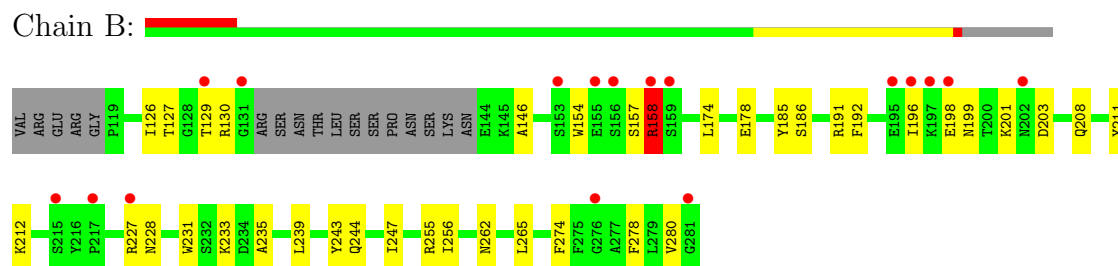
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total 71	O 71	0	0
5	B	58	Total 58	O 58	0	0
5	D	50	Total 50	O 50	0	0
5	R	40	Total 40	O 40	0	0
5	S	39	Total 39	O 39	0	0
5	T	26	Total 26	O 26	0	0



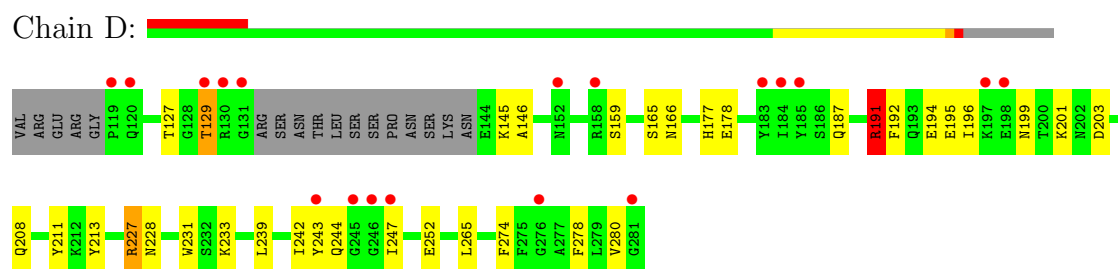
- Molecule 2: APOPTOSIS-2 LIGAND

Chain B:



- Molecule 2: APOPTOSIS-2 LIGAND

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.82Å 111.02Å 130.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.75 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.40) 98.0 (29.75-2.38)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.88 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 98.1	Depositor
R, $R_{free}$	0.222 , 0.267 0.282 , 0.312	Depositor DCC
$R_{free}$ test set	3818 reflections (9.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 26.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 38850 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	R	0.55	0/851	0.82	0/1150
1	S	0.51	0/867	0.77	0/1170
1	T	0.53	0/867	0.83	1/1170 (0.1%)
2	A	0.85	4/1288 (0.3%)	0.86	2/1729 (0.1%)
2	B	0.68	0/1288	0.90	4/1729 (0.2%)
2	D	0.64	0/1288	0.86	2/1729 (0.1%)
All	All	0.66	4/6449 (0.1%)	0.85	9/8677 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	198	GLU	CG-CD	13.26	1.71	1.51
2	A	198	GLU	CD-OE1	9.97	1.36	1.25
2	A	198	GLU	CD-OE2	6.88	1.33	1.25
2	A	194	GLU	CB-CG	-5.27	1.42	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	ARG	NE-CZ-NH2	-9.43	115.59	120.30
2	B	158	ARG	CG-CD-NE	6.93	126.36	111.80
2	B	158	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	T	129	GLU	N-CA-C	-6.62	93.14	111.00
2	D	191	ARG	NE-CZ-NH1	5.57	123.09	120.30
2	D	129	THR	N-CA-C	-5.33	96.62	111.00
2	B	129	THR	N-CA-C	-5.27	96.76	111.00
2	A	198	GLU	N-CA-C	5.20	125.04	111.00
2	A	167	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.



There are no planarity outliers.

## 5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	833	0	755	25	0
1	S	849	0	766	19	0
1	T	849	0	766	27	0
2	A	1253	0	1204	37	0
2	B	1253	0	1204	34	0
2	D	1253	0	1204	31	0
3	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	71	0	0	3	0
5	B	58	0	0	0	0
5	D	50	0	0	4	0
5	R	40	0	0	0	0
5	S	39	0	0	1	0
5	T	26	0	0	0	0
All	All	6576	0	5899	146	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (146) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:158:ARG:HD3	2:B:158:ARG:N	1.75	1.01
2:A:192:PHE:CD1	2:A:194:GLU:HG2	1.97	1.00
2:B:158:ARG:HD3	2:B:158:ARG:H	1.31	0.93
1:R:67:ASP:HB3	2:A:130:ARG:HH12	1.49	0.77
1:T:28:CYS:SG	1:T:34:ILE:HG22	2.26	0.76
2:B:228:ASN:HD22	2:D:239:LEU:H	1.34	0.75
2:A:228:ASN:HD22	2:B:239:LEU:H	1.34	0.75
2:A:239:LEU:H	2:D:228:ASN:HD22	1.35	0.74
1:R:39:ARG:HG2	1:R:39:ARG:HH11	1.55	0.71
2:A:278:PHE:HD2	2:D:247:ILE:HD11	1.57	0.70
1:T:93:GLU:HG2	1:T:94:GLU:N	2.06	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:86:CYS:SG	1:S:92:ARG:HD3	2.31	0.70
2:D:129:THR:HG23	5:D:282:HOH:O	1.90	0.70
1:R:67:ASP:HB3	2:A:130:ARG:NH1	2.07	0.69
1:T:92:ARG:HG3	1:T:92:ARG:HH11	1.60	0.67
1:S:64:THR:H	1:S:81:ASN:HD21	1.40	0.67
1:T:110:GLY:HA2	1:T:128:LYS:HE3	1.76	0.67
1:S:92:ARG:HG2	1:S:96:SER:O	1.95	0.67
2:B:157:SER:HA	2:B:158:ARG:NH1	2.11	0.66
1:T:33:HIS:HD2	1:T:34:ILE:O	1.79	0.66
2:B:247:ILE:HD11	2:D:278:PHE:HD2	1.61	0.66
2:B:158:ARG:CD	2:B:158:ARG:H	2.01	0.66
1:S:76:CYS:HB2	1:S:82:THR:HG22	1.77	0.66
2:A:192:PHE:HD1	2:A:194:GLU:HG2	1.57	0.65
2:A:214:THR:HG23	2:A:215:SER:N	2.13	0.64
1:T:52:THR:HG22	1:T:79:THR:O	1.99	0.62
2:A:208:GLN:HE21	2:A:244:GLN:HE21	1.46	0.62
1:S:64:THR:O	1:S:82:THR:HG21	1.99	0.62
2:B:191:ARG:HG2	2:B:191:ARG:HH11	1.66	0.61
1:R:104:ARG:HD3	1:R:122:ASP:OD2	1.99	0.61
2:B:192:PHE:HB3	2:B:265:LEU:HD22	1.82	0.61
1:T:93:GLU:HG2	1:T:94:GLU:H	1.66	0.60
1:S:74:SER:HB2	1:S:83:VAL:HG23	1.83	0.60
1:R:101:ARG:HB3	2:D:201:LYS:NZ	2.17	0.60
2:A:192:PHE:HB3	2:A:265:LEU:HD22	1.84	0.59
1:T:64:THR:O	1:T:82:THR:HG21	2.03	0.59
2:A:158:ARG:HG2	2:A:161:HIS:HA	1.85	0.59
1:R:76:CYS:HB2	1:R:82:THR:OG1	2.02	0.59
2:A:208:GLN:NE2	2:A:244:GLN:HE21	2.01	0.58
1:T:71:VAL:HG13	1:T:87:GLU:OE1	2.04	0.58
2:D:127:THR:HG22	2:D:274:PHE:HB3	1.85	0.57
1:R:29:PRO:HG2	1:R:32:HIS:CD2	2.39	0.57
1:R:126:VAL:HG22	1:R:127:HIS:H	1.70	0.57
2:A:247:ILE:HD11	2:B:278:PHE:HD2	1.69	0.57
1:T:50:TYR:CZ	1:T:81:ASN:HB2	2.39	0.56
2:B:208:GLN:HE21	2:B:244:GLN:HE21	1.55	0.55
2:D:192:PHE:HB3	2:D:265:LEU:HD22	1.88	0.55
1:S:93:GLU:HG3	1:S:96:SER:OG	2.07	0.55
2:A:191:ARG:CG	2:A:191:ARG:HH11	2.20	0.55
1:T:74:SER:HB2	1:T:80:ARG:HH21	1.71	0.55
2:D:191:ARG:CG	2:D:191:ARG:HH11	2.20	0.55
1:T:59:PHE:CD2	2:D:159:SER:HA	2.42	0.54
2:A:239:LEU:H	2:D:228:ASN:ND2	2.00	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:228:ASN:ND2	2:B:239:LEU:H	2.03	0.54
2:D:146:ALA:HB1	2:D:211:TYR:CE2	2.43	0.54
2:B:278:PHE:CE1	2:B:280:VAL:HG12	2.44	0.53
2:A:278:PHE:CD2	2:D:247:ILE:HD11	2.42	0.53
1:R:101:ARG:HB3	2:D:201:LYS:HZ1	1.74	0.53
1:S:127:HIS:HB3	5:S:144:HOH:O	2.08	0.53
2:B:262:ASN:HB3	2:B:265:LEU:HD12	1.91	0.52
2:B:247:ILE:HD11	2:D:278:PHE:CD2	2.44	0.52
2:A:168:HIS:HB2	5:A:359:HOH:O	2.09	0.52
1:T:33:HIS:CD2	1:T:34:ILE:O	2.62	0.52
2:B:201:LYS:HE3	5:D:330:HOH:O	2.09	0.52
1:R:86:CYS:SG	1:R:92:ARG:HD3	2.50	0.52
1:S:128:LYS:HG3	1:S:128:LYS:O	2.10	0.52
1:R:119:PRO:HG2	1:R:120:TRP:CZ3	2.46	0.51
2:A:227[A]:ARG:NH1	2:B:227[A]:ARG:HH12	2.09	0.50
1:R:31:GLY:HA2	1:R:78:THR:O	2.11	0.50
1:R:67:ASP:CG	2:A:191:ARG:HH22	2.14	0.50
1:R:39:ARG:NH1	1:R:39:ARG:HG2	2.26	0.50
2:D:278:PHE:CE1	2:D:280:VAL:HG12	2.47	0.50
2:B:186:SER:HB3	2:B:208:GLN:NE2	2.28	0.48
2:D:203:ASP:HB3	2:D:231:TRP:CZ3	2.49	0.48
1:R:125:CYS:HB2	2:D:199:ASN:HD21	1.78	0.48
2:D:203:ASP:HA	5:D:297:HOH:O	2.13	0.48
1:T:29:PRO:HG2	1:T:32:HIS:CD2	2.50	0.47
1:S:125:CYS:O	2:A:199:ASN:ND2	2.46	0.47
1:S:59:PHE:CE2	2:B:158:ARG:HB2	2.49	0.47
1:S:74:SER:HB2	1:S:83:VAL:CG2	2.44	0.47
2:D:208:GLN:HE21	2:D:244:GLN:HE21	1.62	0.47
1:R:57:LEU:HB3	1:R:59:PHE:O	2.15	0.46
2:B:146:ALA:HB1	2:B:211:TYR:CE2	2.51	0.46
1:T:22:SER:HA	1:T:23:PRO:HD3	1.75	0.46
2:A:227[A]:ARG:HH12	2:D:227[A]:ARG:NH1	2.13	0.46
1:R:65:ARG:HB3	2:A:130:ARG:HD2	1.99	0.45
2:A:247:ILE:HG13	2:B:185:TYR:OH	2.15	0.45
2:A:270:HIS:HD2	5:A:339:HOH:O	1.99	0.45
2:B:208:GLN:NE2	2:B:244:GLN:HE21	2.14	0.45
2:A:192:PHE:CD1	2:A:194:GLU:CG	2.86	0.45
1:R:126:VAL:HG22	1:R:127:HIS:N	2.32	0.45
1:T:125:CYS:HB2	2:B:199:ASN:OD1	2.16	0.45
2:D:177:HIS:O	2:D:252:GLU:HG3	2.17	0.45
1:S:55:ASN:HB2	5:A:335:HOH:O	2.17	0.45
1:T:114:VAL:HG21	1:T:126:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:243:TYR:C	2:B:243:TYR:CD1	2.91	0.45
1:R:39:ARG:HG3	1:R:40:ASP:N	2.32	0.45
1:S:31:GLY:HA2	1:S:78:THR:O	2.18	0.44
2:A:173:GLU:HG2	2:A:257:PHE:HB3	1.99	0.44
1:R:28:CYS:O	1:R:54:TRP:HA	2.18	0.44
1:S:90:THR:HA	1:S:101:ARG:O	2.18	0.44
1:T:23:PRO:HG3	1:T:41:CYS:SG	2.57	0.44
1:R:96:SER:N	1:R:97:PRO:HD3	2.33	0.44
1:T:31:GLY:HA2	1:T:78:THR:O	2.18	0.44
2:A:231:TRP:CD2	2:B:235:ALA:HA	2.53	0.43
1:R:112:VAL:HG13	1:R:126:VAL:HG12	2.00	0.43
2:D:191:ARG:HG2	2:D:191:ARG:HH11	1.82	0.43
2:B:278:PHE:HE1	2:B:280:VAL:HG12	1.82	0.43
1:T:93:GLU:OE2	1:T:95:ASP:HB2	2.18	0.43
1:T:50:TYR:CE2	1:T:81:ASN:HB2	2.53	0.43
1:T:92:ARG:HG3	1:T:92:ARG:NH1	2.29	0.43
2:A:165:SER:O	2:A:166:ASN:HB2	2.18	0.43
2:A:212:LYS:HA	2:A:255:ARG:O	2.19	0.43
1:R:39:ARG:CG	1:R:39:ARG:NH1	2.82	0.43
2:B:212:LYS:HA	2:B:255:ARG:O	2.19	0.43
1:T:67:ASP:CG	2:D:191:ARG:HH22	2.22	0.42
2:D:191:ARG:CG	2:D:191:ARG:NH1	2.82	0.42
2:B:201:LYS:HB3	2:B:201:LYS:HE2	1.86	0.42
1:S:64:THR:O	1:S:82:THR:CG2	2.66	0.42
1:S:29:PRO:HG2	1:S:32:HIS:CD2	2.54	0.42
2:D:187:GLN:HA	2:D:242:ILE:O	2.20	0.42
2:B:127:THR:HG22	2:B:274:PHE:HB3	2.02	0.42
2:B:126:ILE:HD12	2:B:154:TRP:CB	2.50	0.42
1:S:76:CYS:HB2	1:S:82:THR:CG2	2.47	0.41
2:B:158:ARG:CD	2:B:158:ARG:N	2.56	0.41
2:A:174:LEU:HB2	2:A:256:ILE:HG13	2.01	0.41
2:A:126:ILE:HD12	2:A:154:TRP:CB	2.51	0.41
1:R:64:THR:HG22	1:R:65:ARG:N	2.34	0.41
2:D:191:ARG:HG2	2:D:191:ARG:NH1	2.35	0.41
2:B:174:LEU:HB2	2:B:256:ILE:HG13	2.02	0.41
2:D:165:SER:O	2:D:166:ASN:HB2	2.21	0.41
2:B:203:ASP:HB3	2:B:231:TRP:CZ3	2.56	0.41
1:T:99:MET:HB3	1:T:99:MET:HE2	1.26	0.41
2:A:191:ARG:CG	2:A:191:ARG:NH1	2.82	0.41
1:T:110:GLY:HA2	1:T:128:LYS:CE	2.48	0.41
1:S:114:VAL:HG21	1:S:126:VAL:HG22	2.02	0.41
1:R:119:PRO:HG2	1:R:120:TRP:CE3	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:126:ILE:HD12	2:A:154:TRP:HB3	2.03	0.40
2:D:243:TYR:CD1	2:D:243:TYR:C	2.95	0.40
2:A:121:ARG:NH2	5:D:318:HOH:O	2.51	0.40
2:A:231:TRP:CG	2:B:235:ALA:HA	2.56	0.40
1:T:91:PHE:HB3	1:T:118:THR:O	2.20	0.40
1:T:28:CYS:O	1:T:54:TRP:HA	2.21	0.40
2:D:194:GLU:O	2:D:194:GLU:HG3	2.21	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	R	106/130 (82%)	104 (98%)	2 (2%)	0	100	100
1	S	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
1	T	108/130 (83%)	106 (98%)	2 (2%)	0	100	100
2	A	148/168 (88%)	138 (93%)	8 (5%)	2 (1%)	16	22
2	B	148/168 (88%)	140 (95%)	6 (4%)	2 (1%)	16	22
2	D	148/168 (88%)	137 (93%)	10 (7%)	1 (1%)	30	43
All	All	766/894 (86%)	731 (95%)	30 (4%)	5 (1%)	30	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	157	SER
2	B	198	GLU
2	A	198	GLU
2	B	196	ILE
2	D	196	ILE

### 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	R	99/117 (85%)	94 (95%)	5 (5%)	33	50
1	S	101/117 (86%)	96 (95%)	5 (5%)	34	51
1	T	101/117 (86%)	95 (94%)	6 (6%)	28	42
2	A	134/149 (90%)	126 (94%)	8 (6%)	27	41
2	B	134/149 (90%)	130 (97%)	4 (3%)	53	75
2	D	134/149 (90%)	126 (94%)	8 (6%)	27	41
All	All	703/798 (88%)	667 (95%)	36 (5%)	34	50

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	52	THR
1	R	58	LEU
1	R	87	GLU
1	R	92	ARG
1	R	93	GLU
1	S	22	SER
1	S	81	ASN
1	S	82	THR
1	S	93	GLU
1	S	120	TRP
1	T	22	SER
1	T	37	ASP
1	T	67	ASP
1	T	82	THR
1	T	93	GLU
1	T	112	VAL
2	A	156	SER
2	A	158	ARG
2	A	178	GLU
2	A	191	ARG
2	A	195	GLU
2	A	196	ILE
2	A	214	THR

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Mol	Chain	Res	Type
2	A	233	LYS
2	B	130	ARG
2	B	158	ARG
2	B	178	GLU
2	B	233	LYS
2	D	145	LYS
2	D	178	GLU
2	D	191	ARG
2	D	195	GLU
2	D	213	TYR
2	D	227[A]	ARG
2	D	227[B]	ARG
2	D	233	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	32	HIS
1	R	48	GLN
1	S	32	HIS
1	S	33	HIS
1	S	81	ASN
1	T	32	HIS
1	T	33	HIS
1	T	127	HIS
2	A	208	GLN
2	A	228	ASN
2	A	270	HIS
2	B	208	GLN
2	B	228	ASN
2	B	270	HIS
2	D	208	GLN
2	D	228	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

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 ⓘ

### 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	R	108/130 (83%)	0.43	5 (4%) 31 29	32, 49, 78, 97	0
1	S	110/130 (84%)	1.42	24 (21%) 1 1	29, 47, 81, 96	0
1	T	110/130 (84%)	0.97	13 (11%) 5 5	34, 48, 84, 97	0
2	A	151/168 (89%)	0.83	11 (7%) 15 13	22, 38, 81, 92	2 (1%)
2	B	151/168 (89%)	1.11	17 (11%) 6 5	21, 35, 76, 98	4 (2%)
2	D	151/168 (89%)	0.80	18 (11%) 5 4	22, 39, 80, 95	4 (2%)
All	All	781/894 (87%)	0.93	88 (11%) 6 5	21, 43, 81, 98	10 (1%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	130	SER	8.1
2	D	198	GLU	5.4
1	S	68	SER	5.0
2	D	131	GLY	4.9
1	S	130	SER	4.8
1	T	110	GLY	4.8
1	S	126	VAL	4.7
1	S	39	ARG	4.7
2	A	131	GLY	4.6
2	B	129	THR	4.5
2	A	159	SER	4.4
2	D	119	PRO	4.1
2	B	197	LYS	4.1
1	T	39	ARG	4.1
2	A	281	GLY	4.0
1	T	27	LEU	3.7
2	B	156	SER	3.5
1	T	65	ARG	3.4
2	D	130	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	131	GLY	3.3
1	R	128	LYS	3.2
1	T	120	TRP	3.2
2	D	129	THR	3.1
2	B	159	SER	3.0
2	B	215	SER	3.0
1	T	112	VAL	2.9
2	B	202	ASN	2.9
1	T	34	ILE	2.9
2	B	195	GLU	2.8
2	D	183	TYR	2.8
1	S	120	TRP	2.8
1	R	65	ARG	2.8
1	S	46	TYR	2.7
2	B	196	ILE	2.7
1	S	66	CYS	2.7
2	D	185	TYR	2.7
1	R	127	HIS	2.7
2	B	153	SER	2.7
2	D	158	ARG	2.7
2	D	120	GLN	2.6
1	S	21	SER	2.6
2	D	246	GLY	2.6
1	T	22	SER	2.6
2	A	160	GLY	2.5
1	S	65	ARG	2.5
2	A	198	GLU	2.5
1	S	94	GLU	2.5
1	S	123	ILE	2.5
1	S	29	PRO	2.5
2	A	157	SER	2.5
1	S	40	ASP	2.4
1	T	45	LYS	2.4
2	B	217	PRO	2.4
2	B	198	GLU	2.4
2	A	161	HIS	2.4
2	D	243	TYR	2.4
2	D	276	GLY	2.4
1	S	34	ILE	2.3
2	B	281	GLY	2.3
2	B	155	GLU	2.3
1	T	25	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	184	ILE	2.3
2	B	158	ARG	2.2
2	A	184	ILE	2.2
2	D	247	ILE	2.2
2	B	227[A]	ARG	2.2
1	R	73	LEU	2.2
1	R	34	ILE	2.2
1	S	129	GLU	2.2
2	A	227[A]	ARG	2.2
1	S	35	SER	2.2
1	T	21	SER	2.2
1	S	110	GLY	2.2
2	A	243	TYR	2.1
2	B	276	GLY	2.1
1	S	44	CYS	2.1
1	S	51	SER	2.1
1	S	128	LYS	2.1
2	A	185	TYR	2.1
2	D	245	GLY	2.1
2	D	197	LYS	2.1
1	S	92	ARG	2.0
1	T	71	VAL	2.0
1	S	97	PRO	2.0
1	S	64	THR	2.0
1	S	105	THR	2.0
2	D	281	GLY	2.0
2	D	152	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	A	300	1/1	0.22	3.40	44,44,44,44	0
4	CL	B	400	1/1	0.11	-1.09	29,29,29,29	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.