



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:15 AM GMT

PDB ID : 2GBI
Title : rat DPP-IV with xanthine inhibitor 4
Authors : Longenecker, K.L.; Jakob, C.G.; Fry, E.H.; Wilk, S.
Deposited on : 2006-03-10
Resolution : 3.30 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

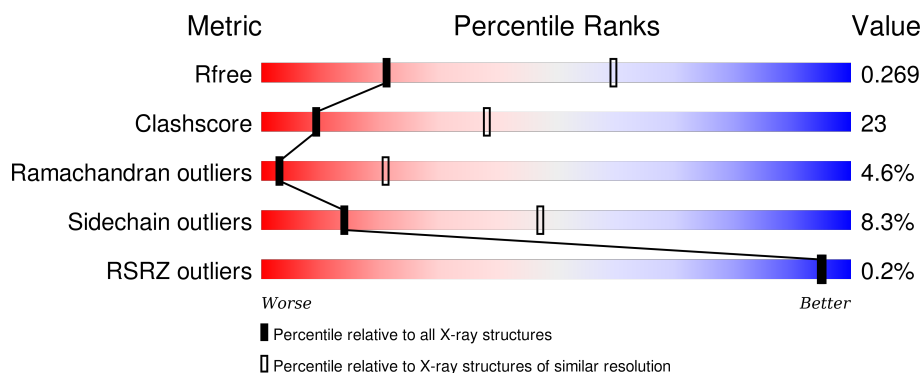
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 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	730	 55% 37% 7% .
1	B	730	 58% 34% 8%

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	XIH	A	901	-	-	-	X

2 Entry composition [i](#)

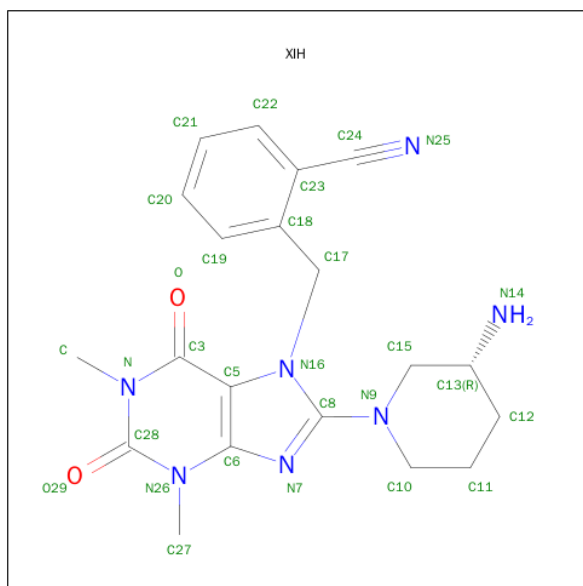
There are 2 unique types of molecules in this entry. The entry contains 11869 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total	C	N	O	S	0	0	0
			5920	3789	981	1124	26			
1	B	730	Total	C	N	O	S	0	0	0
			5920	3789	981	1124	26			

- Molecule 2 is 2-({8-[(3R)-3-AMINOPIPERIDIN-1-YL]-1,3-DIMETHYL-2,6-DIOXO-1,2,3,6-TETRAHYDRO-7H-PURIN-7-YL}METHYL)BENZONITRILE (three-letter code: XIH) (formula: C₂₀H₂₃N₇O₂).

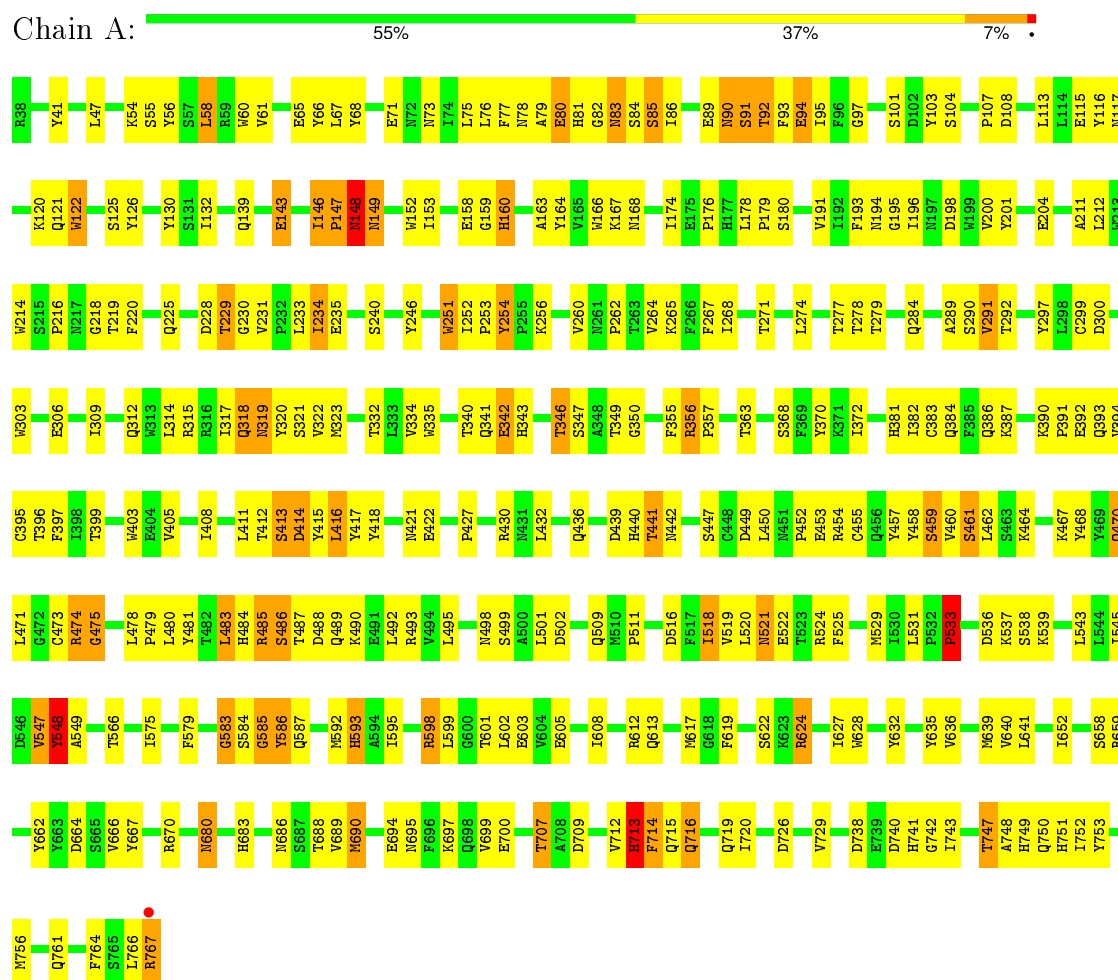


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	20	7	2		

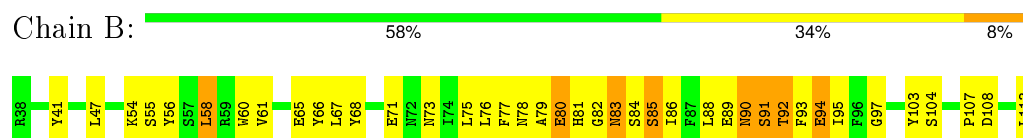
3 Residue-property plots

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: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4



T707	A708	D709	H713	F714	Q715	Q716	Q719	I720	F725	D726	V729	D738	F739	H741	G742	I743	A744	S745	S746	A748	H749	Q750	H751	I752	Y753	M756	Q761	F764	S765	L766	R767																	
I595	R598	L599	G600	T601	L602	E603	R612	F619	S622	K623	R624	I627	W628	Y632	Y635	V636	M639	V640	L641	H642	I643	I652	S658	R659	Y662	D664	S665	V666	R670	D679	I680	H683	N686	S687	T688	V689	M690	E694	K697	Q698	V699	E700						
K490	E491	L492	R493	V494	L495	M498	L501	Q509	W510	P511	D516	F517	I518	V519	L520	M521	E522	T523	R524	F525	M529	I530	L531	P532	R533	D536	R537	S538	K539	L543	L544	I545	D546	V547	R548	A549	T556	I575	F579	G583	S584	Q585	Y586	Q587	M592	H593	A594	
Y418	M421	E422	Y423	K424	P427	R430	M431	L432	Q436	D439	H440	T441	M442	K443	S447	D449	L450	M451	P452	E453	R454	C455	Q456	Y457	Y458	S459	V460	S461	L462	S463	K464	K467	Q470	L471	Q472	C473	R474	Q475	P479	L480	Y481	T482	L483	H484	R485	S486	T487	Q489
Q318	R319	Y320	S321	V322	M323	T332	L333	V334	K335	T339	T340	Q341	E342	H343	T346	S347	A348	G350	F355	R356	P357	I372	H381	I382	C383	Q386	K387	K390	P391	E392	Q393	V394	C395	T396	F397	I398	T399	M403	E404	V405	I408	T412	S413	R414	Y415	L416	Y417	
F220	Q225	D228	Y229	G230	V231	P232	L233	I234	E235	W251	I252	P253	Y254	K255	A257	V260	G261	P262	T263	V264	K265	F266	I268	T271	L274	T277	T278	T279	Q284	A289	S290	V291	T292	Y297	L298	C299	D300	W303	E306	I309	L314	I317	T317					

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	208.55Å 208.55Å 208.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 29.79 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.30) 99.9 (29.79-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.277 0.234 , 0.269	Depositor DCC
R_{free} test set	2293 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.8	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	2 of 49851 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11869	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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

5.1 Standard geometry

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

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	0.45	0/6088	0.71	2/8278 (0.0%)
1	B	0.43	0/6088	0.71	3/8278 (0.0%)
All	All	0.44	0/12176	0.71	5/16556 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	713	HIS	N-CA-C	6.95	129.77	111.00
1	B	713	HIS	N-CA-C	6.87	129.54	111.00
1	B	548	TYR	N-CA-C	-5.90	95.06	111.00
1	A	548	TYR	N-CA-C	-5.87	95.14	111.00
1	B	383	CYS	CA-CB-SG	5.29	123.53	114.00

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	5920	0	5632	267	0
1	B	5920	0	5632	266	0
2	A	29	0	23	3	0
All	All	11869	0	11287	527	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 23.

All (527) 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:174:ILE:H	1:A:174:ILE:HD12	1.20	1.03
1:B:174:ILE:HD12	1:B:174:ILE:H	1.22	1.01
1:A:595:ILE:HD11	1:A:603:GLU:HB3	1.47	0.96
1:B:595:ILE:HD11	1:B:603:GLU:HB3	1.47	0.94
1:A:412:THR:HG22	1:A:414:ASP:H	1.28	0.93
1:B:54:LYS:H	1:B:498:ASN:HD21	1.17	0.92
1:B:412:THR:HG22	1:B:414:ASP:H	1.33	0.91
1:A:349:THR:HB	1:A:593:HIS:HD2	1.37	0.90
1:A:54:LYS:H	1:A:498:ASN:HD21	1.18	0.90
1:A:449:ASP:O	1:A:452:PRO:HD3	1.72	0.89
1:B:449:ASP:O	1:B:452:PRO:HD3	1.73	0.89
1:B:349:THR:HB	1:B:593:HIS:HD2	1.38	0.88
1:A:747:THR:HG21	1:B:726:ASP:HA	1.58	0.83
1:B:54:LYS:H	1:B:498:ASN:ND2	1.75	0.83
1:A:54:LYS:H	1:A:498:ASN:ND2	1.76	0.83
1:A:383:CYS:HB3	1:A:397:PHE:HA	1.59	0.83
1:A:460:VAL:HG22	1:A:461:SER:H	1.44	0.82
1:B:383:CYS:HB3	1:B:397:PHE:HA	1.61	0.82
1:B:639:MET:CE	1:B:689:VAL:HA	2.11	0.81
1:A:79:ALA:O	1:A:80:GLU:HB2	1.82	0.80
1:B:460:VAL:HG22	1:B:461:SER:H	1.45	0.79
1:B:707:THR:CG2	1:B:738:ASP:H	1.95	0.79
1:A:639:MET:CE	1:A:689:VAL:HA	2.13	0.79
1:A:121:GLN:O	1:A:125:SER:HB2	1.82	0.78
1:A:658:SER:H	1:A:716:GLN:NE2	1.81	0.78
1:B:79:ALA:O	1:B:80:GLU:HB2	1.81	0.78
1:A:690:MET:HE3	1:A:720:ILE:HA	1.66	0.78
1:A:234:ILE:HD13	1:A:713:HIS:CE1	2.19	0.77
1:A:707:THR:CG2	1:A:738:ASP:H	1.97	0.76
1:B:690:MET:HE3	1:B:720:ILE:HA	1.66	0.76
1:B:121:GLN:O	1:B:125:SER:HB2	1.85	0.76
1:A:56:TYR:CE2	1:A:495:LEU:HD22	2.20	0.75
1:B:91:SER:O	1:B:93:PHE:N	2.20	0.75
1:A:91:SER:O	1:A:93:PHE:N	2.20	0.74
1:A:726:ASP:HA	1:B:747:THR:HG21	1.68	0.74
1:B:54:LYS:N	1:B:498:ASN:HD21	1.85	0.74
1:A:586:TYR:CD1	1:A:586:TYR:N	2.55	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:VAL:HG22	1:B:461:SER:N	2.02	0.74
1:A:460:VAL:HG22	1:A:461:SER:N	2.01	0.73
1:A:761:GLN:HB3	1:A:767:ARG:HB3	1.70	0.73
1:B:234:ILE:HD13	1:B:713:HIS:CE1	2.23	0.73
1:B:56:TYR:CE2	1:B:495:LEU:HD22	2.24	0.72
1:A:54:LYS:N	1:A:498:ASN:HD21	1.85	0.72
1:B:235:GLU:HG2	1:B:251:TRP:HB3	1.71	0.72
1:B:658:SER:H	1:B:716:GLN:NE2	1.86	0.72
1:A:235:GLU:HG2	1:A:251:TRP:HB3	1.72	0.71
1:B:586:TYR:N	1:B:586:TYR:CD1	2.56	0.71
1:A:662:TYR:OH	1:A:719:GLN:HG2	1.91	0.70
1:A:277:THR:HG22	1:A:278:THR:H	1.57	0.70
1:B:761:GLN:HB3	1:B:767:ARG:HB3	1.74	0.70
1:A:349:THR:HB	1:A:593:HIS:CD2	2.26	0.69
1:B:55:SER:HA	1:B:481:TYR:CE1	2.28	0.69
1:A:107:PRO:HG2	1:A:158:GLU:O	1.92	0.69
1:B:91:SER:HA	1:B:94:GLU:OE1	1.93	0.69
1:B:277:THR:HG22	1:B:278:THR:H	1.58	0.69
1:A:204:GLU:OE2	2:A:901:XIH:N14	2.26	0.68
1:A:652:ILE:HG21	1:A:756:MET:HE3	1.75	0.68
1:A:747:THR:CG2	1:B:726:ASP:HA	2.24	0.68
1:B:485:ARG:HG3	1:B:485:ARG:O	1.93	0.68
1:A:91:SER:HA	1:A:94:GLU:OE1	1.94	0.68
1:A:277:THR:HG21	1:A:279:THR:O	1.93	0.68
1:A:624:ARG:HB2	1:A:624:ARG:HH11	1.58	0.67
1:B:349:THR:HB	1:B:593:HIS:CD2	2.27	0.67
1:B:485:ARG:HD2	1:B:487:THR:HB	1.77	0.67
1:B:277:THR:HG21	1:B:279:THR:O	1.95	0.67
1:B:107:PRO:HG2	1:B:158:GLU:O	1.94	0.67
1:A:518:ILE:CD1	1:A:519:VAL:H	2.08	0.67
1:A:473:CYS:O	1:A:479:PRO:HA	1.95	0.67
1:A:219:THR:O	1:A:271:THR:HB	1.94	0.66
1:B:473:CYS:O	1:B:479:PRO:HA	1.95	0.66
1:B:219:THR:O	1:B:271:THR:HB	1.94	0.66
1:A:412:THR:CG2	1:A:413:SER:N	2.58	0.66
1:B:767:ARG:HH11	1:B:767:ARG:HG3	1.61	0.66
1:B:662:TYR:OH	1:B:719:GLN:HG2	1.96	0.66
1:A:65:GLU:HB3	1:A:76:LEU:HD11	1.78	0.65
1:A:323:MET:O	1:A:342:GLU:O	2.14	0.65
1:A:688:THR:CG2	1:A:690:MET:HG2	2.26	0.65
1:A:55:SER:HA	1:A:481:TYR:CE1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:THR:CG2	1:B:413:SER:N	2.59	0.65
1:A:485:ARG:HD2	1:A:487:THR:HB	1.78	0.65
1:A:518:ILE:HD12	1:A:519:VAL:H	1.62	0.65
1:A:641:LEU:HD22	1:A:699:VAL:HG11	1.77	0.65
1:B:688:THR:CG2	1:B:690:MET:HG2	2.27	0.64
1:A:767:ARG:HG3	1:A:767:ARG:HH11	1.62	0.64
1:A:485:ARG:HG3	1:A:485:ARG:O	1.97	0.64
1:A:195:GLY:C	1:A:211:ALA:HB3	2.18	0.64
1:B:65:GLU:HB3	1:B:76:LEU:HD11	1.78	0.64
1:B:697:LYS:HG2	1:B:729:VAL:HG22	1.79	0.64
1:A:439:ASP:OD1	1:A:441:THR:HB	1.98	0.64
1:B:195:GLY:C	1:B:211:ALA:HB3	2.18	0.64
1:A:612:ARG:HH11	1:A:612:ARG:HG3	1.64	0.63
1:B:518:ILE:CD1	1:B:519:VAL:H	2.11	0.63
1:B:256:LYS:NZ	1:B:713:HIS:HD2	1.96	0.63
1:A:697:LYS:HG2	1:A:729:VAL:HG22	1.80	0.63
1:B:612:ARG:HH11	1:B:612:ARG:HG3	1.63	0.63
1:B:624:ARG:HB2	1:B:624:ARG:HH11	1.61	0.63
1:B:84:SER:O	1:B:85:SER:HB2	1.98	0.62
1:B:439:ASP:OD1	1:B:441:THR:HB	1.99	0.62
1:A:73:ASN:OD1	1:A:90:ASN:N	2.32	0.62
1:B:595:ILE:HG21	1:B:599:LEU:HD23	1.82	0.62
1:B:78:ASN:HB3	1:B:83:ASN:HB3	1.82	0.62
1:A:595:ILE:CG2	1:A:599:LEU:HD23	2.29	0.62
1:A:595:ILE:HG21	1:A:599:LEU:HD23	1.80	0.62
1:B:595:ILE:CG2	1:B:599:LEU:HD23	2.30	0.62
1:B:652:ILE:HG21	1:B:756:MET:HE3	1.81	0.62
1:A:256:LYS:NZ	1:A:713:HIS:HD2	1.98	0.61
1:A:174:ILE:H	1:A:174:ILE:CD1	2.00	0.61
1:B:639:MET:HE3	1:B:689:VAL:HA	1.80	0.61
1:B:707:THR:HG22	1:B:738:ASP:H	1.66	0.61
1:A:639:MET:HE3	1:A:689:VAL:HA	1.83	0.61
1:B:518:ILE:HD12	1:B:519:VAL:H	1.66	0.61
1:B:73:ASN:OD1	1:B:90:ASN:N	2.33	0.60
1:A:712:VAL:HG22	2:A:901:XIH:H21	1.83	0.60
1:A:483:LEU:HB3	1:A:495:LEU:HD11	1.83	0.60
1:B:767:ARG:C	1:B:767:ARG:HD2	2.20	0.60
1:B:641:LEU:HD22	1:B:699:VAL:HG11	1.82	0.60
1:A:713:HIS:O	1:A:714:PHE:CB	2.49	0.60
1:B:713:HIS:O	1:B:714:PHE:CB	2.49	0.60
1:B:323:MET:O	1:B:342:GLU:O	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASN:HB3	1:A:83:ASN:HB3	1.82	0.60
1:B:79:ALA:O	1:B:80:GLU:CB	2.49	0.60
1:A:79:ALA:O	1:A:80:GLU:CB	2.50	0.59
1:B:483:LEU:HB3	1:B:495:LEU:HD11	1.83	0.59
1:A:84:SER:O	1:A:85:SER:HB2	2.01	0.59
1:A:713:HIS:O	1:A:714:PHE:HB3	2.02	0.59
1:A:460:VAL:CG2	1:A:461:SER:H	2.15	0.59
1:A:412:THR:HG22	1:A:413:SER:N	2.17	0.59
1:B:713:HIS:O	1:B:714:PHE:HB3	2.03	0.59
1:A:58:LEU:HD12	1:A:58:LEU:H	1.68	0.58
1:B:583:GLY:O	1:B:584:SER:HB3	2.04	0.58
1:B:412:THR:HG22	1:B:413:SER:N	2.16	0.58
1:A:636:VAL:O	1:A:640:VAL:HG23	2.03	0.58
1:A:583:GLY:O	1:A:584:SER:HB3	2.02	0.58
1:B:408:ILE:HG23	1:B:416:LEU:HD11	1.85	0.58
1:B:383:CYS:CB	1:B:397:PHE:HA	2.33	0.58
1:A:233:LEU:HD23	1:A:253:PRO:HA	1.86	0.58
1:A:383:CYS:CB	1:A:397:PHE:HA	2.33	0.58
1:A:408:ILE:HG23	1:A:416:LEU:HD11	1.85	0.58
1:B:470:GLN:HG2	1:B:471:LEU:N	2.20	0.57
1:B:460:VAL:CG2	1:B:461:SER:H	2.16	0.57
1:B:636:VAL:O	1:B:640:VAL:HG23	2.04	0.57
1:B:264:VAL:HG12	1:B:265:LYS:N	2.20	0.57
1:A:470:GLN:HG2	1:A:471:LEU:N	2.18	0.57
1:A:277:THR:HG22	1:A:278:THR:N	2.20	0.57
1:B:178:LEU:HB3	1:B:179:PRO:HD2	1.87	0.57
1:B:233:LEU:HD23	1:B:253:PRO:HA	1.86	0.56
1:B:632:TYR:O	1:B:635:TYR:HB3	2.04	0.56
1:B:403:TRP:CE3	1:B:422:GLU:HB2	2.40	0.56
1:B:415:TYR:HD2	1:B:436:GLN:HA	1.70	0.56
1:A:415:TYR:HD2	1:A:436:GLN:HA	1.70	0.56
1:B:277:THR:HG22	1:B:278:THR:N	2.20	0.56
1:B:58:LEU:H	1:B:58:LEU:HD12	1.70	0.56
1:A:264:VAL:HG12	1:A:265:LYS:N	2.21	0.56
1:B:320:TYR:CE2	1:B:322:VAL:HG23	2.41	0.56
1:B:403:TRP:CD2	1:B:422:GLU:HB2	2.40	0.56
1:A:178:LEU:HB3	1:A:179:PRO:HD2	1.87	0.56
1:B:462:LEU:N	1:B:462:LEU:HD12	2.21	0.56
1:A:632:TYR:O	1:A:635:TYR:HB3	2.05	0.56
1:A:707:THR:HG22	1:A:738:ASP:H	1.68	0.55
1:B:709:ASP:OD2	1:B:741:HIS:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ARG:HG2	1:A:524:ARG:HH11	1.71	0.55
1:B:116:TYR:O	1:B:117:ASN:HB2	2.06	0.55
1:A:483:LEU:CB	1:A:495:LEU:HD11	2.36	0.55
1:B:267:PHE:CE2	1:B:284:GLN:HB2	2.42	0.55
1:A:317:ILE:HG22	1:A:319:ASN:HB2	1.89	0.55
1:B:47:LEU:HD22	1:B:750:GLN:HA	1.88	0.55
1:A:386:GLN:HG3	1:A:390:LYS:HE3	1.88	0.55
1:B:524:ARG:HH11	1:B:524:ARG:HG2	1.71	0.55
1:A:320:TYR:CE2	1:A:322:VAL:HG23	2.41	0.55
1:A:125:SER:O	1:A:126:TYR:HB3	2.06	0.55
1:B:94:GLU:O	1:B:94:GLU:HG2	2.06	0.54
1:A:403:TRP:CD2	1:A:422:GLU:HB2	2.42	0.54
1:A:658:SER:H	1:A:716:GLN:HE21	1.54	0.54
1:A:767:ARG:HD2	1:A:767:ARG:C	2.27	0.54
1:A:267:PHE:CE2	1:A:284:GLN:HB2	2.43	0.54
1:A:460:VAL:CG2	1:A:461:SER:N	2.70	0.54
1:B:125:SER:O	1:B:126:TYR:HB3	2.06	0.54
1:B:483:LEU:CB	1:B:495:LEU:HD11	2.37	0.54
1:A:447:SER:HB2	1:A:458:TYR:CE1	2.42	0.54
1:B:267:PHE:CD2	1:B:284:GLN:HB2	2.43	0.54
1:A:709:ASP:OD2	1:A:741:HIS:HA	2.08	0.54
1:A:601:THR:HG22	1:A:602:LEU:N	2.23	0.54
1:A:228:ASP:OD1	1:A:262:PRO:HB3	2.07	0.54
1:A:256:LYS:HZ3	1:A:713:HIS:HD2	1.55	0.53
1:A:726:ASP:HA	1:B:747:THR:CG2	2.38	0.53
1:A:292:THR:HG22	1:A:292:THR:O	2.08	0.53
1:A:415:TYR:CD2	1:A:436:GLN:HA	2.43	0.53
1:A:146:ILE:HD12	1:A:153:ILE:HD12	1.91	0.53
1:A:403:TRP:CE3	1:A:422:GLU:HB2	2.43	0.53
1:A:707:THR:HG21	1:A:738:ASP:H	1.73	0.53
1:A:267:PHE:CD2	1:A:284:GLN:HB2	2.43	0.53
1:B:174:ILE:H	1:B:174:ILE:CD1	2.02	0.53
1:A:712:VAL:CG2	2:A:901:XIH:H21	2.39	0.53
1:B:386:GLN:HG3	1:B:390:LYS:HE3	1.90	0.53
1:A:455:CYS:HA	1:A:475:GLY:HA3	1.91	0.53
1:A:547:VAL:HG23	1:A:628:TRP:O	2.08	0.52
1:A:147:PRO:HB2	1:A:166:TRP:CD1	2.44	0.52
1:B:584:SER:O	1:B:585:GLY:O	2.27	0.52
1:B:292:THR:HG22	1:B:292:THR:O	2.09	0.52
1:B:317:ILE:HG22	1:B:319:ASN:HB2	1.91	0.52
1:A:174:ILE:HD12	1:A:174:ILE:N	2.04	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:SER:HB2	1:B:458:TYR:CE1	2.45	0.52
1:B:742:GLY:O	1:B:743:ILE:C	2.48	0.52
1:A:462:LEU:N	1:A:462:LEU:HD12	2.25	0.52
1:B:80:GLU:H	1:B:493:ARG:HH22	1.58	0.52
1:A:47:LEU:HD22	1:A:750:GLN:HA	1.91	0.52
1:A:688:THR:HG21	1:A:690:MET:HG2	1.92	0.52
1:A:485:ARG:HB3	1:A:492:LEU:HD21	1.91	0.52
1:B:60:TRP:CE3	1:B:66:TYR:HB3	2.45	0.52
1:A:94:GLU:HG2	1:A:94:GLU:O	2.08	0.52
1:B:256:LYS:HZ3	1:B:713:HIS:HD2	1.58	0.52
1:B:415:TYR:CD2	1:B:436:GLN:HA	2.44	0.52
1:A:421:ASN:ND2	1:A:427:PRO:HA	2.25	0.52
1:B:659:ARG:HG2	1:B:662:TYR:CE2	2.44	0.52
1:A:612:ARG:NH1	1:A:612:ARG:HG3	2.24	0.52
1:B:228:ASP:OD1	1:B:262:PRO:HB3	2.10	0.52
1:A:116:TYR:O	1:A:117:ASN:HB2	2.09	0.52
1:A:381:HIS:CD2	1:A:399:THR:HG22	2.45	0.52
1:B:146:ILE:HD12	1:B:153:ILE:HD12	1.90	0.52
1:A:699:VAL:HG12	1:A:700:GLU:N	2.24	0.51
1:A:299:CYS:SG	1:A:357:PRO:HD2	2.50	0.51
1:A:314:LEU:CD1	1:A:321:SER:HB2	2.41	0.51
1:B:95:ILE:C	1:B:97:GLY:H	2.13	0.51
1:B:455:CYS:HA	1:B:475:GLY:HA3	1.92	0.51
1:B:688:THR:HG21	1:B:690:MET:HG2	1.92	0.51
1:B:547:VAL:HG23	1:B:628:TRP:O	2.09	0.51
1:A:742:GLY:O	1:A:743:ILE:C	2.49	0.51
1:B:601:THR:HG22	1:B:602:LEU:N	2.25	0.51
1:A:699:VAL:CG1	1:A:700:GLU:N	2.73	0.51
1:A:314:LEU:HD12	1:A:321:SER:HB2	1.92	0.51
1:B:147:PRO:HB2	1:B:166:TRP:CD1	2.46	0.51
1:B:314:LEU:HD12	1:B:321:SER:HB2	1.91	0.51
1:A:412:THR:CG2	1:A:413:SER:H	2.23	0.51
1:A:122:TRP:CH2	1:A:252:ILE:HD11	2.45	0.51
1:B:598:ARG:HD3	1:B:598:ARG:O	2.10	0.51
1:B:485:ARG:HB3	1:B:492:LEU:HD21	1.92	0.51
1:A:95:ILE:C	1:A:97:GLY:H	2.13	0.51
1:A:121:GLN:O	1:A:122:TRP:HB2	2.11	0.51
1:B:612:ARG:HG3	1:B:612:ARG:NH1	2.24	0.51
1:B:421:ASN:ND2	1:B:427:PRO:HA	2.27	0.50
1:B:314:LEU:CD1	1:B:321:SER:HB2	2.41	0.50
1:B:699:VAL:HG12	1:B:700:GLU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:LEU:O	1:B:767:ARG:O	2.30	0.50
1:B:767:ARG:HG3	1:B:767:ARG:NH1	2.27	0.50
1:B:699:VAL:CG1	1:B:700:GLU:N	2.74	0.50
1:A:598:ARG:HD3	1:A:598:ARG:O	2.11	0.50
1:B:196:ILE:N	1:B:211:ALA:HB3	2.27	0.50
1:A:584:SER:O	1:A:585:GLY:O	2.30	0.50
1:B:229:THR:HG22	1:B:230:GLY:N	2.27	0.50
1:A:584:SER:H	1:A:592:MET:HA	1.77	0.50
1:B:462:LEU:H	1:B:462:LEU:HD12	1.77	0.50
1:A:624:ARG:HB2	1:A:624:ARG:NH1	2.26	0.49
1:A:412:THR:HG23	1:A:413:SER:H	1.78	0.49
1:A:80:GLU:H	1:A:493:ARG:HH22	1.59	0.49
1:B:122:TRP:CH2	1:B:252:ILE:HD11	2.48	0.49
1:A:89:GLU:C	1:A:91:SER:N	2.63	0.49
1:A:536:ASP:HB3	1:A:539:LYS:HE2	1.95	0.49
1:A:132:ILE:HG21	1:A:176:PRO:HB3	1.95	0.49
1:B:412:THR:CG2	1:B:413:SER:H	2.25	0.49
1:A:767:ARG:HG3	1:A:767:ARG:NH1	2.28	0.49
1:A:334:VAL:HG12	1:A:335:TRP:N	2.28	0.49
1:B:121:GLN:O	1:B:122:TRP:HB2	2.13	0.49
1:A:659:ARG:HG2	1:A:662:TYR:CE2	2.48	0.49
1:B:511:PRO:HB2	1:B:531:LEU:O	2.13	0.49
1:A:342:GLU:O	1:A:343:HIS:HB2	2.13	0.49
1:B:132:ILE:HG21	1:B:176:PRO:HB3	1.94	0.48
1:A:234:ILE:O	1:A:234:ILE:HG13	2.12	0.48
1:B:658:SER:H	1:B:716:GLN:HE21	1.61	0.48
1:A:314:LEU:HG	1:A:318:GLN:HG2	1.94	0.48
1:A:430:ARG:HG2	1:A:457:TYR:CE1	2.48	0.48
1:A:749:HIS:CE1	1:A:753:TYR:CE1	3.01	0.48
1:B:690:MET:HE3	1:B:720:ILE:CA	2.40	0.48
1:B:299:CYS:SG	1:B:314:LEU:HD22	2.53	0.48
1:B:314:LEU:HG	1:B:318:GLN:HG2	1.95	0.48
1:B:707:THR:HG21	1:B:738:ASP:H	1.72	0.48
1:B:474:ARG:O	1:B:475:GLY:O	2.31	0.48
1:B:381:HIS:CD2	1:B:399:THR:HG22	2.48	0.48
1:A:748:ALA:O	1:A:752:ILE:HG22	2.13	0.48
1:B:78:ASN:O	1:B:81:HIS:O	2.32	0.48
1:B:200:VAL:HG13	1:B:201:TYR:N	2.28	0.48
1:B:624:ARG:NH1	1:B:624:ARG:HB2	2.28	0.48
1:B:441:THR:O	1:B:443:LYS:N	2.44	0.48
1:A:82:GLY:O	1:A:83:ASN:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:TRP:CE3	1:A:66:TYR:HB3	2.48	0.48
1:A:603:GLU:OE1	1:A:603:GLU:N	2.46	0.48
1:A:264:VAL:HG12	1:A:265:LYS:H	1.79	0.48
1:B:75:LEU:HB2	1:B:77:PHE:HE1	1.79	0.48
1:A:104:SER:HB3	1:A:113:LEU:HB2	1.96	0.47
1:A:299:CYS:SG	1:A:314:LEU:HD22	2.54	0.47
1:A:61:VAL:HG21	1:A:67:LEU:HG	1.96	0.47
1:A:583:GLY:HA2	1:A:592:MET:O	2.14	0.47
1:B:430:ARG:HG2	1:B:457:TYR:CE1	2.49	0.47
1:A:148:ASN:HD22	1:A:148:ASN:HA	1.56	0.47
1:A:71:GLU:O	1:A:73:ASN:ND2	2.48	0.47
1:A:601:THR:HG22	1:A:602:LEU:HD23	1.95	0.47
1:B:82:GLY:O	1:B:83:ASN:C	2.52	0.47
1:B:299:CYS:SG	1:B:357:PRO:HD2	2.55	0.47
1:A:543:LEU:HD12	1:A:575:ILE:O	2.15	0.47
1:A:229:THR:HG22	1:A:230:GLY:N	2.30	0.47
1:B:234:ILE:HG13	1:B:234:ILE:O	2.14	0.47
1:A:196:ILE:N	1:A:211:ALA:HB3	2.30	0.47
1:B:584:SER:H	1:B:592:MET:HA	1.79	0.47
1:B:529:MET:HB3	1:B:529:MET:HE2	1.70	0.47
1:A:520:LEU:O	1:A:522:GLU:N	2.48	0.47
1:B:334:VAL:HG12	1:B:335:TRP:N	2.29	0.47
1:A:78:ASN:O	1:A:81:HIS:O	2.33	0.47
1:A:216:PRO:C	1:A:218:GLY:H	2.18	0.47
1:A:467:LYS:C	1:A:486:SER:HB2	2.35	0.47
1:B:680:ASN:ND2	1:B:683:HIS:HB2	2.30	0.47
1:A:583:GLY:HA2	1:A:592:MET:HA	1.97	0.47
1:B:509:GLN:O	1:B:533:PRO:HG3	2.14	0.47
1:B:303:TRP:CE2	1:B:309:ILE:HD12	2.50	0.47
1:A:509:GLN:O	1:A:533:PRO:HG3	2.14	0.47
1:B:601:THR:HG22	1:B:602:LEU:HD23	1.97	0.47
1:B:767:ARG:C	1:B:767:ARG:CD	2.84	0.46
1:A:216:PRO:C	1:A:218:GLY:N	2.69	0.46
1:B:467:LYS:C	1:B:486:SER:HB2	2.35	0.46
1:A:529:MET:HE2	1:A:529:MET:HB3	1.65	0.46
1:B:342:GLU:O	1:B:343:HIS:HB2	2.15	0.46
1:B:75:LEU:HD23	1:B:86:ILE:HA	1.96	0.46
1:B:216:PRO:C	1:B:218:GLY:N	2.68	0.46
1:B:216:PRO:C	1:B:218:GLY:H	2.18	0.46
1:B:488:ASP:O	1:B:489:GLN:HB2	2.15	0.46
1:B:603:GLU:OE1	1:B:603:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:GLU:O	1:B:697:LYS:HG3	2.16	0.46
1:A:694:GLU:O	1:A:697:LYS:HG3	2.15	0.46
1:A:416:LEU:C	1:A:416:LEU:HD12	2.36	0.46
1:A:303:TRP:CE2	1:A:309:ILE:HD12	2.50	0.46
1:B:748:ALA:O	1:B:752:ILE:HG22	2.16	0.46
1:B:289:ALA:C	1:B:291:VAL:H	2.19	0.46
1:A:418:TYR:O	1:A:432:LEU:HD12	2.16	0.46
1:A:277:THR:HG22	1:A:279:THR:H	1.81	0.46
1:A:536:ASP:OD2	1:A:538:SER:OG	2.34	0.46
1:B:121:GLN:O	1:B:122:TRP:CB	2.64	0.46
1:B:741:HIS:O	1:B:741:HIS:CG	2.69	0.46
1:B:583:GLY:HA2	1:B:592:MET:HA	1.98	0.46
1:B:41:TYR:CD2	1:B:566:THR:HG22	2.51	0.46
1:A:511:PRO:HB2	1:A:531:LEU:O	2.15	0.46
1:B:89:GLU:C	1:B:91:SER:N	2.66	0.45
1:A:766:LEU:O	1:A:767:ARG:O	2.34	0.45
1:B:235:GLU:OE2	1:B:251:TRP:HB3	2.16	0.45
1:A:474:ARG:O	1:A:475:GLY:O	2.35	0.45
1:B:160:HIS:HB2	1:B:176:PRO:HD3	1.98	0.45
1:B:392:GLU:C	1:B:393:GLN:HG3	2.37	0.45
1:B:543:LEU:HD12	1:B:575:ILE:O	2.16	0.45
1:B:264:VAL:HG12	1:B:265:LYS:H	1.81	0.45
1:B:488:ASP:OD1	1:B:490:LYS:HB2	2.16	0.45
1:A:121:GLN:O	1:A:122:TRP:CB	2.63	0.45
1:B:71:GLU:O	1:B:73:ASN:ND2	2.50	0.45
1:A:289:ALA:C	1:A:291:VAL:H	2.20	0.45
1:A:91:SER:OG	1:A:92:THR:N	2.50	0.45
1:B:104:SER:HB3	1:B:113:LEU:HB2	1.98	0.45
1:A:235:GLU:OE2	1:A:251:TRP:HB3	2.16	0.45
1:A:382:ILE:HG13	1:A:405:VAL:HG21	1.98	0.45
1:B:163:ALA:HB2	1:B:214:TRP:CZ2	2.52	0.45
1:A:392:GLU:C	1:A:393:GLN:HG3	2.36	0.45
1:A:690:MET:HE3	1:A:720:ILE:CA	2.42	0.45
1:B:290:SER:O	1:B:291:VAL:HG23	2.17	0.45
1:B:80:GLU:HA	1:B:492:LEU:HD13	1.99	0.45
1:A:297:TYR:CE2	1:A:666:VAL:HG22	2.51	0.45
1:A:383:CYS:HB3	1:A:397:PHE:CA	2.40	0.45
1:B:120:LYS:HG2	1:B:121:GLN:N	2.32	0.45
1:A:462:LEU:H	1:A:462:LEU:HD12	1.81	0.45
1:B:216:PRO:O	1:B:306:GLU:OE2	2.35	0.45
1:B:231:VAL:HG22	1:B:260:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:THR:CG2	1:B:279:THR:O	2.64	0.44
1:A:386:GLN:O	1:A:387:LYS:C	2.56	0.44
1:B:536:ASP:HB3	1:B:539:LYS:HE2	1.98	0.44
1:A:163:ALA:HB2	1:A:214:TRP:CZ2	2.52	0.44
1:B:174:ILE:HD12	1:B:174:ILE:N	2.06	0.44
1:A:120:LYS:HG2	1:A:121:GLN:N	2.33	0.44
1:B:320:TYR:HE2	1:B:322:VAL:HG23	1.80	0.44
1:A:200:VAL:HG13	1:A:201:TYR:N	2.32	0.44
1:B:297:TYR:CE2	1:B:666:VAL:HG22	2.52	0.44
1:B:346:THR:HG23	1:B:347:SER:N	2.33	0.44
1:A:320:TYR:HE2	1:A:322:VAL:HG23	1.82	0.44
1:B:318:GLN:OE1	1:B:670:ARG:HD3	2.17	0.44
1:A:41:TYR:CD2	1:A:566:THR:HG22	2.52	0.44
1:A:488:ASP:O	1:A:489:GLN:HB2	2.18	0.44
1:B:193:PHE:O	1:B:225:GLN:HA	2.18	0.44
1:A:318:GLN:OE1	1:A:670:ARG:HD3	2.18	0.44
1:A:160:HIS:HB2	1:A:176:PRO:HD3	1.99	0.44
1:B:61:VAL:HG21	1:B:67:LEU:HG	1.99	0.44
1:B:412:THR:HG23	1:B:413:SER:H	1.81	0.44
1:A:84:SER:O	1:A:85:SER:CB	2.65	0.44
1:B:749:HIS:CE1	1:B:753:TYR:CE1	3.05	0.44
1:A:246:TYR:CZ	1:B:232:PRO:HB2	2.53	0.44
1:A:439:ASP:C	1:A:441:THR:H	2.21	0.44
1:B:215:SER:HB3	1:B:303:TRP:CZ2	2.53	0.44
1:B:545:ILE:HB	1:B:627:ILE:HG13	2.00	0.44
1:A:680:ASN:ND2	1:A:683:HIS:HB2	2.33	0.44
1:B:690:MET:HE2	1:B:719:GLN:C	2.39	0.43
1:B:355:PHE:O	1:B:356:ARG:HB3	2.18	0.43
1:B:707:THR:HG22	1:B:738:ASP:N	2.32	0.43
1:B:277:THR:HG22	1:B:279:THR:H	1.83	0.43
1:A:103:TYR:HA	1:A:113:LEU:O	2.18	0.43
1:A:75:LEU:HD23	1:A:86:ILE:HA	2.00	0.43
1:A:488:ASP:OD1	1:A:490:LYS:HB2	2.18	0.43
1:B:418:TYR:O	1:B:432:LEU:HD12	2.18	0.43
1:B:91:SER:OG	1:B:92:THR:N	2.50	0.43
1:B:484:HIS:ND1	1:B:484:HIS:N	2.66	0.43
1:B:382:ILE:HG13	1:B:405:VAL:HG21	2.00	0.43
1:B:75:LEU:HB2	1:B:77:PHE:CE1	2.53	0.43
1:A:277:THR:CG2	1:A:279:THR:O	2.63	0.43
1:A:75:LEU:HB2	1:A:77:PHE:HE1	1.82	0.43
1:A:454:ARG:HD3	1:A:478:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:PHE:O	1:A:225:GLN:HA	2.18	0.43
1:A:605:GLU:O	1:A:608:ILE:N	2.50	0.43
1:B:688:THR:HG22	1:B:690:MET:N	2.34	0.43
1:A:586:TYR:H	1:A:586:TYR:HD1	1.66	0.43
1:B:714:PHE:O	1:B:715:GLN:C	2.57	0.43
1:B:583:GLY:HA2	1:B:592:MET:O	2.18	0.43
1:A:714:PHE:O	1:A:715:GLN:C	2.58	0.43
1:A:707:THR:HG23	1:A:707:THR:O	2.19	0.43
1:B:548:TYR:O	1:B:549:ALA:HB3	2.19	0.43
1:B:416:LEU:C	1:B:416:LEU:HD12	2.39	0.43
1:A:372:ILE:HA	1:A:381:HIS:O	2.19	0.43
1:B:355:PHE:O	1:B:670:ARG:NH1	2.51	0.43
1:B:200:VAL:CG1	1:B:201:TYR:N	2.82	0.43
1:A:751:HIS:CD2	1:B:725:VAL:HA	2.53	0.43
1:B:120:LYS:CG	1:B:121:GLN:N	2.82	0.42
1:A:332:THR:HG22	1:A:332:THR:O	2.19	0.42
1:A:120:LYS:CG	1:A:121:GLN:N	2.82	0.42
1:B:745:SER:OG	1:B:748:ALA:HB3	2.19	0.42
1:B:194:ASN:OD1	1:B:225:GLN:HG3	2.19	0.42
1:B:341:GLN:OE1	1:B:387:LYS:HE3	2.20	0.42
1:A:306:GLU:HG2	1:A:306:GLU:O	2.19	0.42
1:B:595:ILE:O	1:B:595:ILE:CG2	2.67	0.42
1:A:334:VAL:CG1	1:A:335:TRP:N	2.83	0.42
1:A:341:GLN:OE1	1:A:387:LYS:HE3	2.18	0.42
1:A:332:THR:O	1:A:334:VAL:HG23	2.19	0.42
1:B:498:ASN:HB3	1:B:501:LEU:HB3	2.02	0.42
1:B:707:THR:HG23	1:B:707:THR:O	2.17	0.42
1:A:741:HIS:CG	1:A:741:HIS:O	2.71	0.42
1:A:355:PHE:O	1:A:670:ARG:NH1	2.51	0.42
1:A:545:ILE:HB	1:A:627:ILE:HG13	2.02	0.42
1:A:346:THR:HG23	1:A:347:SER:N	2.34	0.42
1:A:204:GLU:HA	1:A:204:GLU:OE1	2.20	0.42
1:B:680:ASN:HD21	1:B:683:HIS:HB2	1.84	0.42
1:A:220:PHE:HB3	1:A:268:ILE:CG2	2.49	0.42
1:B:439:ASP:C	1:B:441:THR:H	2.23	0.42
1:A:416:LEU:HD12	1:A:417:TYR:N	2.35	0.42
1:A:167:LYS:O	1:A:168:ASN:HB2	2.19	0.42
1:A:688:THR:HG22	1:A:690:MET:N	2.34	0.42
1:A:153:ILE:HG13	1:A:164:TYR:HB3	2.01	0.42
1:B:680:ASN:HD21	1:B:683:HIS:CG	2.38	0.42
1:A:193:PHE:CE2	1:A:198:ASP:HA	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:VAL:HG22	1:A:260:VAL:O	2.19	0.42
1:A:370:TYR:CE2	1:A:384:GLN:CG	3.03	0.42
1:A:690:MET:HE2	1:A:719:GLN:C	2.40	0.42
1:A:381:HIS:CG	1:A:399:THR:HG22	2.54	0.42
1:B:68:TYR:HB3	1:B:77:PHE:CE1	2.55	0.42
1:B:103:TYR:HA	1:B:113:LEU:O	2.20	0.42
1:A:194:ASN:OD1	1:A:225:GLN:HG3	2.20	0.42
1:A:518:ILE:HD13	1:A:519:VAL:H	1.84	0.41
1:B:220:PHE:HB3	1:B:268:ILE:CG2	2.49	0.41
1:A:80:GLU:HA	1:A:492:LEU:HD13	2.01	0.41
1:B:256:LYS:HZ1	1:B:713:HIS:HD2	1.68	0.41
1:B:628:TRP:CE3	1:B:756:MET:HE1	2.55	0.41
1:A:613:GLN:O	1:A:617:MET:HG3	2.20	0.41
1:A:254:TYR:CE1	1:A:713:HIS:CE1	3.08	0.41
1:B:471:LEU:HA	1:B:471:LEU:HD23	1.92	0.41
1:B:372:ILE:HA	1:B:381:HIS:O	2.21	0.41
1:B:193:PHE:CE2	1:B:198:ASP:HA	2.55	0.41
1:B:332:THR:O	1:B:332:THR:HG22	2.21	0.41
1:A:484:HIS:ND1	1:A:484:HIS:N	2.68	0.41
1:B:152:TRP:CD1	1:B:212:LEU:HD12	2.55	0.41
1:A:130:TYR:HB2	1:A:146:ILE:HD13	2.02	0.41
1:B:164:TYR:CE1	1:B:171:TYR:HB2	2.56	0.41
1:B:529:MET:HE1	1:B:531:LEU:HD21	2.01	0.41
1:B:306:GLU:O	1:B:306:GLU:HG2	2.21	0.41
1:B:41:TYR:CD2	1:B:566:THR:CG2	3.03	0.41
1:B:639:MET:HE3	1:B:689:VAL:CA	2.49	0.41
1:A:548:TYR:O	1:A:549:ALA:HB3	2.19	0.41
1:A:520:LEU:O	1:A:521:ASN:C	2.59	0.41
1:B:520:LEU:O	1:B:522:GLU:N	2.53	0.41
1:B:547:VAL:HG12	1:B:548:TYR:N	2.36	0.41
1:B:536:ASP:OD2	1:B:538:SER:OG	2.38	0.41
1:A:363:THR:HG23	1:A:368:SER:O	2.20	0.41
1:B:479:PRO:HG2	1:B:498:ASN:OD1	2.21	0.41
1:A:473:CYS:HB3	1:A:480:LEU:O	2.20	0.41
1:B:61:VAL:CG2	1:B:67:LEU:HG	2.51	0.41
1:A:152:TRP:CD1	1:A:212:LEU:HD12	2.55	0.41
1:A:601:THR:HG22	1:A:602:LEU:CD2	2.51	0.41
1:B:88:LEU:HA	1:B:88:LEU:HD23	1.87	0.41
1:B:254:TYR:C	1:B:254:TYR:CD2	2.94	0.41
1:B:586:TYR:HD1	1:B:586:TYR:H	1.68	0.41
1:A:624:ARG:HG2	1:A:764:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:SER:O	1:B:85:SER:CB	2.65	0.41
1:A:585:GLY:HA3	1:A:587:GLN:HE21	1.85	0.41
1:B:58:LEU:HD12	1:B:58:LEU:N	2.35	0.41
1:A:547:VAL:HG12	1:A:548:TYR:N	2.36	0.41
1:B:153:ILE:HG13	1:B:164:TYR:HB3	2.01	0.41
1:A:355:PHE:O	1:A:356:ARG:HB3	2.20	0.41
1:B:334:VAL:CG1	1:B:335:TRP:N	2.84	0.41
1:B:680:ASN:HD21	1:B:683:HIS:CD2	2.38	0.41
1:B:520:LEU:O	1:B:521:ASN:C	2.60	0.41
1:A:499:SER:O	1:A:502:ASP:HB3	2.21	0.41
1:A:101:SER:HB3	1:A:115:GLU:HG2	2.03	0.41
1:B:458:TYR:HA	1:B:472:GLY:O	2.20	0.41
1:A:61:VAL:CG2	1:A:67:LEU:HG	2.50	0.41
1:A:467:LYS:HD3	1:A:468:TYR:HE1	1.86	0.41
1:B:481:TYR:O	1:B:495:LEU:HB2	2.21	0.40
1:B:251:TRP:N	1:B:251:TRP:CD1	2.89	0.40
1:B:585:GLY:HA3	1:B:587:GLN:HE21	1.86	0.40
1:A:315:ARG:HD2	1:A:320:TYR:HB3	2.03	0.40
1:A:479:PRO:HG2	1:A:498:ASN:OD1	2.21	0.40
1:A:312:GLN:HG2	1:A:323:MET:HG3	2.04	0.40
1:B:624:ARG:HG2	1:B:764:PHE:CD2	2.56	0.40
1:A:749:HIS:CE1	1:A:753:TYR:HE1	2.39	0.40
1:A:75:LEU:HB2	1:A:77:PHE:CE1	2.57	0.40
1:A:411:LEU:HD12	1:A:411:LEU:HA	1.79	0.40
1:A:41:TYR:CD2	1:A:566:THR:CG2	3.04	0.40
1:A:525:PHE:HB3	1:A:579:PHE:CZ	2.57	0.40
1:A:498:ASN:HB3	1:A:501:LEU:HB3	2.03	0.40
1:B:254:TYR:CE1	1:B:713:HIS:CE1	3.10	0.40
1:B:339:THR:O	1:B:342:GLU:HB2	2.22	0.40
1:A:459:SER:HB3	1:A:474:ARG:HE	1.85	0.40
1:B:60:TRP:CG	1:B:463:SER:HA	2.56	0.40
1:A:667:TYR:O	1:A:670:ARG:HB3	2.22	0.40
1:B:299:CYS:SG	1:B:314:LEU:HB2	2.62	0.40
1:B:679:ASP:OD1	1:B:680:ASN:N	2.54	0.40
1:A:68:TYR:HB3	1:A:77:PHE:CE1	2.56	0.40
1:A:383:CYS:HB2	1:A:396:THR:O	2.22	0.40
1:B:256:LYS:O	1:B:257:ALA:C	2.60	0.40
1:B:430:ARG:HA	1:B:430:ARG:HD3	1.88	0.40
1:B:525:PHE:HB3	1:B:579:PHE:CZ	2.57	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	728/730 (100%)	614 (84%)	80 (11%)	34 (5%)	3	20
1	B	728/730 (100%)	619 (85%)	76 (10%)	33 (4%)	3	21
All	All	1456/1460 (100%)	1233 (85%)	156 (11%)	67 (5%)	3	21

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	SER
1	A	92	THR
1	A	274	LEU
1	A	450	LEU
1	A	475	GLY
1	A	521	ASN
1	A	533	PRO
1	A	585	GLY
1	A	619	PHE
1	A	713	HIS
1	B	91	SER
1	B	92	THR
1	B	274	LEU
1	B	450	LEU
1	B	475	GLY
1	B	533	PRO
1	B	585	GLY
1	B	619	PHE
1	B	713	HIS
1	A	80	GLU
1	A	85	SER
1	A	149	ASN
1	A	159	GLY
1	A	714	PHE
1	B	80	GLU

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Mol	Chain	Res	Type
1	B	85	SER
1	B	521	ASN
1	B	714	PHE
1	A	147	PRO
1	B	149	ASN
1	B	159	GLY
1	A	83	ASN
1	A	318	GLN
1	A	440	HIS
1	A	442	ASN
1	B	83	ASN
1	B	147	PRO
1	B	148	ASN
1	B	318	GLN
1	B	424	LYS
1	B	442	ASN
1	A	143	GLU
1	A	148	ASN
1	A	537	LYS
1	A	695	ASN
1	B	121	GLN
1	B	143	GLU
1	B	440	HIS
1	B	461	SER
1	A	240	SER
1	A	290	SER
1	A	291	VAL
1	A	461	SER
1	A	464	LYS
1	B	290	SER
1	B	291	VAL
1	B	464	LYS
1	A	391	PRO
1	B	391	PRO
1	B	356	ARG
1	B	191	VAL
1	A	191	VAL
1	A	356	ARG
1	A	583	GLY
1	B	350	GLY
1	B	583	GLY
1	A	350	GLY

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	643/651 (99%)	590 (92%)	53 (8%)	14	48
1	B	643/651 (99%)	589 (92%)	54 (8%)	14	46
All	All	1286/1302 (99%)	1179 (92%)	107 (8%)	14	47

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	90	ASN
1	A	94	GLU
1	A	108	ASP
1	A	122	TRP
1	A	139	GLN
1	A	143	GLU
1	A	146	ILE
1	A	148	ASN
1	A	149	ASN
1	A	160	HIS
1	A	180	SER
1	A	229	THR
1	A	234	ILE
1	A	251	TRP
1	A	254	TYR
1	A	300	ASP
1	A	319	ASN
1	A	340	THR
1	A	342	GLU
1	A	346	THR
1	A	394	VAL
1	A	395	CYS
1	A	413	SER
1	A	414	ASP
1	A	416	LEU
1	A	441	THR

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Mol	Chain	Res	Type
1	A	453	GLU
1	A	459	SER
1	A	470	GLN
1	A	474	ARG
1	A	483	LEU
1	A	485	ARG
1	A	486	SER
1	A	516	ASP
1	A	518	ILE
1	A	533	PRO
1	A	547	VAL
1	A	548	TYR
1	A	586	TYR
1	A	593	HIS
1	A	598	ARG
1	A	622	SER
1	A	624	ARG
1	A	664	ASP
1	A	680	ASN
1	A	686	ASN
1	A	690	MET
1	A	707	THR
1	A	716	GLN
1	A	740	ASP
1	A	747	THR
1	A	767	ARG
1	B	58	LEU
1	B	90	ASN
1	B	94	GLU
1	B	108	ASP
1	B	122	TRP
1	B	139	GLN
1	B	143	GLU
1	B	146	ILE
1	B	148	ASN
1	B	149	ASN
1	B	160	HIS
1	B	180	SER
1	B	229	THR
1	B	234	ILE
1	B	251	TRP
1	B	254	TYR

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Mol	Chain	Res	Type
1	B	300	ASP
1	B	319	ASN
1	B	340	THR
1	B	342	GLU
1	B	346	THR
1	B	394	VAL
1	B	395	CYS
1	B	413	SER
1	B	414	ASP
1	B	416	LEU
1	B	441	THR
1	B	453	GLU
1	B	459	SER
1	B	470	GLN
1	B	474	ARG
1	B	483	LEU
1	B	484	HIS
1	B	485	ARG
1	B	486	SER
1	B	516	ASP
1	B	518	ILE
1	B	533	PRO
1	B	547	VAL
1	B	548	TYR
1	B	586	TYR
1	B	593	HIS
1	B	598	ARG
1	B	622	SER
1	B	624	ARG
1	B	664	ASP
1	B	680	ASN
1	B	686	ASN
1	B	690	MET
1	B	707	THR
1	B	716	GLN
1	B	740	ASP
1	B	747	THR
1	B	767	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	148	ASN
1	A	177	HIS
1	A	319	ASN
1	A	384	GLN
1	A	484	HIS
1	A	498	ASN
1	A	587	GLN
1	A	593	HIS
1	A	607	GLN
1	A	680	ASN
1	A	698	GLN
1	A	713	HIS
1	A	715	GLN
1	A	716	GLN
1	A	719	GLN
1	A	749	HIS
1	B	90	ASN
1	B	148	ASN
1	B	177	HIS
1	B	319	ASN
1	B	384	GLN
1	B	484	HIS
1	B	498	ASN
1	B	587	GLN
1	B	593	HIS
1	B	607	GLN
1	B	680	ASN
1	B	698	GLN
1	B	713	HIS
1	B	715	GLN
1	B	716	GLN
1	B	719	GLN
1	B	749	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	XIH	A	901	-	25,32,32	3.87	5 (20%)	26,47,47	2.55	5 (19%)

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	XIH	A	901	-	-	0/6/20/20	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	XIH	C12-C13	2.35	1.55	1.51
2	A	901	XIH	C23-C18	3.97	1.46	1.40
2	A	901	XIH	C3-C5	5.41	1.51	1.41
2	A	901	XIH	C6-N26	8.31	1.48	1.39
2	A	901	XIH	C6-N7	15.30	1.47	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	XIH	C17-C18-C19	-4.09	111.73	121.09
2	A	901	XIH	C22-C23-C24	-3.26	113.54	119.37
2	A	901	XIH	C18-C17-N16	2.83	118.00	113.31
2	A	901	XIH	C18-C23-C24	6.97	126.13	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	XIH	C17-C18-C23	8.38	131.40	120.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	XIH	3	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 [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	730/730 (100%)	-0.37	1 (0%) 95 96	4, 31, 79, 187	0
1	B	730/730 (100%)	-0.32	2 (0%) 94 94	5, 37, 92, 161	0
All	All	1460/1460 (100%)	-0.34	3 (0%) 95 95	4, 33, 88, 187	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	767	ARG	3.7
1	B	392	GLU	3.3
1	B	393	GLN	2.4

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	XIH	A	901	29/29	0.92	0.25	2.24	48,48,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.