



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:50 AM GMT

PDB ID : 2BXD  
Title : HUMAN SERUM ALBUMIN COMPLEXED WITH WARFARIN  
Authors : Ghuman, J.; Zunszain, P.A.; Petitpas, I.; Bhattacharya, A.A.; Curry, S.  
Deposited on : 2005-07-26  
Resolution : 3.05 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

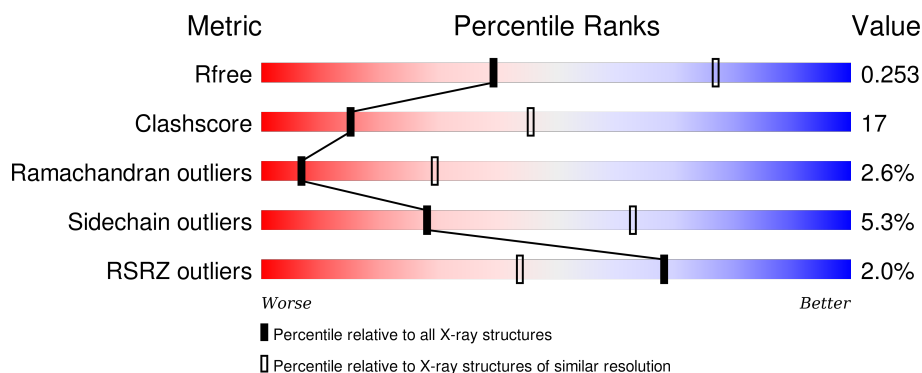
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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))
$R_{free}$	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	585	<div> <div>2%</div> <div>63%</div> <div>34%</div> <div>..</div> </div>
1	B	585	<div> <div>2%</div> <div>65%</div> <div>30%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	RWF	A	2001	-	-	-	X
2	RWF	B	2001	-	-	-	X

## 2 Entry composition [i](#)

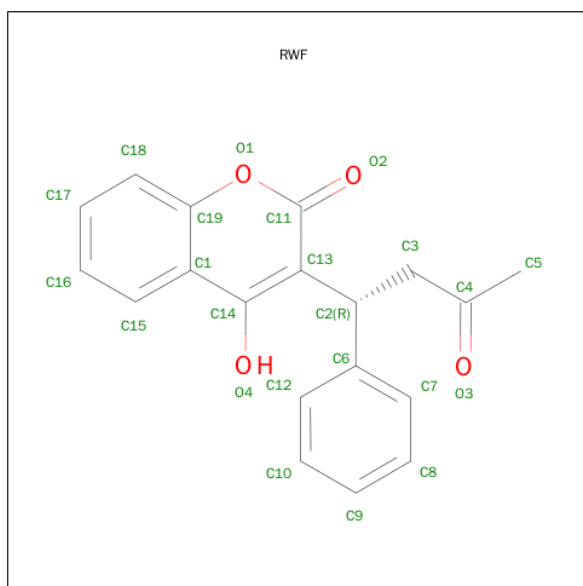
There are 2 unique types of molecules in this entry. The entry contains 8632 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

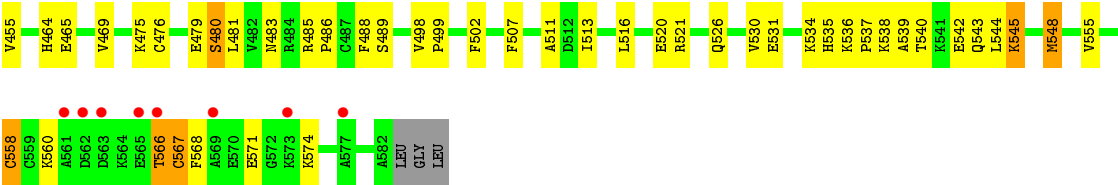
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4323	2727	725	830	41			
1	B	578	Total	C	N	O	S	0	0	0
			4263	2684	719	820	40			

- Molecule 2 is R-WARFARIN (three-letter code: RWF) (formula: C<sub>19</sub>H<sub>16</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	19	4		
2	B	1	Total	C	O	0	0
			23	19	4		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.02Å 55.36Å 119.59Å 81.14° 90.53° 64.79°	Depositor
Resolution (Å)	49.32 – 3.05 49.32 – 3.05	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.32-3.05) 91.6 (49.32-3.05)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 3.07Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.213 , 0.259 0.206 , 0.253	Depositor DCC
$R_{free}$ test set	1106 reflections (4.73%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.8	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 74.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23948 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8632	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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

### 5.1 Standard geometry

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

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	0/4408	0.64	0/5999
1	B	0.38	0/4343	0.61	0/5911
All	All	0.40	0/8751	0.62	0/11910

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

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	4323	0	3976	152	0
1	B	4263	0	3894	137	0
2	A	23	0	15	4	0
2	B	23	0	15	4	0
All	All	8632	0	7900	289	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 (289) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:CYS:SG	1:A:568:PHE:N	2.31	1.03
1:A:67:HIS:HB3	1:A:98:ARG:HH21	1.26	0.98
1:A:94:GLN:O	1:A:98:ARG:HB3	1.70	0.91
1:A:551:PHE:HA	1:A:554:PHE:HD1	1.37	0.86
1:A:551:PHE:HA	1:A:554:PHE:CD1	2.10	0.86
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.59	0.84
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.60	0.83
1:B:39:HIS:O	1:B:43:VAL:HG23	1.81	0.81
1:A:257:ARG:HG3	2:A:2001:RWF:H16	1.62	0.81
1:B:567:CYS:SG	1:B:568:PHE:N	2.53	0.81
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.63	0.79
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.65	0.79
1:B:544:LEU:O	1:B:548:MET:HB2	1.82	0.79
1:A:67:HIS:CB	1:A:98:ARG:HH21	1.95	0.78
1:B:206:PHE:CD2	1:B:481:LEU:HD22	2.18	0.78
1:A:424:VAL:O	1:A:428:ARG:HG3	1.83	0.78
1:A:115:LEU:HD22	1:A:145:ARG:NH1	2.00	0.76
1:B:485:ARG:NH2	1:B:486:PRO:HG3	2.01	0.76
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.70	0.74
1:B:424:VAL:O	1:B:428:ARG:HG3	1.88	0.74
1:B:206:PHE:CE2	1:B:481:LEU:HD13	2.21	0.74
1:A:23:VAL:HG13	1:A:70:PHE:HE2	1.54	0.73
1:A:61:ASN:HD22	1:A:64:LYS:HE3	1.54	0.72
1:A:23:VAL:O	1:A:27:PHE:HD1	1.73	0.72
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.55	0.72
1:B:81:ARG:HE	1:B:88:ALA:HB3	1.53	0.71
1:B:194:ALA:HB1	1:B:455:VAL:HG13	1.72	0.71
1:A:225:LYS:HG2	1:A:299:PRO:HG3	1.72	0.71
1:A:497:TYR:CE2	1:A:537:PRO:HG3	2.25	0.71
1:A:414:LYS:O	1:A:472:ARG:NH1	2.24	0.71
1:B:194:ALA:HB1	1:B:455:VAL:CG1	2.20	0.70
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.74	0.69
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.76	0.68
1:A:199:LYS:HG2	1:A:211:PHE:HE1	1.60	0.67
1:A:497:TYR:HE2	1:A:537:PRO:HG3	1.57	0.67
1:A:98:ARG:CZ	1:A:99:ASN:HB2	2.25	0.66
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.77	0.66
1:B:57:GLU:OE1	1:B:57:GLU:HA	1.96	0.66
1:A:115:LEU:HD22	1:A:145:ARG:HH12	1.58	0.66
1:A:206:PHE:CE2	1:A:481:LEU:HD13	2.30	0.65
1:B:537:PRO:C	1:B:539:ALA:H	1.99	0.65
1:A:564:LYS:O	1:A:566:THR:N	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLU:O	1:B:48:GLU:HG2	1.95	0.65
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.78	0.65
1:A:117:ARG:HB2	1:A:123:MET:CE	2.27	0.65
1:B:545:LYS:HE3	1:B:545:LYS:HA	1.80	0.64
1:A:564:LYS:C	1:A:566:THR:H	2.00	0.64
1:A:512:ASP:O	1:A:515:THR:HG22	1.97	0.64
1:B:483:ASN:O	1:B:486:PRO:HD2	1.97	0.64
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.62	0.63
1:A:98:ARG:NH1	1:A:99:ASN:H	1.95	0.63
1:B:42:LEU:O	1:B:46:VAL:HG23	1.97	0.63
1:A:420:THR:HG23	1:A:530:VAL:HG11	1.81	0.62
1:B:81:ARG:NE	1:B:88:ALA:HB3	2.15	0.62
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.81	0.62
1:A:98:ARG:NH2	1:A:99:ASN:HB2	2.15	0.61
1:B:367:HIS:O	1:B:371:ALA:HB2	2.01	0.61
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.40	0.61
1:B:540:THR:O	1:B:544:LEU:HG	2.01	0.61
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.66	0.61
1:A:376:GLU:O	1:A:379:PRO:HD2	2.01	0.61
1:A:557:LYS:HG2	1:A:558:CYS:N	2.15	0.61
1:A:310:VAL:O	1:A:370:TYR:HE1	1.84	0.61
1:A:49:PHE:O	1:A:49:PHE:HD2	1.83	0.60
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.83	0.60
1:B:279:CYS:HA	1:B:286:LYS:HD2	1.84	0.60
1:B:290:ILE:O	1:B:293:VAL:HG12	2.01	0.60
1:B:511:ALA:C	1:B:513:ILE:H	2.04	0.59
1:A:257:ARG:HG3	2:A:2001:RWF:C16	2.32	0.59
1:B:373:VAL:HG13	1:B:374:PHE:N	2.16	0.59
1:B:372:LYS:O	1:B:375:ASP:HB2	2.01	0.59
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.85	0.59
1:A:551:PHE:CA	1:A:554:PHE:HD1	2.12	0.59
1:B:36:PHE:O	1:B:40:VAL:HG23	2.03	0.59
1:B:544:LEU:O	1:B:548:MET:N	2.34	0.59
1:A:283:LEU:HG	1:A:284:LEU:HD23	1.84	0.58
1:A:279:CYS:HA	1:A:286:LYS:CD	2.33	0.58
1:A:117:ARG:HB2	1:A:123:MET:HE3	1.85	0.58
1:B:499:PRO:HB3	1:B:535:HIS:O	2.04	0.58
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.85	0.57
1:B:186:ARG:O	1:B:190:LYS:HG3	2.03	0.57
1:B:409:VAL:O	1:B:413:LYS:HG3	2.03	0.57
1:A:38:ASP:O	1:A:42:LEU:HG	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LEU:HD11	1:A:526:GLN:HB3	1.87	0.57
1:A:372:LYS:O	1:A:375:ASP:HB2	2.04	0.57
1:A:420:THR:HG23	1:A:530:VAL:CG1	2.35	0.56
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.40	0.56
1:A:49:PHE:CE2	1:A:53:CYS:SG	2.98	0.56
1:B:52:THR:HA	1:B:56:ASP:OD2	2.05	0.56
1:B:571:GLU:HA	1:B:574:LYS:HB3	1.86	0.56
1:B:61:ASN:HB3	1:B:64:LYS:HD2	1.87	0.55
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.07	0.55
1:B:420:THR:HG23	1:B:530:VAL:HG11	1.88	0.55
1:B:98:ARG:O	1:B:101:CYS:HB3	2.06	0.55
1:A:550:ASP:HB3	1:A:554:PHE:HE1	1.71	0.54
1:A:387:LEU:HD22	1:A:485:ARG:NH1	2.21	0.54
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.88	0.54
1:B:276:LYS:HG3	1:B:277:GLU:N	2.22	0.54
1:A:420:THR:O	1:A:424:VAL:HG23	2.06	0.54
1:B:464:HIS:CE1	1:B:469:VAL:H	2.25	0.54
1:A:464:HIS:CE1	1:A:469:VAL:H	2.26	0.54
1:B:25:ILE:O	1:B:29:GLN:HG3	2.07	0.53
1:B:400:GLU:O	1:B:404:GLN:HG3	2.07	0.53
1:A:348:ARG:HG3	1:A:482:VAL:HG12	1.89	0.53
1:B:480:SER:OG	1:B:483:ASN:HB2	2.08	0.53
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.90	0.53
1:B:29:GLN:HG2	1:B:143:ALA:O	2.08	0.53
1:B:483:ASN:C	1:B:486:PRO:HD2	2.29	0.53
1:A:139:LEU:HD21	1:A:158:ALA:HB2	1.90	0.53
1:B:405:ASN:O	1:B:409:VAL:HG23	2.08	0.53
1:A:168:CYS:SG	1:A:177:CYS:C	2.87	0.53
1:B:394:LEU:O	1:B:397:GLN:HG2	2.08	0.53
1:A:117:ARG:HB2	1:A:123:MET:HE1	1.91	0.52
1:A:279:CYS:HA	1:A:286:LYS:HD2	1.92	0.52
1:A:540:THR:O	1:A:544:LEU:HG	2.09	0.52
1:A:323:LYS:HG3	1:A:324:ASP:N	2.25	0.52
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.46	0.51
1:B:81:ARG:HE	1:B:88:ALA:CB	2.23	0.51
1:A:578:ALA:O	1:A:581:ALA:HB3	2.10	0.51
1:B:50:ALA:O	1:B:54:VAL:HG23	2.11	0.51
1:A:405:ASN:O	1:A:409:VAL:HG23	2.10	0.51
1:A:281:LYS:HB2	1:A:282:PRO:CD	2.41	0.51
1:B:32:GLN:NE2	1:B:110:PRO:HG3	2.26	0.51
1:A:395:PHE:CD1	1:A:434:GLY:HA3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:GLY:O	1:A:438:CYS:HB2	2.11	0.51
1:A:6:GLU:O	1:A:9:HIS:HB3	2.10	0.51
1:B:516:LEU:O	1:B:521:ARG:NH2	2.41	0.51
1:A:517:SER:O	1:A:521:ARG:HG3	2.10	0.51
1:B:23:VAL:O	1:B:27:PHE:HD1	1.94	0.51
1:A:485:ARG:HB3	1:A:486:PRO:CD	2.39	0.50
1:B:139:LEU:HD21	1:B:158:ALA:HB2	1.93	0.50
1:B:537:PRO:C	1:B:539:ALA:N	2.64	0.50
1:A:282:PRO:HB2	1:A:285:GLU:OE1	2.11	0.50
1:B:291:ALA:HB1	2:B:2001:RWF:H3C1	1.93	0.50
1:B:536:LYS:O	1:B:539:ALA:HB3	2.12	0.50
1:B:14:LEU:HD13	1:B:22:LEU:HD12	1.92	0.50
1:A:525:LYS:O	1:A:528:ALA:HB3	2.12	0.50
1:B:442:GLU:HA	1:B:445:ARG:HD2	1.94	0.50
1:B:333:GLU:OE1	1:B:336:ARG:HD3	2.12	0.50
1:B:511:ALA:C	1:B:513:ILE:N	2.63	0.50
1:A:290:ILE:O	1:A:293:VAL:HG12	2.12	0.49
1:A:49:PHE:CD2	1:A:49:PHE:C	2.85	0.49
1:B:240:LYS:HE2	1:B:244:GLU:OE2	2.13	0.49
1:B:420:THR:O	1:B:424:VAL:HG23	2.11	0.49
1:A:199:LYS:NZ	2:A:2001:RWF:H5C3	2.28	0.49
1:A:23:VAL:HG13	1:A:27:PHE:HE1	1.78	0.49
1:A:564:LYS:C	1:A:566:THR:N	2.65	0.49
1:A:430:LEU:O	1:A:433:VAL:HG12	2.12	0.49
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.95	0.49
1:A:49:PHE:HE2	1:A:62:CYS:SG	2.36	0.48
1:A:572:GLY:O	1:A:576:VAL:HG23	2.13	0.48
1:B:141:GLU:O	1:B:144:ARG:HG2	2.11	0.48
1:B:151:ALA:CB	1:B:152:PRO:HD3	2.40	0.48
1:B:285:GLU:O	1:B:289:CYS:HB2	2.14	0.48
1:A:279:CYS:HA	1:A:286:LYS:HD3	1.95	0.48
1:B:103:LEU:C	1:B:105:HIS:H	2.17	0.48
1:A:178:LEU:O	1:A:179:LEU:C	2.52	0.48
1:A:551:PHE:O	1:A:555:VAL:HG23	2.13	0.48
1:A:179:LEU:CB	1:A:180:PRO:HD3	2.42	0.48
1:B:398:LEU:O	1:B:402:LYS:HB2	2.14	0.48
1:B:279:CYS:HA	1:B:286:LYS:CD	2.43	0.47
1:A:151:ALA:CB	1:A:152:PRO:HD3	2.39	0.47
1:B:38:ASP:O	1:B:42:LEU:HG	2.14	0.47
1:A:310:VAL:HG23	1:A:311:GLU:N	2.28	0.47
1:A:394:LEU:HG	1:A:398:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLN:O	1:A:98:ARG:HD3	2.15	0.47
1:A:370:TYR:CD1	1:A:370:TYR:C	2.88	0.47
1:A:392:CYS:O	1:A:396:GLU:HG3	2.15	0.47
1:B:345:LEU:O	1:B:349:LEU:HG	2.14	0.47
1:A:67:HIS:O	1:A:68:THR:C	2.52	0.46
1:A:42:LEU:O	1:A:46:VAL:HG23	2.15	0.46
1:B:276:LYS:HE3	1:B:280:GLU:OE2	2.15	0.46
1:B:283:LEU:HG	1:B:284:LEU:N	2.29	0.46
1:A:156:PHE:CE2	1:A:160:ARG:HD2	2.51	0.46
1:A:98:ARG:NH1	1:A:99:ASN:HB2	2.30	0.46
1:A:27:PHE:CD2	1:A:74:LEU:HD21	2.51	0.46
1:A:49:PHE:HD2	1:A:49:PHE:C	2.19	0.46
1:B:333:GLU:O	1:B:336:ARG:HG2	2.15	0.46
1:A:394:LEU:HG	1:A:398:LEU:CD1	2.46	0.46
1:B:141:GLU:O	1:B:145:ARG:HG3	2.16	0.46
1:B:168:CYS:SG	1:B:177:CYS:C	2.95	0.46
1:B:168:CYS:SG	1:B:178:LEU:N	2.89	0.46
1:A:420:THR:HB	1:A:421:PRO:HD3	1.98	0.45
1:A:306:ALA:HA	1:A:310:VAL:HG22	1.97	0.45
1:A:32:GLN:HG2	1:A:144:ARG:O	2.16	0.45
1:A:499:PRO:HG3	1:A:537:PRO:HG2	1.97	0.45
1:B:373:VAL:CG1	1:B:374:PHE:N	2.78	0.45
1:B:199:LYS:HD3	2:B:2001:RWF:H10	1.97	0.45
1:A:151:ALA:O	1:A:154:LEU:N	2.49	0.45
1:B:214:TRP:NE1	1:B:343:VAL:HG11	2.31	0.45
1:B:370:TYR:C	1:B:370:TYR:CD1	2.89	0.45
1:B:410:ARG:O	1:B:414:LYS:HG3	2.17	0.45
1:A:553:ALA:O	1:A:556:GLU:HG2	2.17	0.45
1:A:214:TRP:NE1	1:A:343:VAL:HG11	2.32	0.45
1:B:81:ARG:HG2	1:B:88:ALA:HB3	1.99	0.45
1:B:23:VAL:O	1:B:27:PHE:CD1	2.70	0.45
1:B:310:VAL:HG21	1:B:374:PHE:CE1	2.51	0.45
1:B:54:VAL:HG12	1:B:55:ALA:N	2.32	0.45
1:B:531:GLU:HA	1:B:531:GLU:OE1	2.17	0.45
1:B:81:ARG:HA	1:B:84:TYR:O	2.17	0.45
1:B:323:LYS:HG3	1:B:324:ASP:N	2.31	0.45
1:B:37:GLU:CD	1:B:37:GLU:H	2.20	0.44
1:A:23:VAL:CG1	1:A:27:PHE:CE1	3.00	0.44
1:A:137:LYS:O	1:A:141:GLU:HG2	2.18	0.44
1:B:196:GLN:HA	1:B:196:GLN:NE2	2.32	0.44
1:B:238:LEU:HA	1:B:238:LEU:HD12	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:GLU:O	1:B:543:GLN:C	2.53	0.44
1:A:87:MET:HE3	1:A:105:HIS:HB3	1.99	0.44
1:A:198:LEU:HA	1:A:458:ASN:ND2	2.33	0.44
1:A:98:ARG:HG2	1:A:99:ASN:N	2.31	0.44
1:A:417:GLN:H	1:A:417:GLN:CD	2.19	0.44
1:B:498:VAL:O	1:B:499:PRO:C	2.55	0.44
1:B:366:PRO:O	1:B:369:CYS:N	2.50	0.44
1:B:51:LYS:C	1:B:53:CYS:H	2.21	0.44
1:A:492:GLU:HA	1:A:492:GLU:OE1	2.16	0.44
1:A:366:PRO:O	1:A:367:HIS:C	2.56	0.44
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.40	0.44
1:A:342:SER:HA	1:A:447:PRO:HA	2.00	0.44
1:A:411:TYR:O	1:A:414:LYS:HB2	2.17	0.44
1:B:507:PHE:N	1:B:507:PHE:CD1	2.85	0.44
1:B:425:GLU:OE1	1:B:425:GLU:HA	2.17	0.43
1:B:530:VAL:HG12	1:B:534:LYS:HD2	2.01	0.43
1:B:214:TRP:CE2	1:B:343:VAL:HG11	2.53	0.43
1:A:110:PRO:HB2	1:A:112:LEU:HG	2.00	0.43
1:B:408:LEU:HD21	1:B:424:VAL:HA	2.00	0.43
1:A:81:ARG:CB	1:A:85:GLY:HA2	2.47	0.43
1:A:550:ASP:O	1:A:553:ALA:HB3	2.18	0.43
1:A:23:VAL:CG1	1:A:27:PHE:HE1	2.32	0.43
1:B:475:LYS:O	1:B:479:GLU:HB2	2.19	0.43
1:A:502:PHE:CE1	1:A:504:ALA:HA	2.53	0.43
1:B:127:PHE:O	1:B:131:GLU:HB3	2.18	0.43
1:A:280:GLU:HA	1:A:280:GLU:OE1	2.18	0.43
1:A:331:LEU:HD13	1:A:350:ALA:HB2	2.00	0.43
1:A:536:LYS:N	1:A:537:PRO:CD	2.82	0.42
1:A:310:VAL:CG2	1:A:311:GLU:N	2.82	0.42
1:B:388:ILE:HD12	1:B:449:ALA:HB3	2.00	0.42
1:B:282:PRO:O	1:B:283:LEU:C	2.57	0.42
1:A:417:GLN:CD	1:A:417:GLN:N	2.73	0.42
1:A:153:GLU:O	1:A:157:PHE:HD1	2.02	0.42
1:A:110:PRO:C	1:A:112:LEU:H	2.22	0.42
1:B:558:CYS:C	1:B:560:LYS:H	2.23	0.42
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.92	0.42
1:A:127:PHE:HB2	1:A:134:PHE:CE2	2.55	0.42
1:A:22:LEU:HA	1:A:22:LEU:HD23	1.86	0.42
1:B:255:ASP:O	1:B:258:ALA:N	2.51	0.42
1:A:366:PRO:O	1:A:369:CYS:HB3	2.19	0.42
1:B:30:TYR:CE1	1:B:103:LEU:HD23	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:HIS:NE2	2:B:2001:RWF:H12	2.34	0.42
1:B:153:GLU:O	1:B:157:PHE:HD1	2.02	0.42
1:B:19:PHE:CD2	1:B:19:PHE:C	2.92	0.42
1:A:388:ILE:HD12	1:A:449:ALA:CB	2.50	0.42
1:B:178:LEU:O	1:B:179:LEU:C	2.58	0.42
1:A:345:LEU:O	1:A:349:LEU:HG	2.20	0.42
1:B:76:THR:O	1:B:77:VAL:HG13	2.19	0.42
1:A:507:PHE:N	1:A:507:PHE:CD1	2.87	0.42
1:A:168:CYS:SG	1:A:177:CYS:O	2.78	0.41
1:B:10:ARG:NH1	1:B:255:ASP:OD2	2.52	0.41
1:B:384:PRO:O	1:B:388:ILE:HG12	2.19	0.41
1:B:199:LYS:HD3	2:B:2001:RWF:C10	2.50	0.41
1:A:384:PRO:O	1:A:388:ILE:HG12	2.20	0.41
1:A:464:HIS:HE1	1:A:470:SER:H	1.68	0.41
1:B:78:ALA:C	1:B:80:LEU:N	2.74	0.41
1:B:331:LEU:HD13	1:B:350:ALA:HB2	2.02	0.41
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.88	0.41
1:A:72:ASP:O	1:A:76:THR:HG23	2.20	0.41
1:A:224:PRO:HD2	1:A:296:ASP:HB3	2.01	0.41
1:A:87:MET:O	1:A:90:CYS:HB2	2.21	0.41
1:B:24:LEU:HD13	1:B:43:VAL:HG21	2.02	0.41
1:B:536:LYS:O	1:B:539:ALA:CB	2.69	0.41
1:B:70:PHE:CD1	1:B:70:PHE:N	2.89	0.41
1:B:302:LEU:HA	1:B:302:LEU:HD23	1.96	0.41
1:B:433:VAL:HG13	1:B:434:GLY:N	2.35	0.41
1:B:272:SER:HB3	1:B:275:LEU:HG	2.03	0.41
1:B:32:GLN:HG2	1:B:144:ARG:O	2.20	0.41
1:B:15:GLY:O	1:B:19:PHE:HB3	2.20	0.41
1:A:34:CYS:HA	1:A:35:PRO:HD3	1.74	0.41
1:A:257:ARG:CG	2:A:2001:RWF:H16	2.43	0.40
1:B:81:ARG:HG2	1:B:88:ALA:CB	2.50	0.40
1:A:49:PHE:HE2	1:A:53:CYS:SG	2.43	0.40
1:B:516:LEU:HD22	1:B:520:GLU:CB	2.51	0.40
1:A:78:ALA:C	1:A:80:LEU:N	2.74	0.40
1:A:563:ASP:C	1:A:564:LYS:O	2.57	0.40
1:B:78:ALA:C	1:B:80:LEU:H	2.23	0.40
1:B:476:CYS:HB3	1:B:488:PHE:CE2	2.56	0.40
1:A:311:GLU:O	1:A:312:SER:C	2.59	0.40
1:A:433:VAL:HG23	1:A:452:TYR:HD2	1.86	0.40
1:B:286:LYS:O	1:B:290:ILE:HG13	2.21	0.40
1:B:293:VAL:HG22	1:B:294:GLU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ASN:O	1:A:462:VAL:HG22	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	576/585 (98%)	496 (86%)	64 (11%)	16 (3%)	6	28
1	B	576/585 (98%)	499 (87%)	63 (11%)	14 (2%)	7	31
All	All	1152/1170 (98%)	995 (86%)	127 (11%)	30 (3%)	7	29

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	300	ALA
1	B	54	VAL
1	B	58	SER
1	B	300	ALA
1	A	150	TYR
1	A	565	GLU
1	B	60	GLU
1	B	85	GLY
1	B	129	ASP
1	B	502	PHE
1	B	566	THR
1	A	502	PHE
1	A	557	LYS
1	A	179	LEU
1	A	545	LYS
1	B	150	TYR

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Mol	Chain	Res	Type
1	B	276	LYS
1	A	58	SER
1	A	129	ASP
1	A	276	LYS
1	A	390	GLN
1	A	465	GLU
1	B	77	VAL
1	B	86	GLU
1	B	465	GLU
1	A	315	VAL
1	A	499	PRO
1	A	180	PRO
1	B	179	LEU

### 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	434/511 (85%)	412 (95%)	22 (5%)	29	65
1	B	419/511 (82%)	396 (94%)	23 (6%)	27	61
All	All	853/1022 (84%)	808 (95%)	45 (5%)	28	63

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	TYR
1	A	37	GLU
1	A	49	PHE
1	A	79	THR
1	A	83	THR
1	A	98	ARG
1	A	109	ASN
1	A	179	LEU
1	A	236	THR
1	A	245	CYS

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Mol	Chain	Res	Type
1	A	252	GLU
1	A	255	ASP
1	A	268	GLN
1	A	284	LEU
1	A	323	LYS
1	A	334	TYR
1	A	375	ASP
1	A	435	SER
1	A	467	THR
1	A	471	ASP
1	A	498	VAL
1	A	550	ASP
1	B	38	ASP
1	B	56	ASP
1	B	57	GLU
1	B	58	SER
1	B	68	THR
1	B	82	GLU
1	B	105	HIS
1	B	179	LEU
1	B	212	LYS
1	B	283	LEU
1	B	284	LEU
1	B	323	LYS
1	B	375	ASP
1	B	435	SER
1	B	480	SER
1	B	489	SER
1	B	538	LYS
1	B	545	LYS
1	B	548	MET
1	B	555	VAL
1	B	558	CYS
1	B	566	THR
1	B	567	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	99	ASN
1	A	109	ASN

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Mol	Chain	Res	Type
1	A	338	HIS
1	A	385	GLN
1	A	464	HIS
1	A	483	ASN
1	B	111	ASN
1	B	196	GLN
1	B	221	GLN
1	B	318	ASN
1	B	385	GLN
1	B	464	HIS
1	B	483	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	RWF	A	2001	-	24,25,25	1.61	3 (12%)	23,35,35	1.43	4 (17%)
2	RWF	B	2001	-	24,25,25	1.78	7 (29%)	23,35,35	1.45	4 (17%)

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	RWF	A	2001	-	-	0/12/12/12	0/3/3/3
2	RWF	B	2001	-	-	0/12/12/12	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	RWF	C18-C19	2.02	1.42	1.38
2	B	2001	RWF	C16-C15	2.03	1.41	1.36
2	B	2001	RWF	C11-C13	2.10	1.47	1.40
2	A	2001	RWF	C14-C1	2.13	1.48	1.43
2	A	2001	RWF	C11-C13	2.20	1.47	1.40
2	B	2001	RWF	C7-C6	2.20	1.42	1.39
2	B	2001	RWF	O1-C19	2.37	1.40	1.36
2	B	2001	RWF	C14-C1	2.61	1.49	1.43
2	B	2001	RWF	O3-C4	5.18	1.39	1.21
2	A	2001	RWF	O3-C4	5.22	1.40	1.21

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	RWF	O3-C4-C3	-2.75	116.67	121.70
2	A	2001	RWF	O3-C4-C3	-2.57	116.99	121.70
2	B	2001	RWF	O4-C14-C13	2.51	124.95	121.10
2	A	2001	RWF	O4-C14-C13	2.86	125.48	121.10
2	A	2001	RWF	C15-C1-C14	3.13	125.51	121.57
2	B	2001	RWF	C15-C1-C14	3.24	125.64	121.57
2	A	2001	RWF	C5-C4-C3	3.59	121.57	116.67
2	B	2001	RWF	C5-C4-C3	3.87	121.95	116.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	RWF	4	0
2	B	2001	RWF	4	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	578/585 (98%)	-0.55	9 (1%)	74 52	25, 65, 147, 166	0
1	B	578/585 (98%)	-0.49	14 (2%)	62 37	25, 70, 151, 168	0
All	All	1156/1170 (98%)	-0.52	23 (1%)	68 44	25, 67, 149, 168	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	GLU	6.6
1	A	83	THR	6.2
1	B	83	THR	5.8
1	B	79	THR	4.5
1	A	570	GLU	4.5
1	A	562	ASP	3.8
1	B	562	ASP	3.5
1	B	563	ASP	3.5
1	A	79	THR	3.4
1	B	84	TYR	3.1
1	B	87	MET	3.1
1	B	566	THR	3.0
1	A	87	MET	2.8
1	B	577	ALA	2.8
1	A	569	ALA	2.7
1	B	561	ALA	2.7
1	A	509	PHE	2.5
1	B	573	LYS	2.4
1	B	569	ALA	2.3
1	A	84	TYR	2.3
1	B	565	GLU	2.2
1	B	86	GLU	2.2
1	A	581	ALA	2.1

## 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( $\text{\AA}^2$ )	Q<0.9
2	RWF	A	2001	23/23	0.84	0.38	8.66	111,113,116,117	0
2	RWF	B	2001	23/23	0.74	0.41	5.27	107,113,116,116	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.