

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	1BP5
Title	:	HUMAN SERUM TRANSFERRIN, RECOMBINANT N-TERMINAL LOBE,
		APO FORM
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Deposited on	:	1998-08-12
Resolution	:	2.20 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.20 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.



Matria	Whole archive	Similar resolution		
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
Clashscore	141614	5594 (2.20-2.20)		
Ramachandran outliers	138981	5503 (2.20-2.20)		
Sidechain outliers	138945	5504 (2.20-2.20)		

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain				
1	А	337	65%	31%	••		
1	В	337	66%	28%	•••		
1	С	337	69%	28%	•••		
1	D	337	70%	28%			



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10810 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	200	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	320	2542	1608	436	477	21	0		0
1	1 B	В 328	Total	С	Ν	0	S	0	0	0
			2542	1608	436	477	21	0	0	U
1	C	C 224	Total	С	Ν	0	S	0	0	0
	334	2586	1634	442	489	21	0	0	U	
1 D	224	Total	С	Ν	0	S	0	0	0	
	334	2586	1634	442	489	21	0	0	0	

• Molecule 1 is a protein called PROTEIN (SERUM TRANSFERRIN).

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	136	Total O 136 136	0	0
2	В	121	Total O 121 121	0	0
2	С	158	Total O 158 158	0	0
2	D	139	Total O 139 139	0	0



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. 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. 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.

Note EDS was not executed.



• Molecule 1: PROTEIN (SERUM TRANSFERRIN)

• Molecule 1: PROTEIN (SERUM TRANSFERRIN)





K116 K116 K144 K1445 K147 K1445 K1445 K1475 K1445 K1475 K1485 K1485

• Molecule 1: PROTEIN (SERUM TRANSFERRIN)





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	83.50Å 77.30Å 107.50Å	Depositor	
a, b, c, α , β , γ	90.00° 98.30° 90.00°	Depositor	
Resolution (Å)	6.00 - 2.20	Depositor	
% Data completeness	80.0 (6.00-2.20)	Depositor	
(in resolution range)	00.0 (0.00 2.20)	Depositor	
R_{merge}	0.05	Depositor	
R _{sym}	(Not available)	Depositor	
Refinement program	X-PLOR 3.1	Depositor	
R, R_{free}	0.203 , 0.292	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	10810	wwPDB-VP	
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP	



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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.62	0/2603	0.78	1/3519~(0.0%)	
1	В	0.60	0/2603	0.77	1/3519~(0.0%)	
1	С	0.61	0/2649	0.78	0/3583	
1	D	0.61	0/2649	0.77	1/3583~(0.0%)	
All	All	0.61	0/10504	0.78	3/14204~(0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	С	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	D	163	ASP	CB-CG-OD1	5.08	122.87	118.30
1	А	26	MET	CG-SD-CE	5.05	108.28	100.20
1	В	38	ALA	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	С	68	TYR	Sidechain
1	D	107	PHE	Mainchain



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	А	2542	0	2465	71	0
1	В	2542	0	2465	76	0
1	С	2586	0	2501	69	0
1	D	2586	0	2501	67	0
2	А	136	0	0	5	0
2	В	121	0	0	6	0
2	С	158	0	0	4	0
2	D	139	0	0	1	0
All	All	10810	0	9932	283	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 14.

All (283) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:78:LYS:HD2	1:A:255:SER:HA	1.54	0.89
1:A:310:ASP:HB3	1:A:313:MET:SD	2.15	0.87
1:D:110:ASN:ND2	1:D:111:GLN:HG3	1.91	0.84
1:B:220:ARG:HH22	1:B:236:ASP:HB3	1.43	0.83
1:D:168:PRO:HD2	1:D:169:GLN:OE1	1.79	0.81
1:B:103:LYS:HD2	1:B:224:GLU:HG3	1.61	0.80
1:D:310:ASP:H	1:D:313:MET:HE3	1.49	0.77
1:A:268:ASN:O	1:A:272:GLU:HG2	1.84	0.77
1:A:26:MET:SD	1:A:274:PHE:HE1	2.09	0.75
1:B:217:LYS:HG2	1:B:220:ARG:NH1	2.02	0.73
1:A:268:ASN:HA	1:A:271:GLN:HE21	1.54	0.72
1:D:88:LYS:NZ	1:D:300:HIS:HD2	1.87	0.72
1:A:188:TYR:OH	1:A:206:LYS:HE3	1.90	0.71
1:B:307:PRO:HB2	1:B:308:ARG:HE	1.54	0.71
1:D:68:TYR:O	1:D:71:TYR:HB3	1.90	0.71
1:B:93:THR:CG2	1:B:303:LEU:HD12	2.22	0.70
1:B:210:ILE:HD11	1:B:214:LEU:HD12	1.75	0.69
1:D:88:LYS:HE3	1:D:300:HIS:HB3	1.76	0.68
1:B:261:ASP:HB3	2:B:399:HOH:O	1.93	0.68



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:92:GLN:HA	2:B:419:HOH:O	1.94	0.67	
1:D:110:ASN:HD21	1:D:111:GLN:HG3	1.59	0.67	
1:C:304:LYS:HD3	1:C:305:VAL:N	2.11	0.66	
1:B:103:LYS:HD3	1:B:221:ASP:O	1.96	0.65	
1:B:188:TYR:OH	1:B:206:LYS:HE3	1.96	0.65	
1:C:78:LYS:HD3	1:C:255:SER:HA	1.78	0.65	
1:D:254:ARG:HB2	1:D:258:GLY:HA2	1.80	0.64	
1:A:210:ILE:HG12	1:A:214:LEU:HD12	1.78	0.64	
1:B:93:THR:HG21	1:B:303:LEU:HD12	1.79	0.64	
1:D:30:ILE:CG2	1:D:34:GLY:HA3	2.27	0.64	
1:B:210:ILE:HD11	1:B:214:LEU:CD1	2.28	0.64	
1:A:93:THR:HG21	1:A:303:LEU:HD12	1.80	0.63	
1:A:29:VAL:HG23	1:A:30:ILE:HG13	1.81	0.62	
1:C:276:LYS:HG3	1:C:300:HIS:HA	1.80	0.62	
1:A:158:CYS:HB2	1:A:173:LEU:HB2	1.81	0.62	
1:C:108:GLN:HE22	1:C:232:ARG:HG3	1.65	0.62	
1:A:18:LYS:HD2	1:A:293:LEU:HB2	1.83	0.61	
1:A:46:LEU:HD21	1:A:50:ARG:NH2	2.14	0.61	
1:B:235:VAL:HG22	2:B:446:HOH:O	2.00	0.61	
1:A:188:TYR:CE1	1:A:206:LYS:HG2	2.35	0.61	
1:D:148:LYS:HE3	1:D:167:PHE:HE1	1.67	0.60	
1:B:220:ARG:NH2	1:B:236:ASP:HB3	2.13	0.60	
1:A:276:LYS:HE3	1:A:299:ALA:O	2.02	0.59	
1:D:306:PRO:HB2	1:D:309:MET:SD	2.42	0.59	
1:B:214:LEU:HD13	1:B:220:ARG:HA	1.85	0.59	
1:C:78:LYS:CD	1:C:255:SER:HA	2.33	0.58	
1:A:142:PRO:HD2	2:A:440:HOH:O	2.04	0.58	
1:B:136:TYR:CE2	1:B:329:GLY:HA2	2.38	0.58	
1:D:233:LYS:HD2	1:D:241:CYS:HB2	1.85	0.58	
1:C:35:PRO:HD3	1:C:265:GLU:OE2	2.04	0.57	
1:B:211:PHE:HE1	1:B:220:ARG:HH21	1.52	0.57	
1:B:108:GLN:HB2	1:B:110:ASN:OD1	2.03	0.57	
1:B:158:CYS:HB2	1:B:173:LEU:HB2	1.86	0.57	
1:D:116:LYS:HE3	1:D:155:SER:OG	2.04	0.57	
1:D:6:VAL:HG23	1:D:262:LEU:HG	1.87	0.57	
1:D:310:ASP:N	1:D:313:MET:HE3	2.17	0.56	
1:B:42:LYS:HE3	1:B:51:ALA:HB2	1.88	0.56	
1:D:111:GLN:O	1:D:115:LYS:HE2	2.05	0.56	
1:D:64:ALA:O	1:D:67:VAL:HB	2.05	0.56	
1:D:88:LYS:NZ	1:D:300:HIS:CD2	2.72	0.56	
1:D:71:TYR:O	1:D:76:ASN:HA	2.05	0.56	



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:276:LYS:HE3	1:B:299:ALA:O	2.06	0.56
1:C:116:LYS:HA	1:C:156:GLY:O	2.05	0.56
1:B:217:LYS:HG2	1:B:220:ARG:HH11	1.67	0.55
1:D:310:ASP:OD1	1:D:313:MET:HG3	2.06	0.55
1:D:269:GLN:OE1	1:D:273:HIS:CE1	2.59	0.55
1:B:214:LEU:CD1	1:B:220:ARG:HA	2.37	0.55
1:D:6:VAL:HB	1:D:266:LEU:HD22	1.89	0.55
1:B:216:ASN:HB2	1:B:219:ASP:CG	2.27	0.54
1:D:88:LYS:HZ1	1:D:300:HIS:HD2	1.56	0.54
1:B:310:ASP:OD2	1:B:313:MET:SD	2.65	0.54
1:C:308:ARG:N	1:C:308:ARG:HH11	2.06	0.54
1:A:108:GLN:HE22	1:A:232:ARG:HG3	1.71	0.54
1:A:146:LEU:O	1:A:150:VAL:HG23	2.08	0.54
1:A:306:PRO:O	1:A:309:MET:HB2	2.08	0.53
1:A:305:VAL:HG13	1:A:306:PRO:HD2	1.91	0.53
1:C:287:SER:HB3	1:C:290:GLY:O	2.09	0.53
1:B:224:GLU:O	1:B:225:LEU:HD23	2.09	0.53
1:B:307:PRO:O	1:B:308:ARG:HB2	2.09	0.53
1:D:145:PRO:HG2	1:D:148:LYS:CB	2.39	0.53
1:B:214:LEU:HD11	1:B:223:TYR:CD1	2.44	0.52
1:D:121:GLY:HA2	1:D:160:PRO:HD2	1.90	0.52
1:A:30:ILE:HG23	1:A:31:PRO:HD2	1.91	0.52
1:A:148:LYS:HB2	1:A:167:PHE:CE1	2.45	0.52
1:C:276:LYS:NZ	1:C:299:ALA:O	2.41	0.52
1:D:108:GLN:H	1:D:111:GLN:HB2	1.73	0.52
1:C:70:ALA:HB1	1:C:77:LEU:HB2	1.91	0.52
1:B:125:SER:HA	1:B:129:ASN:HB2	1.92	0.52
1:C:6:VAL:CG2	1:C:262:LEU:HG	2.40	0.52
1:A:275:GLY:HA3	2:A:404:HOH:O	2.09	0.52
1:C:217:LYS:HG2	1:C:220:ARG:NH2	2.25	0.52
1:D:70:ALA:HB1	1:D:77:LEU:HD12	1.92	0.52
1:A:310:ASP:HB3	1:A:313:MET:CG	2.39	0.51
1:C:84:PHE:CD2	1:C:303:LEU:HG	2.46	0.51
1:C:42:LYS:HE3	1:C:51:ALA:HB2	1.92	0.51
1:C:94:PHE:CE2	1:C:247:PRO:HD3	2.46	0.51
1:A:125:SER:HA	1:A:129:ASN:HB2	1.93	0.51
1:D:94:PHE:HA	1:D:246:VAL:O	2.10	0.51
1:D:210:ILE:HD13	1:D:235:VAL:HG11	1.91	0.51
1:A:80:VAL:HG23	1:A:81:VAL:HG23	1.92	0.51
1:A:103:LYS:HE3	1:A:221:ASP:O	2.11	0.51
1:C:78:LYS:CE	1:C:255:SER:HA	2.41	0.50



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:49:ILE:HG21	1:C:70:ALA:HA	1.92	0.50	
1:C:158:CYS:HB2	1:C:173:LEU:HB2	1.92	0.50	
1:C:80:VAL:HG11	1:C:260:GLU:HB3	1.94	0.50	
1:A:7:ARG:HG2	1:A:38:ALA:HB3	1.94	0.50	
1:D:48:CYS:O	1:D:52:ILE:HG13	2.12	0.50	
1:D:145:PRO:HG2	1:D:148:LYS:HB2	1.94	0.50	
1:C:145:PRO:HG2	1:C:148:LYS:HB3	1.93	0.49	
1:D:30:ILE:HG22	1:D:31:PRO:O	2.12	0.49	
1:D:68:TYR:CD2	1:D:323:ILE:HD13	2.47	0.49	
1:D:293:LEU:O	1:D:294:LEU:HB2	2.12	0.49	
1:B:4:LYS:HD2	1:B:33:ASP:O	2.11	0.49	
1:B:143:ARG:O	1:B:144:LYS:HD3	2.12	0.49	
1:C:94:PHE:HA	1:C:246:VAL:O	2.13	0.49	
1:C:261:ASP:HB3	2:C:493:HOH:O	2.11	0.49	
1:C:113:ARG:CG	1:C:113:ARG:HH11	2.25	0.49	
1:D:70:ALA:HB1	1:D:77:LEU:HB2	1.95	0.49	
1:D:272:GLU:O	1:D:278:LYS:HD2	2.13	0.49	
1:A:192:PHE:CE1	1:A:210:ILE:HG13	2.48	0.49	
1:B:116:LYS:NZ	1:B:155:SER:O	2.45	0.49	
1:B:254:ARG:HG2	2:B:429:HOH:O	2.13	0.49	
1:C:304:LYS:HD3	1:C:305:VAL:H	1.78	0.49	
1:C:310:ASP:OD1	1:C:313:MET:HG3	2.12	0.49	
1:D:195:LEU:HB2	1:D:203:ALA:HB2	1.94	0.48	
1:C:148:LYS:HB2	1:C:167:PHE:CE1	2.49	0.48	
1:B:6:VAL:HB	1:B:266:LEU:HD22	1.95	0.48	
1:C:210:ILE:HD13	1:C:235:VAL:HG11	1.96	0.48	
1:B:37:VAL:HG22	1:B:266:LEU:HD21	1.96	0.48	
1:C:207:HIS:HB2	1:C:238:TYR:CG	2.49	0.48	
1:B:120:THR:HG22	1:B:188:TYR:HA	1.96	0.48	
1:B:84:PHE:HB2	1:B:91:PRO:HB2	1.97	0.47	
1:B:249:HIS:CG	1:B:296:LYS:HE2	2.48	0.47	
1:D:29:VAL:HG21	1:D:274:PHE:CZ	2.50	0.47	
1:B:96:TYR:HB2	1:B:207:HIS:HB3	1.96	0.47	
1:D:7:ARG:HA	1:D:38:ALA:HB3	1.96	0.47	
1:D:26:MET:CE	1:D:266:LEU:HD12	2.44	0.47	
1:D:107:PHE:H	1:D:232:ARG:NH2	2.12	0.47	
1:C:4:LYS:C	1:C:262:LEU:HD21	2.34	0.47	
1:C:188:TYR:CE1	1:C:206:LYS:HG2	2.50	0.47	
1:C:265:GLU:O	1:C:269:GLN:HG2	2.13	0.47	
1:C:274:PHE:CD1	1:C:282:PHE:HB3	2.49	0.47	
1:D:5:THR:CG2	1:D:38:ALA:HB2	2.44	0.47	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:46:LEU:O	1:B:50:ARG:HG3	2.14	0.47
1:B:85:TYR:CE1	1:B:248:SER:OG	2.65	0.47
1:B:211:PHE:HE1	1:B:220:ARG:NH2	2.12	0.47
1:C:88:LYS:HD3	1:C:88:LYS:N	2.30	0.47
1:D:22:PHE:HA	1:D:282:PHE:CZ	2.50	0.47
1:C:6:VAL:HB	1:C:266:LEU:HD22	1.97	0.46
1:D:86:GLY:O	1:D:300:HIS:NE2	2.48	0.46
1:A:207:HIS:CG	1:A:208:SER:N	2.83	0.46
1:B:217:LYS:HA	1:B:220:ARG:HD3	1.97	0.46
1:C:79:PRO:HB3	1:C:250:THR:HG21	1.98	0.46
1:D:4:LYS:HD2	1:D:34:GLY:O	2.15	0.46
1:B:26:MET:SD	1:B:274:PHE:HE2	2.38	0.46
1:A:324:ARG:HD2	1:A:328:GLU:OE2	2.15	0.46
1:B:93:THR:HG23	1:B:303:LEU:HD12	1.97	0.46
1:B:307:PRO:HB2	1:B:308:ARG:NE	2.28	0.46
1:C:84:PHE:HD2	1:C:303:LEU:HG	1.79	0.46
1:B:141:GLU:OE1	1:B:142:PRO:HA	2.16	0.46
1:C:188:TYR:CZ	1:C:206:LYS:HG2	2.50	0.46
1:A:181:THR:HG22	2:A:425:HOH:O	2.15	0.45
1:A:26:MET:SD	1:A:274:PHE:CE1	2.99	0.45
1:A:225:LEU:HG	1:A:235:VAL:HA	1.98	0.45
1:A:310:ASP:HB3	1:A:313:MET:HG3	1.97	0.45
1:C:71:TYR:HD1	2:C:408:HOH:O	1.99	0.45
1:A:46:LEU:HG	1:A:50:ARG:NH1	2.30	0.45
1:A:83:GLU:OE1	1:A:299:ALA:HB2	2.15	0.45
1:A:268:ASN:HA	1:A:271:GLN:HG2	1.99	0.45
1:B:194:CYS:O	1:B:199:ALA:HB3	2.16	0.45
1:B:6:VAL:HG23	1:B:262:LEU:HG	1.99	0.45
1:B:317:TYR:CE1	1:B:318:GLU:HG3	2.52	0.45
1:C:291:LYS:HE2	1:C:291:LYS:HB3	1.65	0.45
1:D:71:TYR:OH	1:D:312:LYS:HD3	2.17	0.45
1:D:30:ILE:HG23	1:D:31:PRO:HD2	1.98	0.45
1:A:154:PHE:O	1:A:169:GLN:NE2	2.49	0.45
1:B:144:LYS:HA	1:B:145:PRO:C	2.37	0.45
1:B:85:TYR:N	1:B:85:TYR:CD1	2.84	0.44
1:B:253:ALA:HB1	2:B:345:HOH:O	2.16	0.44
1:A:85:TYR:HE1	1:A:248:SER:HG	1.58	0.44
1:A:96:TYR:CE2	1:A:245:GLN:HG3	2.52	0.44
1:A:46:LEU:HG	1:A:50:ARG:CZ	2.47	0.44
1:B:85:TYR:O	1:B:91:PRO:HA	2.18	0.44
1:B:276:LYS:HG3	1:B:300:HIS:HA	1.99	0.44



		Interatomic	nic Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:268:ASN:HA	1:A:271:GLN:NE2	2.28	0.44	
1:B:107:PHE:HA	1:B:111:GLN:OE1	2.17	0.44	
1:A:320:VAL:O	1:A:324:ARG:HG3	2.18	0.44	
1:C:81:VAL:HG12	1:C:82:ALA:N	2.33	0.44	
1:A:37:VAL:HG22	1:A:266:LEU:HD21	1.99	0.44	
1:C:7:ARG:HA	1:C:38:ALA:HB3	1.99	0.44	
1:C:128:TRP:O	1:C:131:PRO:HG2	2.17	0.44	
1:C:258:GLY:O	1:C:259:LYS:HB2	2.18	0.44	
1:B:319:TYR:CE2	1:B:323:ILE:HD11	2.53	0.43	
1:A:70:ALA:O	1:A:75:ASN:HB2	2.18	0.43	
1:B:310:ASP:N	1:B:313:MET:SD	2.86	0.43	
1:D:71:TYR:HB2	1:D:311:ALA:CB	2.48	0.43	
1:D:99:ALA:HB3	1:D:226:LEU:HB2	2.00	0.43	
1:A:70:ALA:HB1	1:A:77:LEU:HB2	1.99	0.43	
1:A:120:THR:OG1	1:A:127:GLY:HA3	2.19	0.43	
1:A:228:LEU:HD12	2:A:411:HOH:O	2.18	0.43	
1:D:324:ARG:HD2	1:D:328:GLU:OE2	2.18	0.43	
1:B:188:TYR:CD1	1:B:209:THR:OG1	2.71	0.43	
1:A:4:LYS:HB3	1:A:34:GLY:O	2.18	0.43	
1:B:5:THR:HA	1:B:36:SER:O	2.17	0.43	
1:B:208:SER:O	1:B:212:GLU:HG3	2.19	0.43	
1:C:121:GLY:HA2	1:C:160:PRO:HD2	1.99	0.43	
1:D:88:LYS:HZ2	1:D:300:HIS:CD2	2.37	0.43	
1:A:188:TYR:HD1	1:A:209:THR:HG1	1.64	0.43	
1:B:30:ILE:HG23	1:B:31:PRO:HD2	2.00	0.43	
1:B:112:LEU:HD23	1:B:112:LEU:HA	1.90	0.43	
1:C:22:PHE:O	1:C:26:MET:HG2	2.19	0.43	
1:D:183:ASN:HB3	1:D:186:PHE:HB2	1.99	0.43	
1:B:7:ARG:HA	1:B:38:ALA:HB3	2.00	0.43	
1:A:105:SER:H	1:A:232:ARG:HH12	1.67	0.43	
1:D:158:CYS:HB2	1:D:173:LEU:HB2	2.01	0.43	
1:A:6:VAL:N	1:A:36:SER:O	2.42	0.42	
1:C:69:ASP:HA	1:C:72:LEU:HD12	2.01	0.42	
1:C:142:PRO:HA	2:C:434:HOH:O	2.18	0.42	
1:C:323:ILE:O	1:C:327:ARG:HG3	2.18	0.42	
1:D:94:PHE:CE2	1:D:247:PRO:HD3	2.54	0.42	
1:D:118:CYS:HB2	1:D:203:ALA:HA	2.00	0.42	
1:D:214:LEU:O	1:D:220:ARG:NH1	2.52	0.42	
1:B:35:PRO:HB3	1:B:262:LEU:CD1	2.50	0.42	
1:C:25:HIS:HB3	1:C:274:PHE:CZ	2.55	0.42	
1:A:31:PRO:HB2	1:A:33:ASP:OD2	2.20	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:103:LYS:CE	1:A:221:ASP:O	2.67	0.42	
1:B:103:LYS:HD2	1:B:224:GLU:CG	2.42	0.42	
1:B:228:LEU:HD12	2:B:400:HOH:O	2.20	0.42	
1:C:31:PRO:HB2	1:C:33:ASP:OD2	2.19	0.42	
1:C:71:TYR:O	1:C:76:ASN:HA	2.18	0.42	
1:D:103:LYS:HA	1:D:224:GLU:OE1	2.18	0.42	
1:A:6:VAL:CG2	1:A:262:LEU:HG	2.49	0.42	
1:A:144:LYS:HD3	1:A:144:LYS:HA	1.67	0.42	
1:B:148:LYS:HB2	1:B:167:PHE:CE1	2.54	0.42	
1:D:316:GLY:O	1:D:320:VAL:HG23	2.20	0.42	
1:D:25:HIS:CD2	1:D:282:PHE:HB2	2.55	0.42	
1:C:45:TYR:O	1:C:49:ILE:HG13	2.20	0.42	
1:A:48:CYS:O	1:A:52:ILE:HG13	2.20	0.42	
1:A:149:ALA:HA	2:A:380:HOH:O	2.19	0.42	
1:C:78:LYS:HE2	1:C:255:SER:HA	2.02	0.42	
1:C:160:PRO:C	1:C:161:CYS:SG	2.98	0.42	
1:D:268:ASN:O	1:D:272:GLU:HG2	2.20	0.42	
1:A:317:TYR:CZ	1:A:318:GLU:HG3	2.54	0.41	
1:D:27:LYS:NZ	1:D:36:SER:HB3	2.35	0.41	
1:D:232:ARG:O	1:D:233:LYS:HG3	2.20	0.41	
1:A:19:CYS:C	1:A:39:CYS:SG	2.98	0.41	
1:A:184:GLN:HG3	1:A:185:TYR:CD1	2.55	0.41	
1:A:266:LEU:O	1:A:270:ALA:HB2	2.20	0.41	
1:A:276:LYS:O	1:A:277:ASP:HB2	2.19	0.41	
1:C:108:GLN:HA	1:C:108:GLN:HE21	1.85	0.41	
1:C:214:LEU:HD23	1:C:214:LEU:HA	1.86	0.41	
1:A:285:PHE:CD1	1:A:299:ALA:HB3	2.55	0.41	
1:B:135:LEU:O	1:B:138:ASP:HB2	2.20	0.41	
1:D:110:ASN:ND2	1:D:110:ASN:C	2.74	0.41	
1:A:107:PHE:HA	1:A:111:GLN:OE1	2.21	0.41	
1:A:210:ILE:CG1	1:A:214:LEU:HD12	2.49	0.41	
1:C:26:MET:O	1:C:30:ILE:HG12	2.21	0.41	
1:C:228:LEU:HD23	1:C:228:LEU:HA	1.77	0.41	
1:A:84:PHE:HA	1:A:92:GLN:O	2.20	0.41	
1:C:107:PHE:H	1:C:232:ARG:NH2	2.19	0.41	
1:D:151:ALA:HA	2:D:433:HOH:O	2.19	0.41	
1:D:305:VAL:HG13	1:D:306:PRO:HD2	2.00	0.41	
1:B:145:PRO:HD2	1:B:148:LYS:HE2	2.03	0.41	
1:B:186:PHE:O	1:B:190:GLY:HA3	2.20	0.41	
1:C:296:LYS:NZ	2:C:435:HOH:O	2.52	0.41	
1:B:174:CYS:SG	1:B:174:CYS:O	2.78	0.41	



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:A:306:PRO:HA	1:A:307:PRO:HD3	1.74	0.41
1:C:17:THR:HG22	1:C:289:HIS:CE1	2.56	0.41
1:C:304:LYS:HD3	1:C:305:VAL:O	2.21	0.41
1:D:105:SER:OG	1:D:232:ARG:NH2	2.51	0.41
1:D:145:PRO:HG2	1:D:148:LYS:HB3	2.02	0.41
1:A:115:LYS:HB3	1:A:201:ASP:OD2	2.20	0.41
1:B:219:ASP:HA	1:B:222:GLN:OE1	2.21	0.41
1:C:108:GLN:HA	1:C:108:GLN:NE2	2.36	0.41
1:A:268:ASN:O	1:A:271:GLN:HG2	2.20	0.40
1:B:193:LYS:NZ	1:B:197:ASP:OD2	2.51	0.40
1:B:217:LYS:HA	1:B:220:ARG:HB2	2.03	0.40
1:C:144:LYS:HA	1:C:145:PRO:C	2.40	0.40
1:C:272:GLU:O	1:C:278:LYS:HE2	2.21	0.40
1:B:110:ASN:OD1	1:B:111:GLN:HG3	2.21	0.40
1:A:151:ALA:O	1:A:169:GLN:NE2	2.55	0.40
1:C:82:ALA:O	1:C:302:PHE:HA	2.21	0.40
1:C:90:ASP:N	1:C:91:PRO:CD	2.85	0.40
1:C:225:LEU:HB2	1:C:241:CYS:SG	2.62	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	Perce	ntiles
1	А	326/337~(97%)	307 (94%)	19 (6%)	0	100	100
1	В	326/337~(97%)	305~(94%)	19~(6%)	2(1%)	25	26
1	С	332/337~(98%)	319 (96%)	12 (4%)	1 (0%)	41	46
1	D	332/337~(98%)	313 (94%)	18 (5%)	1 (0%)	41	46
All	All	1316/1348~(98%)	1244 (94%)	68 (5%)	4 (0%)	41	46

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	D	125	SER
1	В	125	SER
1	В	329	GLY
1	С	205	VAL

5.3.2 Protein sidechains (i)

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	\mathbf{s}
1	А	273/281~(97%)	260~(95%)	13~(5%)	25 32	
1	В	273/281~(97%)	256~(94%)	17~(6%)	18 21	
1	С	278/281~(99%)	265~(95%)	13~(5%)	26 33	
1	D	278/281~(99%)	270~(97%)	8(3%)	42 54	
All	All	1102/1124 (98%)	1051 (95%)	51 (5%)	27 34	

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	33	ASP
1	А	71	TYR
1	А	78	LYS
1	А	182	LEU
1	А	217	LYS
1	А	234	PRO
1	А	249	HIS
1	А	252	VAL
1	А	256	MET
1	А	261	ASP
1	А	274	PHE
1	А	291	LYS
1	А	308	ARG
1	В	32	SER
1	В	33	ASP
1	В	66	LEU
1	В	71	TYR
1	В	88	LYS



Mol	Chain	Res	Type
1	В	105	SER
1	В	236	ASP
1	В	249	HIS
1	В	261	ASP
1	В	272	GLU
1	В	277	ASP
1	В	281	GLU
1	В	291	LYS
1	В	308	ARG
1	В	309	MET
1	В	310	ASP
1	В	313	MET
1	С	32	SER
1	С	88	LYS
1	С	113	ARG
1	С	122	LEU
1	С	148	LYS
1	С	217	LYS
1	С	249	HIS
1	С	255	SER
1	С	256	MET
1	С	280	LYS
1	C	284	LEU
1	C	291	LYS
1	С	308	ARG
1	D	56	GLU
1	D	169	GLN
1	D	182	LEU
1	D	236	ASP
1	D	249	HIS
1	D	261	ASP
1	D	308	ARG
1	D	336	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	92	GLN
1	А	108	GLN
1	А	169	GLN
1	В	76	ASN
1	В	108	GLN



Mol	Chain	Res	Type
1	В	213	ASN
1	В	283	GLN
1	С	108	GLN
1	D	75	ASN
1	D	92	GLN
1	D	108	GLN
1	D	110	ASN
1	D	273	HIS
1	D	283	GLN
1	D	300	HIS

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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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

