



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:49 PM GMT

PDB ID : 1QRK
Title : HUMAN FACTOR XIII WITH STRONTIUM BOUND IN THE ION SITE
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Deposited on : 1999-06-14
Resolution : 2.50 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

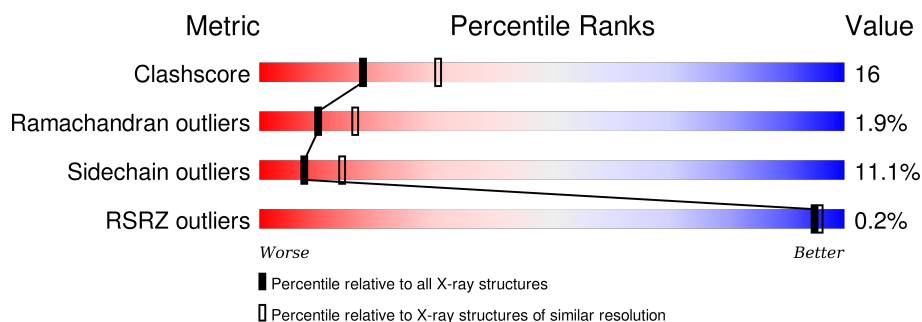
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	731	
1	B	731	

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	SR	A	732	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11492 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 PROTEIN (COAGULATION FACTOR XIII).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	700	Total	C	N	O	S	0	0	0
			5610	3557	966	1061	26			
1	B	705	Total	C	N	O	S	0	0	0
			5650	3583	973	1068	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	651	GLU	GLN	CONFLICT	UNP P00488
B	651	GLU	GLN	CONFLICT	UNP P00488

- Molecule 2 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Sr	0	0
			1	1		
2	A	1	Total	Sr	0	0
			1	1		

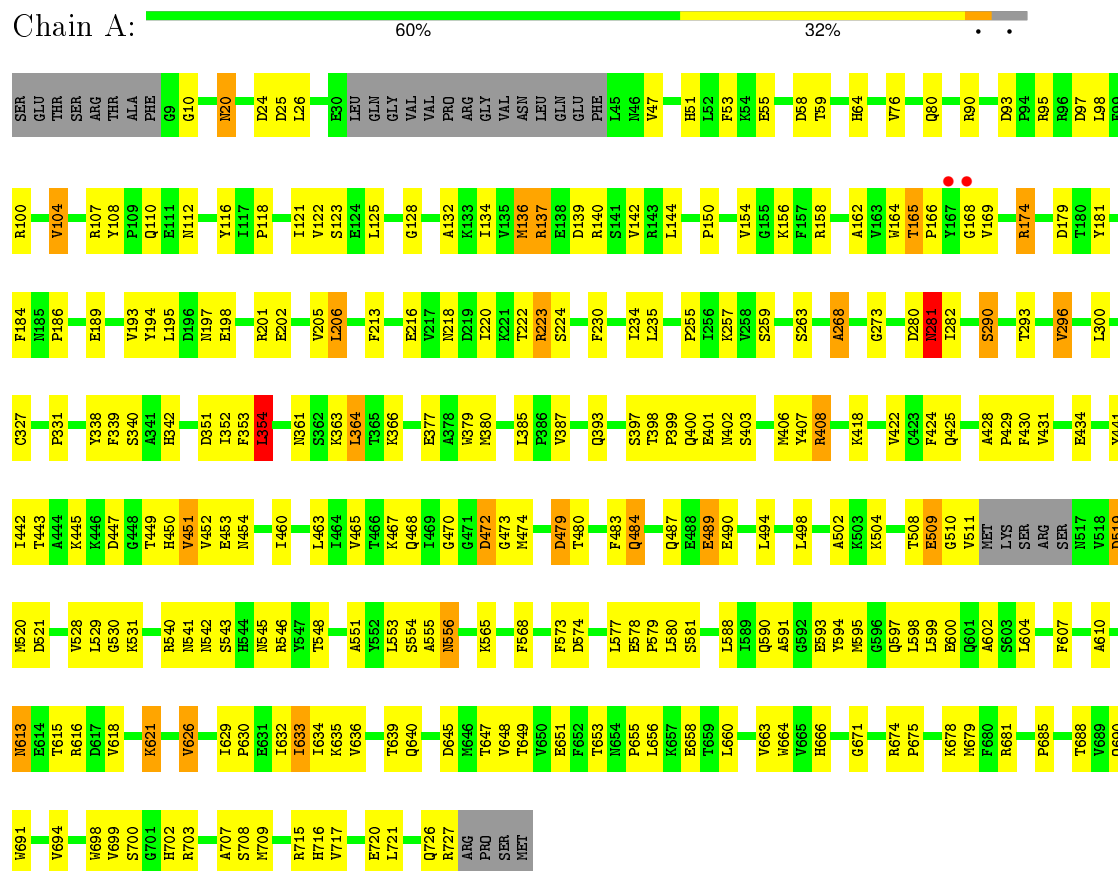
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	115	Total	O	0	0
			115	115		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PROTEIN (COAGULATION FACTOR XIII)



D722	T639	I549	M474	K392	D271	V161
V723	Q640	Y552	I477	S397	E272	T165
Q724	V641	Y552	Q484	T398	L275	G168
I725	V642	A555	Q484	P399	M281	V169
Q726	G643	N556	Q487	Q400	P289	L170
R727	G643	I557	E488	E401	I171	A173
ARG	M646	T561	E489	I402	D297	T172
PRO	T647	Q565	E490	D404	D297	S173
SER	T647	Q565	R491	G405	L300	R174
MET	T653	K565	L492	N406	E301	I182
	N654	F568	E495	Y407	L183	L183
	P655	K569	L498	R408	F184	F184
	L656	D574	A502	C409	S305	E306
	R657	L577	P411	G410	E306	E306
	E658	E578	A502	Q415	V309	C188
	T659	F579	P505	V422	R310	E189
	L660	L580	L506	Q425	Y311	A192
	R661	F581	N507	THR	R326	V193
	W664	F582	THR	F426	C327	E198
	V665	K583	GLY	D427	I330	E202
	H666	K584	VAL	A428	T336	L206
	L667	E585	MET	F429	N337	V211
	M676	L588	LYS	F430	Y338	T212
	M679	I589	SER	V431	F339	F213
	E682	Q590	ARG	E434	S340	E216
	T683	A591	S516	V435	A341	N218
	R684	Y594	N517	V435	R342	D219
	P685	L599	V518	R436	N344	T220
	N686	E600	D519	S437	E217	K221
	E693	S603	M520	D438	E216	R223
	V694	L604	D521	L439	N347	Y227
	C695	T609	F522	I440	N347	F230
	R696	A610	E523	Y441	L348	L235
	P697	R611	V524	I442	Q349	K247
	W698	I612	E525	T443	M350	K252
	V699	M613	N526	A444	L354	S259
	S700	R612	A527	K446	E355	V261
	R703	L613	W528	L529	E356	N267
	K704	R616	F533	V451	V360	A268
	L705	D617	R534	V452	N361	K269
	I706	V618	L535	V455	S362	D270
	A707	L619	S536	D456	K363	
	S708	A620	I537	H459	K366	
	W709	K621	T538	I460	W370	
	S713	T625	N541	G461	E377	
	L714	T625	N541	K462	M380	
	R715	I632	S543	L463	T381	
	H716	I633	H544	I464	K269	
	W717	K634	N545	V465	R382	
	E720	K635	R546	T466		
	L721	V636	Y547	K467		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.90Å 72.32Å 135.03Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 72.32 – 2.20	Depositor EDS
% Data completeness (in resolution range)	78.5 (10.00-2.50) 62.6 (72.32-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.183 , 0.275 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 95.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 60194 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11492	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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](#)

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

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	0.56	0/5741	0.79	1/7792 (0.0%)
1	B	0.60	0/5782	0.81	3/7847 (0.0%)
All	All	0.58	0/11523	0.80	4/15639 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	LEU	CA-CB-CG	5.76	128.56	115.30
1	B	170	LEU	N-CA-C	-5.73	95.53	111.00
1	B	588	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	26	LEU	CA-CB-CG	5.05	126.91	115.30

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	5610	0	5467	166	0
1	B	5650	0	5495	189	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	115	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	115	0	0	4	0
All	All	11492	0	10962	353	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 16.

All (353) 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:331:PRO:HG2	1:A:379:TRP:HB3	1.46	0.97
1:B:544:HIS:HA	1:B:579:PRO:HB3	1.52	0.90
1:B:44:PHE:O	1:B:45:LEU:HB2	1.73	0.87
1:A:709:MET:HB3	1:A:717:VAL:HB	1.58	0.85
1:B:591:ALA:HA	1:B:594:TYR:CE2	2.15	0.82
1:A:128:GLY:HA2	1:A:150:PRO:HD2	1.61	0.81
1:A:198:GLU:O	1:A:202:GLU:HG3	1.80	0.81
1:A:632:ILE:HD11	1:A:709:MET:HB2	1.64	0.79
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.66	0.76
1:B:90:ARG:HH11	1:B:90:ARG:HG3	1.50	0.76
1:B:435:VAL:HG21	1:B:464:ILE:HD11	1.69	0.75
1:A:100:ARG:HG2	1:A:164:TRP:HE1	1.51	0.75
1:A:128:GLY:HA2	1:A:150:PRO:CD	2.16	0.75
1:B:647:THR:HG23	1:B:694:VAL:HG22	1.69	0.74
1:A:443:THR:HG23	1:A:451:VAL:HG13	1.70	0.74
1:B:697:PRO:CB	1:B:725:ILE:HD13	2.19	0.73
1:B:632:ILE:HD11	1:B:709:MET:HB2	1.71	0.73
1:B:443:THR:HB	1:B:451:VAL:HG13	1.70	0.73
1:B:657:LYS:HE2	1:B:686:ASN:HD21	1.55	0.72
1:A:442:ILE:HG12	1:A:452:VAL:HG12	1.72	0.72
1:A:290:SER:HB3	1:A:716:HIS:HD2	1.56	0.70
1:B:52:LEU:O	1:B:54:LYS:N	2.25	0.70
1:B:440:ILE:HD12	1:B:455:VAL:HG12	1.74	0.70
1:B:642:VAL:HG21	1:B:700:SER:HB3	1.73	0.69
1:B:128:GLY:HA2	1:B:150:PRO:HD3	1.74	0.69
1:A:193:VAL:HG13	1:A:331:PRO:HD2	1.74	0.68
1:A:656:LEU:HD12	1:A:660:LEU:HD21	1.75	0.67
1:A:635:LYS:HG3	1:A:649:THR:HB	1.75	0.67
1:B:703:ARG:NE	1:B:703:ARG:HA	2.09	0.67
1:A:402:ASN:HA	1:A:430:PHE:CZ	2.29	0.66
1:A:551:ALA:HB3	1:A:573:PHE:HB2	1.78	0.66
1:B:542:ASN:O	1:B:580:LEU:HD23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ASP:O	1:B:98:LEU:HD12	1.96	0.65
1:B:656:LEU:HD12	1:B:660:LEU:HD21	1.79	0.65
1:A:541:ASN:HB2	1:A:577:LEU:HD13	1.79	0.64
1:A:206:LEU:O	1:A:230:PHE:HE2	1.78	0.64
1:A:636:VAL:HG12	1:A:648:VAL:HG22	1.78	0.64
1:A:498:LEU:HA	1:A:502:ALA:HB3	1.79	0.64
1:B:213:PHE:CD2	1:B:222:THR:HG22	2.33	0.64
1:B:642:VAL:CG2	1:B:700:SER:HB3	2.28	0.63
1:A:653:THR:HG23	1:A:688:THR:OG1	1.98	0.63
1:B:445:LYS:NZ	1:B:445:LYS:HB3	2.13	0.63
1:A:154:VAL:HG21	1:A:184:PHE:CE2	2.33	0.62
1:B:544:HIS:CA	1:B:579:PRO:HB3	2.25	0.62
1:B:68:LYS:HG3	1:B:230:PHE:CE1	2.34	0.62
1:A:290:SER:HB3	1:A:716:HIS:CD2	2.35	0.62
1:A:653:THR:O	1:A:655:PRO:HD3	1.99	0.62
1:B:549:ILE:HG23	1:B:610:ALA:HB1	1.82	0.62
1:B:247:MET:HA	3:B:1032:HOH:O	2.00	0.61
1:B:235:LEU:HA	1:B:327:CYS:SG	2.40	0.61
1:B:524:VAL:HG11	1:B:625:THR:HG21	1.83	0.61
1:B:337:ASN:HD21	1:B:461:GLY:HA2	1.65	0.61
1:A:220:ILE:HG21	1:A:474:MET:HE2	1.82	0.60
1:B:90:ARG:NH1	1:B:90:ARG:HG3	2.16	0.60
1:A:98:LEU:HD23	1:A:164:TRP:HB2	1.83	0.60
1:A:521:ASP:OD1	1:A:621:LYS:HE2	2.01	0.60
1:A:630:PRO:HG3	1:A:655:PRO:HG3	1.82	0.60
1:B:223:ARG:NH2	3:B:6078:HOH:O	2.33	0.60
1:A:377:GLU:HA	1:A:393:GLN:O	2.02	0.60
1:A:487:GLN:HB3	1:A:489:GLU:HG2	1.84	0.59
1:B:139:ASP:HB2	3:B:2023:HOH:O	2.03	0.59
1:B:213:PHE:O	1:B:336:THR:HG21	2.01	0.59
1:B:439:LEU:HB2	1:B:456:ASP:HB3	1.85	0.59
1:B:697:PRO:HB2	1:B:725:ILE:HD13	1.82	0.59
1:B:54:LYS:HG3	1:B:55:GLU:H	1.67	0.59
1:B:522:PHE:CD2	1:B:535:LEU:HD21	2.38	0.59
1:A:64:HIS:CD2	1:A:76:VAL:HG12	2.37	0.59
1:B:487:GLN:HA	1:B:487:GLN:OE1	2.02	0.58
1:A:484:GLN:H	1:A:487:GLN:NE2	1.99	0.58
1:A:280:ASP:O	1:A:282:ILE:N	2.36	0.58
1:B:490:GLU:HG3	1:B:491:ARG:N	2.18	0.58
1:A:529:LEU:HD21	1:A:598:LEU:CD1	2.33	0.57
1:B:17:ASN:ND2	1:B:115:THR:HG21	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:HIS:ND1	1:B:434:GLU:OE2	2.36	0.57
1:B:281:ASN:OD1	1:B:600:GLU:HG3	2.04	0.57
1:B:636:VAL:HG11	1:B:723:VAL:HG11	1.86	0.57
1:A:100:ARG:HG2	1:A:164:TRP:NE1	2.19	0.57
1:B:154:VAL:HG21	1:B:184:PHE:CD2	2.40	0.57
1:B:616:ARG:O	1:B:616:ARG:HD2	2.05	0.57
1:A:353:PHE:O	1:A:361:ASN:HB3	2.05	0.57
1:A:385:LEU:HD22	1:A:424:PHE:HB3	1.86	0.56
1:B:30:GLU:HB3	1:B:169:VAL:HG22	1.87	0.56
1:A:107:ARG:HG2	1:A:107:ARG:O	2.04	0.56
1:A:634:ILE:HD12	1:A:720:GLU:HA	1.88	0.56
1:B:522:PHE:HB3	1:B:537:ILE:HG23	1.87	0.56
1:A:281:ASN:ND2	1:A:715:ARG:NH1	2.53	0.56
1:B:47:VAL:HG12	1:B:88:PHE:CE1	2.41	0.55
1:B:685:PRO:O	1:B:686:ASN:HB2	2.06	0.55
1:B:65:HIS:O	1:B:68:LYS:HD2	2.06	0.55
1:B:101:VAL:O	1:B:118:PRO:O	2.25	0.55
1:A:484:GLN:HG2	1:A:487:GLN:HG3	1.88	0.55
1:A:189:GLU:HA	1:A:194:TYR:CG	2.42	0.55
1:B:442:ILE:HG12	1:B:452:VAL:HG12	1.88	0.55
1:A:154:VAL:HG21	1:A:184:PHE:CD2	2.42	0.55
1:B:705:LEU:O	1:B:720:GLU:HA	2.07	0.55
1:A:399:PRO:HA	1:A:407:TYR:O	2.06	0.55
1:A:508:THR:HB	1:A:511:VAL:HG21	1.87	0.54
1:B:350:MET:HB2	1:B:439:LEU:HD23	1.89	0.54
1:A:257:LYS:HG3	1:B:403:SER:O	2.07	0.54
1:B:659:THR:HG22	1:B:685:PRO:HD3	1.88	0.54
1:B:600:GLU:HG2	1:B:715:ARG:HH11	1.72	0.54
1:A:578:GLU:HB3	1:A:579:PRO:HD2	1.88	0.54
1:B:122:VAL:HG12	1:B:132:ALA:O	2.08	0.54
1:B:17:ASN:HD22	1:B:115:THR:HG21	1.73	0.53
1:A:530:GLY:HA2	1:A:595:MET:SD	2.48	0.53
1:A:591:ALA:HA	1:A:594:TYR:CE2	2.43	0.53
1:A:468:GLN:CD	1:A:473:GLY:HA3	2.29	0.53
1:B:275:LEU:HD23	1:B:309:VAL:O	2.09	0.53
1:A:26:LEU:HD11	1:A:104:VAL:HG11	1.89	0.53
1:B:484:GLN:N	1:B:484:GLN:OE1	2.41	0.53
1:A:546:ARG:HB2	1:A:577:LEU:O	2.07	0.53
1:A:520:MET:HG2	1:A:521:ASP:N	2.24	0.53
1:A:633:ILE:HG22	1:A:651:GLU:HG2	1.91	0.53
1:B:211:VAL:HG22	1:B:467:LYS:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:LYS:HG3	1:B:705:LEU:H	1.74	0.53
1:B:338:TYR:O	1:B:339:PHE:HB2	2.09	0.52
1:A:64:HIS:HE1	1:A:80:GLN:HB3	1.74	0.52
1:B:657:LYS:HE2	1:B:686:ASN:ND2	2.23	0.52
1:A:361:ASN:ND2	1:A:364:LEU:HD22	2.25	0.52
1:A:636:VAL:CG1	1:A:648:VAL:HG22	2.39	0.52
1:A:116:TYR:CE2	1:A:118:PRO:HG3	2.45	0.52
1:B:76:VAL:O	1:B:182:ILE:HA	2.10	0.52
1:A:24:ASP:O	1:A:158:ARG:NH2	2.42	0.52
1:B:634:ILE:HD11	1:B:707:ALA:HB2	1.91	0.51
1:A:93:ASP:O	1:A:97:ASP:HB2	2.10	0.51
1:B:269:LYS:O	1:B:270:ASP:HB3	2.11	0.51
1:B:667:LEU:HD23	1:B:676:MET:CE	2.40	0.51
1:A:666:HIS:HB2	1:A:708:SER:OG	2.09	0.51
1:A:615:THR:O	1:A:616:ARG:HB2	2.11	0.51
1:B:71:ASN:HB3	1:B:75:ILE:HD11	1.92	0.51
1:A:342:HIS:ND1	1:A:434:GLU:OE2	2.44	0.51
1:A:20:ASN:ND2	1:A:20:ASN:O	2.44	0.51
1:B:135:VAL:HG12	1:B:143:ARG:O	2.10	0.51
1:B:348:LEU:HD12	1:B:498:LEU:HD11	1.93	0.51
1:A:64:HIS:HE1	1:A:80:GLN:CB	2.25	0.51
1:A:658:GLU:C	1:A:685:PRO:HG3	2.32	0.50
1:A:401:GLU:HA	1:A:406:MET:H	1.75	0.50
1:A:528:VAL:HB	1:A:531:LYS:HD2	1.91	0.50
1:B:401:GLU:HA	1:B:406:MET:H	1.76	0.50
1:B:555:ALA:HB1	1:B:568:PHE:CZ	2.47	0.50
1:B:382:ARG:NH2	1:B:411:PRO:O	2.45	0.50
1:B:697:PRO:HB3	1:B:725:ILE:HD13	1.92	0.50
1:A:449:THR:HG22	1:A:450:HIS:H	1.77	0.50
1:B:54:LYS:O	1:B:55:GLU:O	2.29	0.50
1:A:197:ASN:O	1:A:201:ARG:HG3	2.12	0.50
1:A:674:ARG:HG3	1:A:675:PRO:HD2	1.94	0.50
1:A:64:HIS:CE1	1:A:80:GLN:HB3	2.47	0.49
1:A:442:ILE:HA	1:A:452:VAL:HA	1.94	0.49
1:B:704:LYS:HD3	1:B:722:ASP:OD1	2.12	0.49
1:B:541:ASN:HB2	1:B:577:LEU:HD23	1.93	0.49
1:B:377:GLU:HB3	1:B:392:TRP:CE3	2.46	0.49
1:A:602:ALA:O	1:A:626:VAL:HA	2.11	0.49
1:B:518:VAL:HG11	1:B:549:ILE:HD11	1.94	0.49
1:A:90:ARG:NH2	1:A:97:ASP:OD1	2.46	0.49
1:B:12:ARG:HH11	1:B:12:ARG:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:VAL:CG2	1:B:464:ILE:HD11	2.40	0.49
1:A:594:TYR:CD1	1:A:595:MET:N	2.81	0.49
1:B:247:MET:HE2	1:B:261:VAL:HG11	1.95	0.49
1:B:139:ASP:O	1:B:140:ARG:HB2	2.12	0.49
1:B:64:HIS:O	1:B:77:ARG:HD2	2.13	0.48
1:B:112:ASN:HB3	1:B:113:LYS:HG2	1.94	0.48
1:B:47:VAL:HG12	1:B:88:PHE:HE1	1.78	0.48
1:B:524:VAL:CG1	1:B:625:THR:HG21	2.42	0.48
1:A:281:ASN:HD21	1:A:715:ARG:NH1	2.11	0.48
1:A:565:LYS:HB2	1:A:599:LEU:HD11	1.95	0.48
1:B:213:PHE:CE2	1:B:222:THR:HG22	2.48	0.48
1:B:582:PHE:HD1	1:B:583:LYS:N	2.11	0.48
1:A:162:ALA:HB1	1:A:169:VAL:CG1	2.43	0.48
1:A:651:GLU:HB3	1:A:690:GLN:HG3	1.96	0.48
1:B:348:LEU:HD11	1:B:502:ALA:HB1	1.95	0.48
1:B:305:SER:O	1:B:306:GLU:HB2	2.13	0.48
1:A:156:LYS:HD2	1:A:181:TYR:CZ	2.49	0.48
1:A:122:VAL:CG2	1:A:125:LEU:HD23	2.44	0.48
1:A:206:LEU:O	1:A:230:PHE:CE2	2.65	0.48
1:B:549:ILE:HA	1:B:611:ARG:O	2.14	0.48
1:B:310:ARG:HB3	1:B:311:TYR:CD1	2.49	0.48
1:A:703:ARG:HA	1:A:703:ARG:NE	2.29	0.47
1:B:11:ARG:HG3	1:B:11:ARG:HH11	1.79	0.47
1:A:213:PHE:CD2	1:A:222:THR:HG22	2.49	0.47
1:A:338:TYR:O	1:A:339:PHE:HB2	2.15	0.47
1:B:667:LEU:HD23	1:B:676:MET:HE1	1.97	0.47
1:A:121:ILE:HG21	1:A:134:ILE:HD11	1.95	0.47
1:A:100:ARG:CG	1:A:164:TRP:HE1	2.24	0.47
1:B:706:ILE:N	1:B:706:ILE:HD12	2.29	0.47
1:B:703:ARG:HE	1:B:703:ARG:HA	1.78	0.47
1:A:663:VAL:O	1:A:679:MET:HA	2.14	0.47
1:B:704:LYS:HG3	1:B:705:LEU:N	2.30	0.47
1:B:724:GLN:CD	1:B:724:GLN:N	2.67	0.47
1:A:186:PRO:HG3	1:A:205:VAL:HG21	1.97	0.47
1:B:664:TRP:CE2	1:B:679:MET:HG3	2.50	0.47
1:B:709:MET:HB3	1:B:717:VAL:HB	1.96	0.47
1:B:30:GLU:O	1:B:168:GLY:HA3	2.15	0.46
1:B:81:SER:HA	1:B:146:ILE:O	2.15	0.46
1:B:536:SER:HB3	1:B:584:LYS:HE3	1.97	0.46
1:B:696:ARG:NH2	1:B:698:TRP:HA	2.30	0.46
1:A:352:ILE:HG21	1:A:441:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:GLN:O	1:A:727:ARG:HB2	2.14	0.46
1:A:281:ASN:HD21	1:A:715:ARG:HH11	1.64	0.46
1:B:122:VAL:HG11	1:B:125:LEU:HD23	1.97	0.46
1:A:698:TRP:CD1	1:A:699:VAL:HG23	2.49	0.46
1:B:153:ILE:HG23	1:B:252:ARG:HB2	1.98	0.46
1:A:519:ASP:HB2	1:A:540:ARG:HB3	1.97	0.46
1:B:569:LYS:HE2	1:B:589:ILE:HD13	1.98	0.46
1:B:529:LEU:HD11	1:B:656:LEU:CD2	2.45	0.46
1:A:280:ASP:C	1:A:282:ILE:H	2.20	0.46
1:B:636:VAL:HB	1:B:646:MET:CE	2.46	0.46
1:B:267:ASN:OD1	1:B:399:PRO:HG3	2.15	0.46
1:A:134:ILE:HG23	1:A:142:VAL:CG1	2.45	0.46
1:B:552:TYR:N	1:B:609:THR:O	2.47	0.46
1:B:684:ARG:HB3	1:B:685:PRO:HD2	1.97	0.45
1:B:71:ASN:CB	1:B:75:ILE:HD11	2.46	0.45
1:A:484:GLN:O	1:A:487:GLN:HB2	2.16	0.45
1:B:64:HIS:O	1:B:65:HIS:HB2	2.17	0.45
1:B:161:VAL:H	1:B:172:THR:HG1	1.63	0.45
1:B:193:VAL:HG21	1:B:330:ILE:HG23	1.99	0.45
1:B:537:ILE:O	1:B:585:GLU:N	2.46	0.45
1:A:678:LYS:HD2	1:A:691:TRP:CD1	2.51	0.45
1:A:193:VAL:HG13	1:A:331:PRO:CD	2.44	0.45
1:B:603:SER:HA	1:B:625:THR:O	2.17	0.45
1:B:122:VAL:N	1:B:132:ALA:O	2.45	0.45
1:A:107:ARG:HD2	1:A:108:TYR:CZ	2.52	0.45
1:B:211:VAL:CG2	1:B:467:LYS:HB2	2.46	0.45
1:B:193:VAL:CG2	1:B:330:ILE:HG23	2.47	0.45
1:A:296:VAL:HB	3:A:6039:HOH:O	2.16	0.45
1:A:235:LEU:HA	1:A:327:CYS:SG	2.57	0.45
1:A:443:THR:HG22	1:A:453:GLU:HG2	1.99	0.45
1:B:600:GLU:HG2	1:B:715:ARG:NH1	2.32	0.45
1:B:348:LEU:HD12	1:B:498:LEU:CD1	2.46	0.45
1:B:525:GLU:HG3	1:B:525:GLU:O	2.17	0.45
1:A:556:ASN:N	1:A:556:ASN:ND2	2.65	0.44
1:B:422:VAL:HB	1:B:429:PRO:HG3	1.99	0.44
1:A:220:ILE:HG21	1:A:474:MET:CE	2.47	0.44
1:A:51:HIS:CE1	1:A:53:PHE:CD1	3.05	0.44
1:B:341:ALA:HB2	1:B:460:ILE:HD13	1.98	0.44
1:A:504:LYS:HE2	1:A:504:LYS:HB3	1.52	0.44
1:B:431:VAL:O	1:B:434:GLU:HB2	2.16	0.44
1:B:310:ARG:HB3	1:B:311:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:ARG:HA	1:B:682:GLU:HA	1.99	0.44
1:B:193:VAL:HG13	1:B:193:VAL:O	2.17	0.44
1:A:255:PRO:HB2	1:A:380:MET:HE2	1.98	0.44
1:B:455:VAL:HG23	1:B:455:VAL:O	2.17	0.44
1:A:352:ILE:HG21	1:A:441:TYR:HE1	1.81	0.44
1:B:380:MET:HG3	1:B:381:THR:O	2.17	0.44
1:A:629:ILE:HG21	1:A:717:VAL:HG22	1.99	0.44
1:A:553:LEU:HD23	1:A:553:LEU:C	2.38	0.44
1:A:122:VAL:HG21	1:A:125:LEU:HD23	1.99	0.44
1:B:643:GLY:HA2	1:B:696:ARG:NE	2.32	0.44
1:A:354:LEU:CD2	1:A:618:VAL:HG11	2.47	0.44
1:B:666:HIS:HB2	1:B:708:SER:OG	2.18	0.44
1:B:14:VAL:HG22	1:B:15:PRO:O	2.18	0.44
1:B:520:MET:O	1:B:521:ASP:HB2	2.17	0.44
1:B:105:ILE:CG2	1:B:115:THR:HG22	2.48	0.43
1:A:460:ILE:H	1:A:460:ILE:HD12	1.82	0.43
1:B:548:THR:O	1:B:612:ILE:HA	2.17	0.43
1:B:42:GLN:HA	1:B:44:PHE:CE2	2.52	0.43
1:B:654:ASN:HB3	1:B:686:ASN:H	1.83	0.43
1:B:440:ILE:CD1	1:B:455:VAL:HG12	2.46	0.43
1:B:459:HIS:O	1:B:462:LYS:HG2	2.18	0.43
1:B:356:GLU:H	1:B:446:LYS:HZ2	1.67	0.43
1:A:555:ALA:HB1	1:A:568:PHE:CE1	2.53	0.43
1:A:422:VAL:HB	1:A:429:PRO:HG3	2.01	0.43
1:B:402:ASN:HA	1:B:430:PHE:CZ	2.53	0.43
1:A:666:HIS:O	1:A:707:ALA:HA	2.17	0.43
1:A:158:ARG:HG2	1:A:174:ARG:NH2	2.34	0.43
1:A:467:LYS:HE2	1:A:472:ASP:HA	2.01	0.43
1:B:653:THR:O	1:B:655:PRO:HD3	2.19	0.43
1:A:223:ARG:NH1	1:A:224:SER:O	2.52	0.43
1:A:610:ALA:O	1:A:618:VAL:HA	2.18	0.43
1:A:363:LYS:O	1:A:366:LYS:HE2	2.19	0.43
1:B:158:ARG:HG2	1:B:174:ARG:NH2	2.33	0.43
1:B:366:LYS:HD3	1:B:366:LYS:HA	1.78	0.42
1:A:418:LYS:HD2	1:A:480:THR:O	2.19	0.42
1:A:509:GLU:HB2	1:A:510:GLY:H	1.65	0.42
1:B:42:GLN:OE1	1:B:44:PHE:CE2	2.72	0.42
1:A:268:ALA:HA	1:A:273:GLY:HA3	2.01	0.42
1:B:187:TRP:HH2	1:B:206:LEU:HD22	1.84	0.42
1:A:702:HIS:ND1	1:A:702:HIS:C	2.72	0.42
1:A:553:LEU:HD23	1:A:554:SER:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:GLY:HA3	3:B:6001:HOH:O	2.19	0.42
1:A:548:THR:HB	1:A:613:ASN:HB2	2.01	0.42
1:A:165:THR:HB	1:A:166:PRO:HD2	2.00	0.42
1:B:518:VAL:O	1:B:619:LEU:HD11	2.19	0.42
1:B:220:ILE:HG23	1:B:338:TYR:OH	2.20	0.42
1:A:556:ASN:N	1:A:556:ASN:HD22	2.17	0.42
1:A:132:ALA:HB1	1:A:144:LEU:HD22	2.02	0.42
1:A:263:SER:OG	1:A:408:ARG:HD3	2.18	0.42
1:A:578:GLU:HB2	1:A:581:SER:HB2	2.02	0.42
1:B:620:ALA:O	1:B:621:LYS:HG2	2.20	0.42
1:A:418:LYS:HE3	1:A:479:ASP:O	2.19	0.42
1:B:370:TRP:HA	1:B:561:THR:O	2.20	0.42
1:A:300:LEU:HA	1:A:300:LEU:HD23	1.76	0.42
1:B:134:ILE:HG23	1:B:142:VAL:CG1	2.50	0.42
1:B:659:THR:HG21	1:B:684:ARG:HH11	1.85	0.42
1:B:557:ILE:HD12	1:B:568:PHE:CD1	2.55	0.42
1:B:546:ARG:NH1	1:B:578:GLU:OE2	2.53	0.42
1:A:545:ASN:N	1:A:579:PRO:HB3	2.35	0.42
1:B:11:ARG:HG3	1:B:11:ARG:NH1	2.35	0.42
1:A:671:GLY:HA2	1:A:698:TRP:CE2	2.55	0.42
1:B:198:GLU:O	1:B:202:GLU:HB2	2.19	0.42
1:B:409:CYS:HB3	1:B:427:ASP:HB2	2.02	0.42
1:A:206:LEU:HA	1:A:206:LEU:HD12	1.91	0.41
1:B:646:MET:HE3	1:B:646:MET:HB2	1.75	0.41
1:B:666:HIS:O	1:B:707:ALA:HA	2.19	0.41
1:B:664:TRP:CZ3	1:B:679:MET:HB2	2.55	0.41
1:B:29:VAL:CG1	1:B:31:LEU:HG	2.50	0.41
1:A:216:GLU:OE2	1:A:218:ASN:HB2	2.20	0.41
1:B:660:LEU:HD22	1:B:713:SER:OG	2.20	0.41
1:B:565:LYS:HB2	1:B:599:LEU:HD11	2.01	0.41
1:B:425:GLN:HB2	1:B:426:PHE:CD2	2.56	0.41
1:A:494:LEU:HG	1:A:498:LEU:HD23	2.02	0.41
1:A:428:ALA:N	1:A:429:PRO:CD	2.84	0.41
1:A:136:MET:HG2	1:A:137:ARG:N	2.35	0.41
1:B:42:GLN:OE1	1:B:44:PHE:HE2	2.02	0.41
1:A:402:ASN:HA	1:A:430:PHE:CE1	2.55	0.41
1:A:483:PHE:CD1	1:A:489:GLU:HG3	2.55	0.41
1:A:671:GLY:HA2	1:A:698:TRP:NE1	2.35	0.41
1:B:465:VAL:HG21	1:B:474:MET:SD	2.60	0.41
1:B:56:ARG:HG2	1:B:56:ARG:H	1.55	0.41
1:B:86:ILE:HD11	1:B:144:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:O	1:A:443:THR:HA	2.21	0.41
1:A:634:ILE:HD11	1:A:707:ALA:HB2	2.03	0.41
1:A:664:TRP:CE3	1:A:679:MET:HB2	2.56	0.41
1:A:498:LEU:HA	1:A:498:LEU:HD13	1.83	0.41
1:B:289:PRO:HD3	1:B:311:TYR:HB2	2.03	0.41
1:A:234:ILE:HD13	1:A:300:LEU:HD21	2.03	0.41
1:A:202:GLU:HA	1:A:206:LEU:HB2	2.02	0.41
1:A:354:LEU:HD23	1:A:618:VAL:HG11	2.03	0.41
1:B:676:MET:CE	1:B:693:GLU:HG3	2.50	0.41
1:A:400:GLN:O	1:A:406:MET:HA	2.21	0.41
1:A:568:PHE:HB2	1:A:593:GLU:O	2.21	0.41
1:B:344:ASN:O	1:B:347:ASN:HB2	2.21	0.41
1:B:527:ALA:HB2	1:B:533:PHE:CB	2.43	0.41
1:B:54:LYS:O	1:B:55:GLU:C	2.60	0.41
1:A:494:LEU:O	1:A:498:LEU:HD23	2.21	0.41
1:B:549:ILE:CG2	1:B:610:ALA:HB1	2.48	0.41
1:A:351:ASP:OD2	1:B:112:ASN:OD1	2.39	0.41
1:B:609:THR:HG22	1:B:620:ALA:HB2	2.03	0.41
1:A:165:THR:HG23	1:A:168:GLY:O	2.21	0.41
1:A:445:LYS:HB3	1:A:447:ASP:OD1	2.21	0.41
1:B:45:LEU:HD22	1:B:97:ASP:HB3	2.03	0.40
1:B:227:TYR:CD2	1:B:326:ARG:NH1	2.90	0.40
1:A:206:LEU:HD12	1:A:230:PHE:CZ	2.57	0.40
1:B:464:ILE:HG22	1:B:477:ILE:HG13	2.02	0.40
1:A:353:PHE:O	1:A:361:ASN:CB	2.69	0.40
1:B:300:LEU:HD23	1:B:300:LEU:HA	1.90	0.40
1:A:174:ARG:NH2	1:A:179:ASP:OD1	2.55	0.40
1:B:445:LYS:HZ3	1:B:445:LYS:HB3	1.85	0.40
1:A:449:THR:HG22	1:A:450:HIS:N	2.36	0.40
1:B:192:ALA:O	1:B:381:THR:HG23	2.21	0.40
1:A:647:THR:HA	1:A:694:VAL:HA	2.04	0.40
1:A:543:SER:O	1:A:580:LEU:HD12	2.21	0.40
1:A:164:TRP:N	1:A:164:TRP:CD1	2.88	0.40
1:A:281:ASN:ND2	1:A:600:GLU:OE1	2.55	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	694/731 (95%)	631 (91%)	52 (8%)	11 (2%)	12	21
1	B	699/731 (96%)	613 (88%)	71 (10%)	15 (2%)	9	14
All	All	1393/1462 (95%)	1244 (89%)	123 (9%)	26 (2%)	10	16

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	281	ASN
1	B	45	LEU
1	B	53	PHE
1	B	55	GLU
1	B	613	ASN
1	A	139	ASP
1	A	470	GLY
1	B	56	ARG
1	B	219	ASP
1	B	505	PRO
1	A	509	GLU
1	A	613	ASN
1	B	487	GLN
1	A	10	GLY
1	A	296	VAL
1	A	472	ASP
1	B	268	ALA
1	B	362	SER
1	B	406	MET
1	A	136	MET
1	A	268	ALA
1	B	60	ASN
1	B	252	ARG
1	B	405	GLY

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Mol	Chain	Res	Type
1	B	91	PRO

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	616/644 (96%)	559 (91%)	57 (9%)	11	21
1	B	619/644 (96%)	539 (87%)	80 (13%)	5	10
All	All	1235/1288 (96%)	1098 (89%)	137 (11%)	8	14

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	25	ASP
1	A	47	VAL
1	A	58	ASP
1	A	59	THR
1	A	95	ARG
1	A	104	VAL
1	A	110	GLN
1	A	112	ASN
1	A	123	SER
1	A	137	ARG
1	A	140	ARG
1	A	165	THR
1	A	174	ARG
1	A	195	LEU
1	A	206	LEU
1	A	223	ARG
1	A	259	SER
1	A	281	ASN
1	A	290	SER
1	A	293	THR
1	A	340	SER

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Mol	Chain	Res	Type
1	A	354	LEU
1	A	364	LEU
1	A	387	VAL
1	A	397	SER
1	A	398	THR
1	A	403	SER
1	A	408	ARG
1	A	425	GLN
1	A	431	VAL
1	A	451	VAL
1	A	454	ASN
1	A	463	LEU
1	A	465	VAL
1	A	479	ASP
1	A	484	GLN
1	A	489	GLU
1	A	490	GLU
1	A	519	ASP
1	A	542	ASN
1	A	556	ASN
1	A	574	ASP
1	A	588	LEU
1	A	590	GLN
1	A	597	GLN
1	A	604	LEU
1	A	607	PHE
1	A	621	LYS
1	A	626	VAL
1	A	633	ILE
1	A	639	THR
1	A	640	GLN
1	A	645	ASP
1	A	681	ARG
1	A	700	SER
1	A	721	LEU
1	B	12	ARG
1	B	14	VAL
1	B	20	ASN
1	B	25	ASP
1	B	47	VAL
1	B	58	ASP
1	B	59	THR

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Mol	Chain	Res	Type
1	B	68	LYS
1	B	76	VAL
1	B	95	ARG
1	B	104	VAL
1	B	110	GLN
1	B	140	ARG
1	B	143	ARG
1	B	148	SER
1	B	165	THR
1	B	172	THR
1	B	174	ARG
1	B	189	GLU
1	B	193	VAL
1	B	202	GLU
1	B	206	LEU
1	B	216	GLU
1	B	217	VAL
1	B	223	ARG
1	B	235	LEU
1	B	247	MET
1	B	259	SER
1	B	272	GLU
1	B	297	ASP
1	B	301	GLU
1	B	310	ARG
1	B	340	SER
1	B	347	ASN
1	B	354	LEU
1	B	360	VAL
1	B	363	LYS
1	B	397	SER
1	B	406	MET
1	B	408	ARG
1	B	415	GLN
1	B	431	VAL
1	B	434	GLU
1	B	435	VAL
1	B	437	SER
1	B	463	LEU
1	B	465	VAL
1	B	487	GLN
1	B	489	GLU

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Mol	Chain	Res	Type
1	B	490	GLU
1	B	492	LEU
1	B	495	GLU
1	B	498	LEU
1	B	517	ASN
1	B	520	MET
1	B	525	GLU
1	B	526	ASN
1	B	538	THR
1	B	544	HIS
1	B	557	ILE
1	B	565	LYS
1	B	574	ASP
1	B	578	GLU
1	B	582	PHE
1	B	589	ILE
1	B	604	LEU
1	B	609	THR
1	B	613	ASN
1	B	616	ARG
1	B	617	ASP
1	B	635	LYS
1	B	639	THR
1	B	640	GLN
1	B	647	THR
1	B	657	LYS
1	B	696	ARG
1	B	713	SER
1	B	721	LEU
1	B	724	GLN
1	B	726	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	281	ASN
1	A	421	HIS
1	A	450	HIS
1	A	487	GLN
1	A	556	ASN
1	A	686	ASN

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Mol	Chain	Res	Type
1	A	716	HIS
1	A	726	GLN
1	B	46	ASN
1	B	307	ASN
1	B	322	ASN
1	B	337	ASN
1	B	421	HIS
1	B	468	GLN
1	B	545	ASN
1	B	613	ASN
1	B	686	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	700/731 (95%)	-0.69	2 (0%) 94 95	8, 31, 66, 83	0
1	B	705/731 (96%)	-0.68	1 (0%) 95 96	4, 28, 71, 85	0
All	All	1405/1462 (96%)	-0.68	3 (0%) 95 96	4, 29, 68, 85	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	577	LEU	2.9
1	A	168	GLY	2.6
1	A	167	TYR	2.3

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, 95th 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(\AA^2)	Q<0.9
2	SR	A	732	1/1	0.99	0.17	2.07	51,51,51,51	0
2	SR	B	732	1/1	0.99	0.14	0.58	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.