



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:08 PM GMT

PDB ID : 1E78
Title : CRYSTAL STRUCTURE OF HUMAN SERUM ALBUMIN
Authors : Bhattacharya, A.A.; Curry, S.; Franks, N.P.
Deposited on : 2000-08-25
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

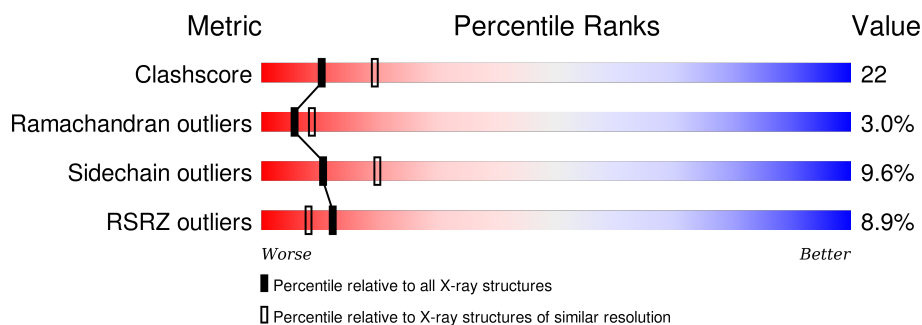
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 ≥ 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>8%</div> <div>60%</div> <div>34%</div> <div>5%</div> </div>
1	B	585	<div> <div>10%</div> <div>61%</div> <div>33%</div> <div>5%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8664 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
			4339	2743	725	830	41			
1	B	578	Total	C	N	O	S	0	0	0
			4265	2692	718	815	40			

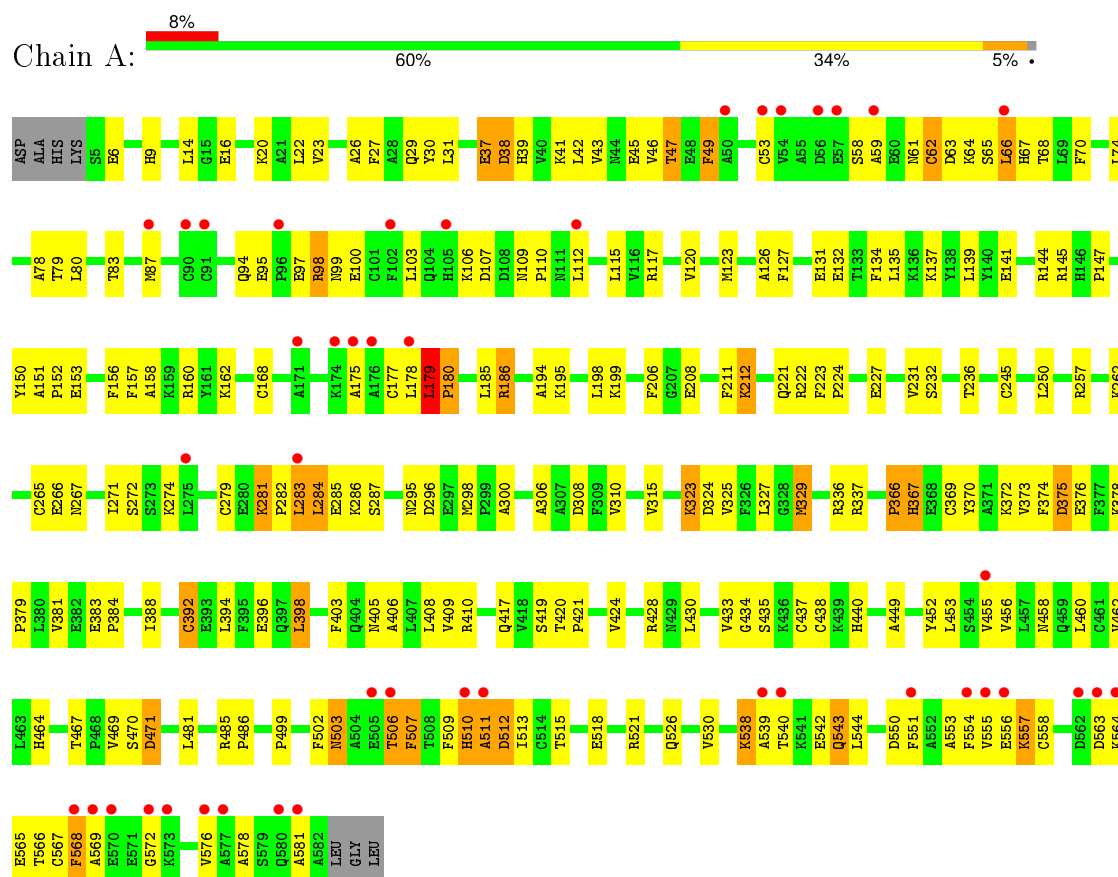
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		
2	B	29	Total	O	0	0
			29	29		

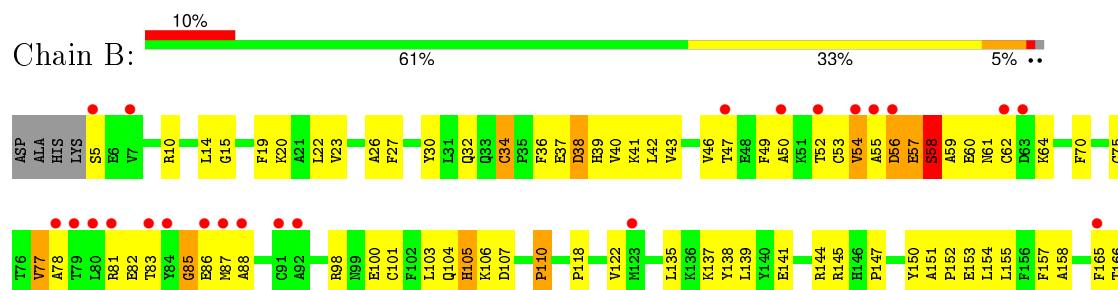
3 Residue-property plots [i](#)

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: SERUM ALBUMIN



• Molecule 1: SERUM ALBUMIN



C567	K483	Q597	S287	E167
F568	R484	L398	R288	C168
A569	R485	G399	I289	C169
E570	P486			
E571		K402	V293	K174
G572	S489	F403	E294	A175
K573		Q404	N295	A176
K574	K500	N405		C177
L575	E501		A300	L178
V576	F502	L408	V310	P180
N503	N503	V409		P180
A504	A504	R410	D314	R186
E505	E505	Y411		
S579	T506		N318	
Q580	F507	K414	K323	K190
A581	T508	T420	D324	A194
A582	H510	P421		L198
LEU	A511	V424	E333	K199
GLY	H512	E425		
LEU	I513	V426	R336	F206
	T515	S427	R337	K212
	L516	R428		A213
		N429	D340	W214
	E520	L430	Y341	A215
	H521		S342	V216
		V433	G434	Q221
	Q526	G434	V344	V231
		S435	L345	S232
	L529			V235
	V530	C438	L349	K240
	E531		A364	E244
	H535	E442		C245
		R445	D365	
	K538	N446	P367	D249
	A539	P447	E368	L250
	T540	V455	Y370	L251
	K541		A371	E252
	E542		K372	
	Q543	N458	V373	S272
	L544	Q459	F374	L275
	K545	L460	D375	K276
	A546	C461		E277
	V547	V462	K378	C279
	N548	L463	P379	E280
		R464		K281
	V555		E383	P282
	E556	T467	P384	L283
	K557	V468	Q385	L284
	C558	S470		E285
	C559		I388	K286
	K560	K475		
	A561			
	D562	E479	C392	
	D563	S480	E393	
	K564	L481	L394	
	E565			
	T566	V482		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.84Å 55.62Å 120.27Å 81.22° 91.08° 64.28°	Depositor
Resolution (Å)	40.00 – 2.60 36.16 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.00-2.60) 90.4 (36.16-2.58)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.58Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.247 , 0.277 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 82.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 37936 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8664	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0.33	0/4425	0.55	0/6018
1	B	0.34	0/4347	0.54	3/5916 (0.1%)
All	All	0.33	0/8772	0.55	3/11934 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	540	THR	N-CA-C	8.09	132.84	111.00
1	B	541	LYS	N-CA-C	6.79	129.34	111.00
1	B	58	SER	CA-C-N	-5.05	106.10	117.20

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	4339	0	4009	196	0
1	B	4265	0	3898	163	0
2	A	31	0	0	4	0
2	B	29	0	0	5	0
All	All	8664	0	7907	359	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 22.

All (359) 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:557:LYS:NZ	1:B:571:GLU:HG3	1.58	1.18
1:A:503:ASN:HB2	1:A:506:THR:OG1	1.56	1.04
1:B:557:LYS:HZ1	1:B:571:GLU:HG3	1.05	1.01
1:A:94:GLN:O	1:A:98:ARG:HB3	1.60	1.00
1:A:503:ASN:HB3	1:A:506:THR:H	1.31	0.96
1:B:378:LYS:HB2	1:B:379:PRO:HD3	1.50	0.93
1:A:557:LYS:HG2	1:A:558:CYS:N	1.86	0.89
1:A:67:HIS:HB3	1:A:98:ARG:HH21	1.35	0.89
1:A:410:ARG:HD3	2:A:2020:HOH:O	1.76	0.84
1:A:392:CYS:O	1:A:396:GLU:HG3	1.79	0.83
1:A:98:ARG:NH2	1:A:99:ASN:HB2	1.94	0.83
1:A:503:ASN:HB2	1:A:506:THR:CB	2.09	0.82
1:A:186:ARG:HD3	2:A:2007:HOH:O	1.76	0.82
1:A:557:LYS:HG2	1:A:558:CYS:H	1.44	0.82
1:B:81:ARG:HE	1:B:88:ALA:HB3	1.43	0.81
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.46	0.80
1:A:376:GLU:O	1:A:379:PRO:HD2	1.82	0.80
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.63	0.80
1:A:507:PHE:CZ	1:A:509:PHE:HZ	2.01	0.79
1:A:503:ASN:HB3	1:A:506:THR:N	1.98	0.77
1:B:39:HIS:O	1:B:43:VAL:HG23	1.85	0.77
1:A:507:PHE:CD1	1:A:507:PHE:O	2.39	0.75
1:A:283:LEU:HG	1:A:284:LEU:HD23	1.67	0.75
1:A:152:PRO:HB2	1:A:257:ARG:HH11	1.52	0.75
1:A:23:VAL:O	1:A:27:PHE:HD1	1.67	0.75
1:A:98:ARG:CZ	1:A:99:ASN:HB2	2.16	0.75
1:B:557:LYS:HZ1	1:B:571:GLU:CG	1.95	0.74
1:A:503:ASN:HB2	1:A:506:THR:HG1	1.53	0.73
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.71	0.73
1:A:61:ASN:HB3	1:A:64:LYS:HD2	1.70	0.73
1:A:564:LYS:O	1:A:566:THR:N	2.17	0.73
1:A:424:VAL:O	1:A:428:ARG:HG3	1.89	0.73
1:A:540:THR:HG23	1:A:544:LEU:CD1	2.17	0.72
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.70	0.72
1:A:503:ASN:CB	1:A:506:THR:CB	2.68	0.71
1:B:81:ARG:NE	1:B:88:ALA:HB3	2.06	0.71
1:B:34:CYS:HB3	1:B:39:HIS:NE2	2.05	0.71
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.71	0.71
1:A:557:LYS:CG	1:A:558:CYS:N	2.54	0.70
1:B:480:SER:HB2	2:B:2024:HOH:O	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.57	0.69
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.72	0.69
1:A:540:THR:HG23	1:A:544:LEU:HD11	1.74	0.69
1:B:507:PHE:CD1	1:B:507:PHE:O	2.46	0.69
1:A:323:LYS:HG3	1:A:324:ASP:N	2.07	0.68
1:B:279:CYS:HA	1:B:286:LYS:HD2	1.73	0.68
1:A:420:THR:HG23	1:A:530:VAL:HG11	1.77	0.67
1:B:511:ALA:HA	1:B:568:PHE:CZ	2.28	0.67
1:A:540:THR:CG2	1:A:544:LEU:HD11	2.23	0.67
1:A:117:ARG:HB2	1:A:123:MET:CE	2.25	0.67
1:A:420:THR:HG23	1:A:530:VAL:CG1	2.25	0.66
1:B:378:LYS:HB2	1:B:379:PRO:CD	2.25	0.66
1:B:394:LEU:HD11	1:B:398:LEU:HD11	1.78	0.66
1:B:310:VAL:HG21	1:B:374:PHE:CE1	2.31	0.65
1:B:212:LYS:O	1:B:216:VAL:HG23	1.94	0.65
1:A:538:LYS:O	1:A:540:THR:N	2.30	0.65
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.76	0.65
1:A:39:HIS:O	1:A:43:VAL:HG23	1.96	0.65
1:A:306:ALA:HA	1:A:310:VAL:HG22	1.79	0.65
1:B:373:VAL:HG13	1:B:374:PHE:N	2.12	0.65
1:A:503:ASN:CB	1:A:506:THR:HB	2.27	0.64
1:A:464:HIS:CE1	1:A:469:VAL:H	2.15	0.64
1:B:394:LEU:O	1:B:397:GLN:HG2	1.97	0.64
1:B:52:THR:HA	1:B:56:ASP:OD2	1.98	0.63
1:A:198:LEU:HA	1:A:458:ASN:ND2	2.13	0.63
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.80	0.63
1:B:36:PHE:O	1:B:40:VAL:HG23	1.99	0.63
1:B:199:LYS:HG3	2:B:2010:HOH:O	1.99	0.63
1:B:557:LYS:HZ2	1:B:571:GLU:HG3	1.59	0.63
1:A:543:GLN:O	1:A:544:LEU:C	2.37	0.63
1:B:50:ALA:O	1:B:54:VAL:HG23	1.99	0.63
1:A:66:LEU:HD23	2:A:2015:HOH:O	1.97	0.62
1:B:276:LYS:HE3	1:B:280:GLU:OE2	1.99	0.62
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.81	0.62
1:B:342:SER:OG	1:B:344:VAL:HG23	1.99	0.62
1:A:502:PHE:CE1	1:A:507:PHE:CZ	2.86	0.62
1:A:117:ARG:HB2	1:A:123:MET:HE3	1.82	0.62
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.82	0.62
1:A:279:CYS:HA	1:A:286:LYS:HD2	1.81	0.62
1:A:394:LEU:HG	1:A:398:LEU:HD11	1.82	0.62
1:B:81:ARG:HE	1:B:88:ALA:CB	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ASN:HB3	1:B:64:LYS:HD2	1.82	0.61
1:A:283:LEU:HG	1:A:284:LEU:N	2.15	0.61
1:A:464:HIS:HE1	1:A:470:SER:H	1.48	0.61
1:A:282:PRO:HB2	1:A:285:GLU:OE1	2.00	0.61
1:A:434:GLY:O	1:A:438:CYS:HB2	2.00	0.61
1:B:531:GLU:O	1:B:535:HIS:HD2	1.83	0.61
1:A:564:LYS:C	1:A:566:THR:H	2.02	0.60
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.83	0.60
1:A:366:PRO:O	1:A:369:CYS:N	2.35	0.60
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.83	0.60
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.33	0.60
1:B:107:ASP:O	1:B:110:PRO:HD3	2.01	0.60
1:B:375:ASP:O	1:B:378:LYS:HG3	2.02	0.60
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.83	0.59
1:A:507:PHE:CE2	1:A:509:PHE:HZ	2.19	0.59
1:A:366:PRO:O	1:A:367:HIS:C	2.41	0.59
1:A:110:PRO:HB2	1:A:112:LEU:HG	1.85	0.59
1:A:511:ALA:O	1:A:513:ILE:N	2.35	0.59
1:B:420:THR:HB	1:B:421:PRO:HD3	1.85	0.59
1:A:507:PHE:O	1:A:509:PHE:CE1	2.56	0.59
1:A:325:VAL:HG12	1:A:329:MET:CE	2.32	0.59
1:B:42:LEU:O	1:B:46:VAL:HG23	2.03	0.59
1:A:67:HIS:CB	1:A:98:ARG:HH21	2.12	0.59
1:B:293:VAL:HG22	1:B:294:GLU:N	2.17	0.59
1:B:323:LYS:HG3	1:B:324:ASP:N	2.17	0.59
1:B:186:ARG:O	1:B:190:LYS:HG3	2.02	0.58
1:A:153:GLU:O	1:A:157:PHE:HD1	1.86	0.58
1:B:475:LYS:O	1:B:479:GLU:HB2	2.03	0.58
1:A:199:LYS:HG2	1:A:211:PHE:HE2	1.68	0.58
1:A:553:ALA:O	1:A:556:GLU:HG2	2.03	0.57
1:A:42:LEU:O	1:A:46:VAL:HG23	2.04	0.57
1:A:430:LEU:O	1:A:433:VAL:HG12	2.02	0.57
1:B:23:VAL:O	1:B:27:PHE:HD1	1.87	0.57
1:A:511:ALA:C	1:A:513:ILE:H	2.07	0.57
1:A:139:LEU:HD21	1:A:158:ALA:HB2	1.86	0.57
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.03	0.57
1:A:408:LEU:HD22	1:A:530:VAL:CG2	2.35	0.56
1:B:507:PHE:HD1	1:B:507:PHE:O	1.88	0.56
1:A:100:GLU:HA	1:A:100:GLU:OE1	2.05	0.56
1:B:426:VAL:HG21	1:B:460:LEU:HB2	1.87	0.56
1:B:571:GLU:HA	1:B:574:LYS:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:PHE:HE1	1:A:507:PHE:CZ	2.23	0.56
1:B:507:PHE:CE2	1:B:509:PHE:HZ	2.24	0.56
1:B:563:ASP:OD2	1:B:565:GLU:O	2.24	0.56
1:B:430:LEU:O	1:B:433:VAL:HG12	2.05	0.55
1:A:98:ARG:NH1	1:A:99:ASN:H	2.04	0.55
1:A:208:GLU:O	1:A:212:LYS:HB2	2.05	0.55
1:A:325:VAL:HG12	1:A:329:MET:HE2	1.89	0.55
1:B:540:THR:O	1:B:544:LEU:CG	2.55	0.55
1:B:428:ARG:HD3	2:B:2020:HOH:O	2.06	0.55
1:A:66:LEU:H	1:A:66:LEU:HD13	1.71	0.54
1:A:554:PHE:HE1	1:A:568:PHE:CE1	2.25	0.54
1:A:567:CYS:SG	1:A:568:PHE:N	2.80	0.54
1:B:194:ALA:HB1	1:B:455:VAL:HG13	1.89	0.54
1:A:262:LYS:O	1:A:266:GLU:HG3	2.07	0.54
1:A:126:ALA:HB2	2:A:2004:HOH:O	2.07	0.54
1:B:459:GLN:O	1:B:462:VAL:HG22	2.09	0.53
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.91	0.53
1:B:464:HIS:CE1	1:B:469:VAL:H	2.26	0.53
1:B:153:GLU:O	1:B:157:PHE:HD1	1.91	0.53
1:B:424:VAL:O	1:B:428:ARG:HG3	2.08	0.53
1:B:398:LEU:O	1:B:402:LYS:HB2	2.08	0.53
1:B:541:LYS:HA	1:B:544:LEU:HD12	1.91	0.53
1:B:571:GLU:OE1	1:B:574:LYS:HD2	2.09	0.53
1:A:49:PHE:HE1	1:A:62:CYS:SG	2.32	0.53
1:B:384:PRO:O	1:B:388:ILE:HG12	2.10	0.52
1:A:100:GLU:OE1	1:A:103:LEU:HD12	2.09	0.52
1:A:23:VAL:HG13	1:A:70:PHE:HE1	1.73	0.52
1:B:394:LEU:CD1	1:B:398:LEU:HD11	2.38	0.52
1:B:516:LEU:HD22	1:B:520:GLU:CB	2.39	0.52
1:A:408:LEU:HD11	1:A:526:GLN:HB3	1.91	0.52
1:B:367:HIS:O	1:B:371:ALA:HB2	2.09	0.52
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.74	0.52
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.91	0.52
1:A:156:PHE:HE1	1:A:285:GLU:HG3	1.74	0.52
1:B:531:GLU:O	1:B:535:HIS:CD2	2.62	0.52
1:B:100:GLU:O	1:B:104:GLN:HG3	2.10	0.52
1:A:405:ASN:O	1:A:409:VAL:HG23	2.09	0.52
1:A:131:GLU:O	1:A:134:PHE:N	2.39	0.52
1:B:240:LYS:HE2	1:B:244:GLU:OE2	2.10	0.52
1:A:117:ARG:HB2	1:A:123:MET:HE1	1.92	0.51
1:A:518:GLU:HA	1:A:521:ARG:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ALA:C	1:A:513:ILE:N	2.63	0.51
1:B:511:ALA:C	1:B:513:ILE:H	2.13	0.51
1:B:405:ASN:O	1:B:409:VAL:HG23	2.11	0.51
1:B:283:LEU:HG	1:B:284:LEU:N	2.25	0.51
1:B:15:GLY:O	1:B:19:PHE:HB3	2.11	0.51
1:B:23:VAL:O	1:B:27:PHE:CD1	2.64	0.51
1:A:372:LYS:O	1:A:375:ASP:HB2	2.11	0.51
1:B:372:LYS:O	1:B:375:ASP:HB2	2.12	0.50
1:A:61:ASN:C	1:A:63:ASP:H	2.15	0.50
1:B:32:GLN:NE2	1:B:110:PRO:HG3	2.27	0.50
1:B:14:LEU:HD13	1:B:22:LEU:HD12	1.94	0.50
1:B:310:VAL:CG2	1:B:374:PHE:CE1	2.94	0.50
1:A:115:LEU:HD22	1:A:145:ARG:NH1	2.27	0.50
1:B:399:GLY:O	1:B:403:PHE:HB2	2.12	0.50
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.93	0.50
1:A:464:HIS:HE1	1:A:469:VAL:H	1.60	0.49
1:A:512:ASP:O	1:A:515:THR:HG22	2.13	0.49
1:A:31:LEU:HG	1:A:74:LEU:HD22	1.93	0.49
1:B:54:VAL:HG12	1:B:55:ALA:N	2.26	0.49
1:A:381:VAL:O	1:A:384:PRO:HD2	2.12	0.49
1:B:333:GLU:O	1:B:337:ARG:HG3	2.11	0.49
1:B:166:THR:CG2	2:B:2007:HOH:O	2.61	0.49
1:B:373:VAL:CG1	1:B:374:PHE:N	2.76	0.49
1:B:540:THR:O	1:B:544:LEU:HG	2.12	0.49
1:A:66:LEU:HD13	1:A:66:LEU:N	2.28	0.48
1:A:540:THR:HG23	1:A:544:LEU:CG	2.43	0.48
1:A:471:ASP:N	1:A:471:ASP:OD1	2.41	0.48
1:A:135:LEU:HD11	1:A:162:LYS:HD3	1.95	0.48
1:A:43:VAL:O	1:A:47:THR:OG1	2.30	0.48
1:A:373:VAL:HG13	1:A:374:PHE:N	2.29	0.48
1:A:543:GLN:HG2	1:A:544:LEU:H	1.78	0.48
1:B:571:GLU:OE1	1:B:571:GLU:HA	2.13	0.48
1:A:420:THR:O	1:A:424:VAL:HG23	2.13	0.48
1:B:198:LEU:HA	1:B:458:ASN:ND2	2.28	0.48
1:A:376:GLU:C	1:A:379:PRO:HD2	2.34	0.48
1:B:57:GLU:O	1:B:58:SER:C	2.51	0.48
1:B:290:ILE:O	1:B:293:VAL:HG12	2.13	0.48
1:A:14:LEU:HD13	1:A:22:LEU:HD12	1.95	0.48
1:B:293:VAL:CG2	1:B:294:GLU:N	2.77	0.48
1:A:38:ASP:O	1:A:42:LEU:HG	2.13	0.48
1:A:449:ALA:O	1:A:453:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:GLU:C	1:B:544:LEU:N	2.67	0.47
1:A:137:LYS:O	1:A:141:GLU:HG2	2.14	0.47
1:B:141:GLU:O	1:B:145:ARG:HG3	2.13	0.47
1:A:61:ASN:HD22	1:A:64:LYS:HE3	1.80	0.47
1:B:141:GLU:OE1	1:B:144:ARG:HD3	2.14	0.47
1:B:310:VAL:HG21	1:B:374:PHE:CD1	2.49	0.47
1:B:194:ALA:HB1	1:B:455:VAL:CG1	2.43	0.47
1:A:222:ARG:C	1:A:224:PRO:HD3	2.35	0.47
1:A:227:GLU:O	1:A:231:VAL:HG23	2.13	0.47
1:B:19:PHE:CD1	1:B:19:PHE:C	2.88	0.47
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.49	0.47
1:B:516:LEU:O	1:B:521:ARG:NH2	2.46	0.47
1:A:310:VAL:O	1:A:370:TYR:HE1	1.98	0.46
1:A:306:ALA:CA	1:A:310:VAL:HG22	2.45	0.46
1:A:578:ALA:O	1:A:581:ALA:HB3	2.15	0.46
1:B:206:PHE:CE2	1:B:481:LEU:HD13	2.51	0.46
1:B:442:GLU:HA	1:B:445:ARG:HD2	1.96	0.46
1:A:420:THR:HB	1:A:421:PRO:HD3	1.96	0.46
1:A:49:PHE:CE1	1:A:53:CYS:SG	3.09	0.46
1:A:221:GLN:O	1:A:224:PRO:HD3	2.16	0.46
1:A:370:TYR:CD1	1:A:370:TYR:C	2.89	0.46
1:A:38:ASP:OD1	1:A:38:ASP:N	2.46	0.46
1:A:178:LEU:O	1:A:179:LEU:C	2.54	0.46
1:A:117:ARG:HG3	1:A:117:ARG:O	2.16	0.46
1:A:567:CYS:O	1:A:569:ALA:N	2.48	0.46
1:A:127:PHE:HB2	1:A:134:PHE:CE2	2.51	0.46
1:B:137:LYS:O	1:B:141:GLU:HG2	2.16	0.46
1:A:152:PRO:HB2	1:A:257:ARG:NH1	2.24	0.46
1:B:34:CYS:HB3	1:B:39:HIS:CD2	2.50	0.46
1:B:34:CYS:HB3	1:B:39:HIS:HE2	1.79	0.46
1:A:419:SER:HB2	1:A:421:PRO:HD2	1.98	0.46
1:B:22:LEU:HD21	1:B:155:LEU:HD11	1.97	0.46
1:A:542:GLU:O	1:A:543:GLN:C	2.52	0.45
1:A:384:PRO:O	1:A:388:ILE:HG12	2.15	0.45
1:A:572:GLY:O	1:A:576:VAL:HG23	2.16	0.45
1:B:249:ASP:HB3	1:B:252:GLU:OE1	2.17	0.45
1:B:374:PHE:O	1:B:375:ASP:C	2.54	0.45
1:B:507:PHE:HD1	1:B:507:PHE:H	1.64	0.45
1:B:483:ASN:C	1:B:486:PRO:HD2	2.36	0.45
1:A:518:GLU:OE1	1:A:521:ARG:HD2	2.15	0.45
1:B:70:PHE:N	1:B:70:PHE:CD1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PRO:CB	1:A:257:ARG:HH11	2.26	0.45
1:A:485:ARG:HB3	1:A:486:PRO:CD	2.45	0.45
1:A:279:CYS:HA	1:A:286:LYS:CD	2.44	0.45
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.16	0.45
1:B:458:ASN:HB2	2:B:2022:HOH:O	2.16	0.45
1:B:141:GLU:HA	1:B:141:GLU:OE1	2.17	0.45
1:A:41:LYS:O	1:A:45:GLU:HG3	2.16	0.45
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.52	0.45
1:A:6:GLU:O	1:A:9:HIS:HB3	2.16	0.45
1:A:95:GLU:O	1:A:98:ARG:NH1	2.50	0.44
1:B:563:ASP:OD2	1:B:565:GLU:C	2.55	0.44
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.99	0.44
1:A:66:LEU:HB3	1:A:70:PHE:CE2	2.53	0.44
1:A:540:THR:HG23	1:A:544:LEU:HG	1.99	0.44
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.98	0.44
1:B:540:THR:O	1:B:544:LEU:CB	2.66	0.44
1:A:507:PHE:CE2	1:A:509:PHE:CZ	3.02	0.44
1:B:38:ASP:O	1:B:41:LYS:HB3	2.17	0.44
1:B:563:ASP:O	1:B:564:LYS:O	2.35	0.44
1:A:141:GLU:O	1:A:145:ARG:HG3	2.17	0.44
1:B:276:LYS:HG3	1:B:277:GLU:N	2.30	0.44
1:A:540:THR:HG21	1:A:544:LEU:HD11	1.98	0.44
1:B:314:ASP:O	1:B:318:ASN:ND2	2.51	0.44
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.48	0.44
1:A:78:ALA:C	1:A:80:LEU:H	2.21	0.44
1:A:417:GLN:HB2	1:A:470:SER:HB2	2.00	0.44
1:B:38:ASP:N	1:B:38:ASP:OD1	2.48	0.44
1:B:278:CYS:HB3	1:B:289:CYS:HB3	1.89	0.44
1:A:509:PHE:O	1:A:510:HIS:C	2.57	0.44
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.58	0.44
1:A:16:GLU:O	1:A:20:LYS:HB2	2.18	0.43
1:B:434:GLY:O	1:B:438:CYS:HB2	2.18	0.43
1:A:97:GLU:C	1:A:99:ASN:N	2.71	0.43
1:A:115:LEU:HD22	1:A:145:ARG:HH12	1.83	0.43
1:A:179:LEU:CB	1:A:180:PRO:HD3	2.48	0.43
1:B:529:LEU:HD13	1:B:548:MET:HG2	2.00	0.43
1:A:168:CYS:SG	1:A:177:CYS:C	2.97	0.43
1:B:81:ARG:HG2	1:B:88:ALA:CB	2.48	0.43
1:A:509:PHE:N	1:A:509:PHE:CD1	2.85	0.43
1:A:23:VAL:HG13	1:A:27:PHE:HE1	1.83	0.43
1:A:61:ASN:C	1:A:63:ASP:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PHE:O	1:A:49:PHE:HD1	2.01	0.43
1:A:564:LYS:C	1:A:566:THR:N	2.63	0.43
1:A:464:HIS:CE1	1:A:470:SER:H	2.32	0.43
1:B:139:LEU:HD21	1:B:158:ALA:HB2	2.00	0.43
1:B:539:ALA:O	1:B:540:THR:HG23	2.19	0.43
1:A:298:MET:SD	1:A:337:ARG:HA	2.59	0.43
1:B:511:ALA:C	1:B:513:ILE:N	2.72	0.43
1:B:56:ASP:N	1:B:56:ASP:OD1	2.52	0.43
1:B:49:PHE:O	1:B:53:CYS:SG	2.77	0.43
1:B:507:PHE:N	1:B:507:PHE:CD1	2.86	0.43
1:B:70:PHE:N	1:B:70:PHE:HD1	2.16	0.43
1:B:10:ARG:HA	1:B:10:ARG:HD3	1.79	0.43
1:B:118:PRO:HB2	1:B:122:VAL:HB	2.01	0.43
1:B:373:VAL:HG13	1:B:374:PHE:H	1.84	0.42
1:A:437:CYS:O	1:A:440:HIS:HB2	2.19	0.42
1:A:551:PHE:O	1:A:555:VAL:HG23	2.19	0.42
1:A:107:ASP:O	1:A:147:PRO:HG3	2.18	0.42
1:B:139:LEU:HD22	1:B:154:LEU:HG	2.00	0.42
1:A:366:PRO:O	1:A:369:CYS:HB3	2.18	0.42
1:A:78:ALA:C	1:A:80:LEU:N	2.72	0.42
1:B:366:PRO:O	1:B:369:CYS:N	2.52	0.42
1:A:61:ASN:O	1:A:63:ASP:N	2.53	0.42
1:A:458:ASN:O	1:A:462:VAL:HG13	2.19	0.42
1:A:554:PHE:CE1	1:A:568:PHE:CE1	3.07	0.42
1:A:131:GLU:O	1:A:132:GLU:C	2.56	0.42
1:A:141:GLU:OE1	1:A:144:ARG:HD3	2.20	0.42
1:B:364:ALA:O	1:B:366:PRO:HD3	2.19	0.42
1:A:452:TYR:O	1:A:456:VAL:HG23	2.19	0.42
1:A:563:ASP:C	1:A:564:LYS:O	2.55	0.42
1:A:394:LEU:O	1:A:398:LEU:HG	2.19	0.42
1:B:103:LEU:C	1:B:105:HIS:H	2.23	0.42
1:A:65:SER:O	1:A:66:LEU:C	2.58	0.42
1:B:333:GLU:OE1	1:B:336:ARG:HD3	2.19	0.42
1:A:223:PHE:N	1:A:224:PRO:HD3	2.34	0.42
1:B:165:PHE:O	1:B:169:CYS:HB2	2.20	0.42
1:A:553:ALA:O	1:A:557:LYS:HB3	2.20	0.42
1:B:38:ASP:O	1:B:42:LEU:HG	2.19	0.42
1:A:67:HIS:O	1:A:68:THR:C	2.57	0.42
1:B:563:ASP:O	1:B:564:LYS:C	2.56	0.42
1:A:49:PHE:CD1	1:A:49:PHE:C	2.93	0.41
1:B:135:LEU:O	1:B:138:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:THR:HG22	1:B:544:LEU:HG	2.02	0.41
1:B:464:HIS:CE1	1:B:470:SER:H	2.38	0.41
1:A:403:PHE:O	1:A:406:ALA:HB3	2.21	0.41
1:A:267:ASN:O	1:A:271:ILE:HD12	2.20	0.41
1:B:168:CYS:SG	1:B:177:CYS:C	2.99	0.41
1:B:384:PRO:O	1:B:385:GLN:C	2.58	0.41
1:B:23:VAL:HG13	1:B:27:PHE:CE1	2.56	0.41
1:B:464:HIS:HE1	1:B:470:SER:H	1.67	0.41
1:A:460:LEU:O	1:A:460:LEU:HD12	2.20	0.41
1:B:85:GLY:C	1:B:87:MET:H	2.24	0.41
1:B:5:SER:HA	1:B:62:CYS:O	2.21	0.41
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.60	0.41
1:A:160:ARG:HD3	1:A:185:LEU:HD21	2.01	0.41
1:A:394:LEU:CG	1:A:398:LEU:HD11	2.48	0.41
1:A:274:LYS:HE3	1:A:296:ASP:HA	2.02	0.41
1:B:345:LEU:O	1:B:349:LEU:HG	2.21	0.41
1:B:507:PHE:CZ	1:B:509:PHE:HZ	2.39	0.41
1:B:408:LEU:HD23	1:B:408:LEU:HA	1.96	0.40
1:B:367:HIS:HA	1:B:370:TYR:CZ	2.56	0.40
1:B:37:GLU:CD	1:B:37:GLU:H	2.24	0.40
1:B:75:CYS:HA	1:B:78:ALA:HB3	2.03	0.40
1:B:178:LEU:O	1:B:179:LEU:C	2.59	0.40
1:B:231:VAL:O	1:B:235:VAL:HG23	2.22	0.40
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.43	0.40
1:B:340:ASP:O	1:B:447:PRO:HD3	2.21	0.40
1:A:367:HIS:HA	1:A:370:TYR:CZ	2.56	0.40
1:A:206:PHE:CE2	1:A:481:LEU:HD13	2.55	0.40
1:A:327:LEU:HA	1:A:327:LEU:HD23	1.96	0.40
1:B:272:SER:HB3	1:B:275:LEU:HG	2.04	0.40
1:B:221:GLN:O	1:B:295:ASN:HB3	2.22	0.40
1:B:98:ARG:O	1:B:101:CYS:HB3	2.21	0.40
1:B:411:TYR:HA	1:B:414:LYS:HD3	2.04	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	576/585 (98%)	496 (86%)	60 (10%)	20 (4%)	4	6
1	B	576/585 (98%)	503 (87%)	59 (10%)	14 (2%)	7	13
All	All	1152/1170 (98%)	999 (87%)	119 (10%)	34 (3%)	5	8

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	300	ALA
1	A	511	ALA
1	A	538	LYS
1	A	539	ALA
1	B	54	VAL
1	B	60	GLU
1	B	300	ALA
1	B	538	LYS
1	B	566	THR
1	A	512	ASP
1	A	565	GLU
1	A	568	PHE
1	B	58	SER
1	B	85	GLY
1	B	539	ALA
1	A	58	SER
1	A	150	TYR
1	A	510	HIS
1	A	557	LYS
1	A	37	GLU
1	A	62	CYS
1	A	179	LEU
1	A	499	PRO
1	B	86	GLU
1	B	540	THR
1	A	180	PRO
1	A	315	VAL
1	A	367	HIS
1	B	564	LYS
1	A	366	PRO

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Mol	Chain	Res	Type
1	B	77	VAL
1	B	110	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	437/511 (86%)	399 (91%)	38 (9%)	13	24
1	B	418/511 (82%)	374 (90%)	44 (10%)	8	16
All	All	855/1022 (84%)	773 (90%)	82 (10%)	10	20

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	TYR
1	A	37	GLU
1	A	38	ASP
1	A	47	THR
1	A	49	PHE
1	A	66	LEU
1	A	79	THR
1	A	83	THR
1	A	87	MET
1	A	98	ARG
1	A	109	ASN
1	A	179	LEU
1	A	186	ARG
1	A	195	LYS
1	A	212	LYS
1	A	232	SER
1	A	236	THR
1	A	245	CYS
1	A	281	LYS
1	A	283	LEU

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Mol	Chain	Res	Type
1	A	284	LEU
1	A	287	SER
1	A	295	ASN
1	A	308	ASP
1	A	323	LYS
1	A	329	MET
1	A	336	ARG
1	A	375	ASP
1	A	392	CYS
1	A	398	LEU
1	A	435	SER
1	A	467	THR
1	A	471	ASP
1	A	503	ASN
1	A	506	THR
1	A	507	PHE
1	A	543	GLN
1	A	550	ASP
1	B	20	LYS
1	B	34	CYS
1	B	38	ASP
1	B	47	THR
1	B	56	ASP
1	B	57	GLU
1	B	58	SER
1	B	77	VAL
1	B	82	GLU
1	B	83	THR
1	B	105	HIS
1	B	150	TYR
1	B	179	LEU
1	B	212	LYS
1	B	232	SER
1	B	245	CYS
1	B	281	LYS
1	B	283	LEU
1	B	284	LEU
1	B	287	SER
1	B	323	LYS
1	B	324	ASP
1	B	336	ARG
1	B	337	ARG

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Mol	Chain	Res	Type
1	B	344	VAL
1	B	375	ASP
1	B	392	CYS
1	B	398	LEU
1	B	410	ARG
1	B	435	SER
1	B	467	THR
1	B	480	SER
1	B	489	SER
1	B	500	LYS
1	B	507	PHE
1	B	540	THR
1	B	544	LEU
1	B	545	LYS
1	B	548	MET
1	B	555	VAL
1	B	557	LYS
1	B	566	THR
1	B	567	CYS
1	B	568	PHE

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

Mol	Chain	Res	Type
1	A	61	ASN
1	A	99	ASN
1	A	109	ASN
1	A	385	GLN
1	A	464	HIS
1	A	483	ASN
1	A	503	ASN
1	B	111	ASN
1	B	196	GLN
1	B	318	ASN
1	B	385	GLN
1	B	464	HIS
1	B	483	ASN
1	B	535	HIS
1	B	543	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	578/585 (98%)	0.32	44 (7%) 17 12	28, 66, 136, 150	0
1	B	578/585 (98%)	0.43	59 (10%) 9 5	30, 72, 139, 150	0
All	All	1156/1170 (98%)	0.38	103 (8%) 12 8	28, 69, 138, 150	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	577	ALA	10.0
1	B	562	ASP	8.7
1	B	573	LYS	8.6
1	B	576	VAL	8.1
1	B	569	ALA	8.0
1	A	539	ALA	7.5
1	A	570	GLU	7.5
1	A	572	GLY	7.4
1	B	572	GLY	7.4
1	B	563	ASP	6.9
1	B	578	ALA	6.7
1	B	570	GLU	6.4
1	B	558	CYS	5.6
1	A	510	HIS	5.5
1	B	91	CYS	5.3
1	A	577	ALA	5.1
1	B	566	THR	4.9
1	A	506	THR	4.8
1	B	54	VAL	4.8
1	A	554	PHE	4.8
1	A	568	PHE	4.5
1	B	87	MET	4.4
1	B	504	ALA	4.4
1	B	559	CYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	568	PHE	4.3
1	A	569	ALA	4.1
1	A	576	VAL	4.1
1	A	580	GLN	4.1
1	A	555	VAL	4.0
1	B	560	LYS	4.0
1	B	513	ILE	3.9
1	B	62	CYS	3.9
1	B	92	ALA	3.9
1	A	505	GLU	3.8
1	B	580	GLN	3.8
1	B	539	ALA	3.7
1	B	79	THR	3.7
1	A	178	LEU	3.7
1	B	78	ALA	3.7
1	B	7	VAL	3.7
1	B	83	THR	3.6
1	B	175	ALA	3.6
1	A	562	ASP	3.5
1	B	508	THR	3.5
1	A	175	ALA	3.4
1	B	581	ALA	3.3
1	B	505	GLU	3.2
1	B	503	ASN	3.2
1	A	573	LYS	3.2
1	A	176	ALA	3.2
1	B	52	THR	3.2
1	B	275	LEU	2.9
1	A	275	LEU	2.9
1	B	55	ALA	2.9
1	A	54	VAL	2.9
1	B	174	LYS	2.9
1	B	84	TYR	2.9
1	A	283	LEU	2.8
1	A	551	PHE	2.8
1	B	81	ARG	2.7
1	B	515	THR	2.7
1	A	91	CYS	2.7
1	A	105	HIS	2.7
1	A	563	ASP	2.7
1	B	516	LEU	2.7
1	A	171	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	87	MET	2.6
1	B	502	PHE	2.6
1	A	50	ALA	2.6
1	A	174	LYS	2.6
1	A	540	THR	2.6
1	B	50	ALA	2.6
1	B	47	THR	2.6
1	A	564	LYS	2.6
1	B	86	GLU	2.6
1	B	278	CYS	2.6
1	B	63	ASP	2.5
1	B	555	VAL	2.5
1	B	5	SER	2.5
1	A	56	ASP	2.4
1	A	511	ALA	2.3
1	B	88	ALA	2.3
1	A	53	CYS	2.3
1	A	455	VAL	2.3
1	B	365	ASP	2.3
1	A	57	GLU	2.3
1	B	165	PHE	2.3
1	A	66	LEU	2.2
1	A	96	PRO	2.2
1	A	59	ALA	2.2
1	B	567	CYS	2.2
1	A	556	GLU	2.2
1	B	56	ASP	2.2
1	A	581	ALA	2.2
1	B	540	THR	2.2
1	B	80	LEU	2.2
1	B	575	LEU	2.1
1	A	102	PHE	2.1
1	B	123	MET	2.1
1	A	90	CYS	2.1
1	A	112	LEU	2.0
1	B	370	TYR	2.0
1	B	547	VAL	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.