



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:56 AM GMT

PDB ID : 2EXX  
Title : Crystal structure of HSCARG from Homo sapiens in complex with NADP  
Authors : Dai, X.; Chen, Q.; Yao, D.; Liang, Y.; Dong, Y.; Gu, X.; Zheng, X.; Luo, M.  
Deposited on : 2005-11-09  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

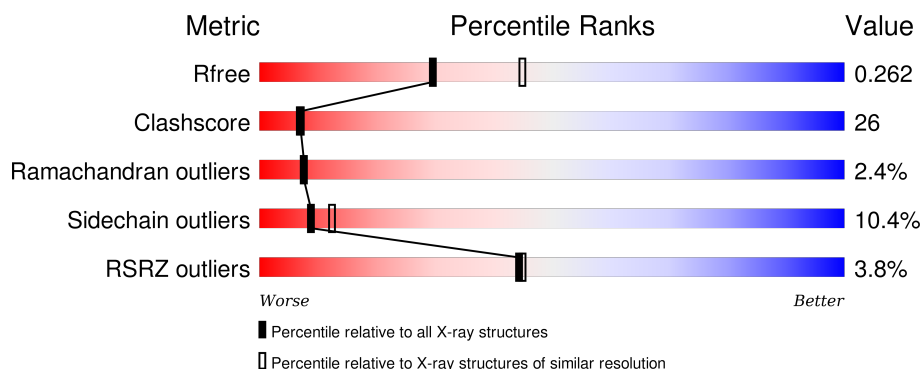
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	306	<div> <div>67%</div> <div>27%</div> <div>6%</div> </div>
1	B	306	<div> <div>7%</div> <div>45%</div> <div>38%</div> <div>8%</div> <div>9%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	2647	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4736 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.

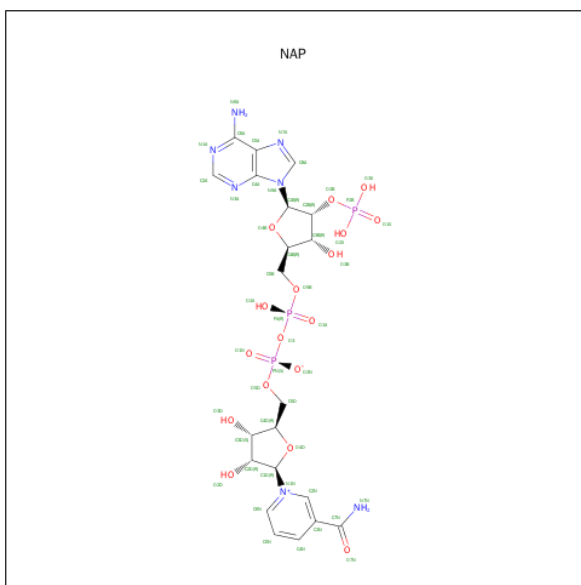
- Molecule 1 is a protein called HSCARG protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2392	1523	416	442	11			
1	B	279	Total	C	N	O	S	0	0	0
			2200	1398	384	408	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	CLONING ARTIFACT	GB 13938446
A	-5	TYR	-	CLONING ARTIFACT	GB 13938446
A	-4	LYS	-	CLONING ARTIFACT	GB 13938446
A	-3	LYS	-	CLONING ARTIFACT	GB 13938446
A	-2	ALA	-	CLONING ARTIFACT	GB 13938446
A	-1	GLY	-	CLONING ARTIFACT	GB 13938446
A	0	LEU	-	CLONING ARTIFACT	GB 13938446
B	-6	LEU	-	CLONING ARTIFACT	GB 13938446
B	-5	TYR	-	CLONING ARTIFACT	GB 13938446
B	-4	LYS	-	CLONING ARTIFACT	GB 13938446
B	-3	LYS	-	CLONING ARTIFACT	GB 13938446
B	-2	ALA	-	CLONING ARTIFACT	GB 13938446
B	-1	GLY	-	CLONING ARTIFACT	GB 13938446
B	0	LEU	-	CLONING ARTIFACT	GB 13938446

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			48	21	7	17	3	
								0
								0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			6	3	3		
						0	
							0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total 63	O 63	0	0
4	B	27	Total 27	O 27	0	0

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 ( $\text{RSRZ} > 2$ ). 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.

Chain A:

Token	Category
L-6	Green
Y-5	Green
M1	Green
K4	Orange
K5	Orange
L6	Orange
V7	Green
F10	Green
G11	Green
G12	Green
T13	Green
G14	Green
A15	Green
Q16	Green
G17	Green
R22	Green
L25	Green
F26	Green
D27	Green
G28	Green
F29	Green
F30	Green
K31	Green
V32	Green
K33	Green
V34	Green
V35	Green
T36	Green
R37	Green
K38	Green
K41	Green
K42	Green
A43	Orange
L47	Yellow
A52	Yellow
Q56	Yellow
G57	Yellow
D61	Green
T64	Orange
G65	Orange
E66	Orange
L67	Orange
A68	Orange
L69	Green
R80	Orange
Y81	Orange
F90	Orange

Chain B:

Amino Acid	Percentage
LEU	7%
TYR	45%
LVS	38%
LVS	38%
LVS	38%
ALA	38%
GLY	38%
LEU	38%
MET	38%
VAL	38%
ASP	38%
K4	38%
V7	38%
V8	38%
V9	38%
F10	38%
G11	38%
G12	38%
T13	38%
Q16	38%
G17	38%
L24	38%
L25	38%
E26	38%
K31	38%
V34	38%
V35	38%
T36	38%
R37	38%
N38	38%
P39	38%
R40	38%
K41	38%
A44	38%
K45	38%
Q50	38%
Q56	38%
G57	38%
D58	38%
Q59	38%
D60	38%
D61	38%
Q62	38%
V63	38%
I64	38%
M65	38%
E66	38%
L67	38%
A68	38%
L69	38%
T75	38%
F76	38%
I77	38%
V78	38%
T79	38%
H80	38%
Y81	38%
W82	38%
E83	38%
Q87	38%
E90	38%
V91	38%
Q92	38%
Q93	38%
I96	38%
L97	38%
L100	38%
A101	38%
R102	38%
R103	38%
H107	38%
Y111	38%
S112	38%
G113	38%
L114	38%
E115	38%
N116	38%
I117	38%
K118	38%
K119	38%
L120	38%
G123	38%
R124	38%
L125	38%
A126	38%
A127	38%
A128	38%
H129	38%
F130	38%
D131	38%
G132	38%
K133	38%
G134	38%
E135	38%
V136	38%
E137	38%
I143	38%
G144	38%
V145	38%
P146	38%
M147	38%
T148	38%
S149	38%
V150	38%
R151	38%
L152	38%
P153	38%
G154	38%
Y155	38%
F156	38%
E157	38%
H162	38%
Q166	38%
K167	38%
A168	38%
P169	38%
D170	38%
G171	38%
K172	38%
S173	38%
Y174	38%
L175	38%
LEU	38%
SER	38%
LEU	38%
PRO	38%
THR	38%
GLY	38%
ASP	38%
V183	38%
G187	38%
M188	38%
S189	38%
V190	38%
S191	38%
D192	38%
M203	38%
P204	38%
E205	38%
K206	38%
Y207	38%
Q210	38%
G213	38%
L214	38%
S215	38%
T216	38%
T220	38%
A221	38%
E222	38%
E223	38%
Y224	38%
L228	38%
H231	38%
T232	38%
R233	38%
K234	38%
V235	38%
V236	38%
M241	38%
T242	38%
F243	38%
E244	38%
D245	38%
Y246	38%
E247	38%
F248	38%
LEU	38%
GLY	38%
PHE	38%
PRO	38%
GLY	38%
ALA	38%
ARG	38%
D256	38%
L257	38%
A258	38%
K259	38%
M260	38%
F261	38%
R262	38%
F263	38%
L266	38%
D269	38%
R270	38%
D271	38%
L272	38%
E273	38%
L274	38%
L283	38%
E290	38%
Q291	38%
E292	38%
K293	38%
F296	38%
ASN	38%
LEU	38%
LEU	38%

## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.30Å 223.30Å 223.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 34.05 – 2.41	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.40) 95.3 (34.05-2.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.19 (at 2.42Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.233 , 0.265 0.232 , 0.262	Depositor DCC
$R_{free}$ test set	1687 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.093 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 33999 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.39	0/2438	0.69	0/3292
1	B	0.39	0/2240	0.69	2/3021 (0.1%)
All	All	0.39	0/4678	0.69	2/6313 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	TYR	N-CA-C	6.26	127.90	111.00
1	B	167	LYS	N-CA-C	-6.26	94.11	111.00

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	2392	0	2427	93	0
1	B	2200	0	2219	156	0
2	A	48	0	24	9	0
3	A	6	0	8	1	0
4	A	63	0	0	2	0
4	B	27	0	0	0	0
All	All	4736	0	4678	246	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 26.

All (246) 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:11:GLY:HA2	2:A:3698:NAP:O3B	1.57	1.04
1:B:172:LYS:HE2	1:B:224:TYR:HB3	1.42	1.01
1:B:166:GLN:C	1:B:168:ALA:H	1.61	1.01
1:B:168:ALA:HB1	1:B:169:PRO:HD2	1.41	1.00
1:B:37:ARG:H	1:B:37:ARG:HD3	1.29	0.94
1:B:168:ALA:CB	1:B:169:PRO:HD2	2.00	0.92
1:B:175:LEU:HD23	1:B:175:LEU:H	1.32	0.91
1:B:166:GLN:C	1:B:168:ALA:N	2.24	0.90
1:B:220:THR:HG22	1:B:222:GLU:H	1.37	0.90
1:B:13:THR:HG22	1:B:37:ARG:NH2	1.88	0.88
1:B:56:GLN:CD	1:B:56:GLN:H	1.79	0.86
1:B:57:GLY:HA3	1:B:64:ILE:HG21	1.58	0.85
1:B:8:VAL:HB	1:B:75:THR:HG23	1.56	0.85
1:B:46:GLU:HG3	1:B:50:GLN:NE2	1.95	0.82
1:A:36:THR:HG22	1:A:38:ASN:H	1.44	0.81
1:B:168:ALA:O	1:B:170:ASP:N	2.12	0.81
1:B:168:ALA:HB1	1:B:169:PRO:CD	2.11	0.81
1:A:216:THR:CG2	1:A:284:THR:HA	2.12	0.79
1:B:57:GLY:CA	1:B:64:ILE:HD13	2.13	0.79
1:A:216:THR:HG21	1:A:283:LEU:O	1.82	0.79
1:A:180:THR:HG21	1:A:221:ALA:H	1.48	0.79
1:B:37:ARG:H	1:B:37:ARG:CD	1.92	0.78
1:A:232:THR:O	1:A:233:ARG:HG2	1.84	0.77
1:B:37:ARG:N	1:B:37:ARG:HD3	1.98	0.77
1:B:175:LEU:N	1:B:175:LEU:HD23	2.01	0.75
1:B:107:HIS:O	1:B:146:PRO:HG2	1.88	0.73
1:B:57:GLY:HA2	1:B:64:ILE:HD13	1.70	0.73
1:B:13:THR:HG22	1:B:37:ARG:CZ	2.18	0.73
1:B:128:ALA:O	1:B:129:HIS:HB2	1.88	0.73
1:A:14:GLY:HA3	2:A:3698:NAP:H51A	1.70	0.73
1:A:193:LEU:O	1:A:196:VAL:HG13	1.89	0.72
1:A:65:MET:HE3	1:A:65:MET:HA	1.71	0.72
1:B:58:ASP:N	1:B:58:ASP:OD2	2.23	0.71
1:B:12:GLY:HA3	1:B:34:VAL:HG13	1.72	0.70
1:A:65:MET:HA	1:A:65:MET:CE	2.22	0.70
1:B:116:ASN:HD22	1:B:119:LYS:H	1.38	0.69
1:B:69:LEU:HD21	1:B:75:THR:HG21	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PHE:O	1:A:298:LEU:HD12	1.91	0.69
1:A:168:ALA:HB2	1:A:175:LEU:HD13	1.73	0.69
1:B:7:VAL:HG11	1:B:24:LEU:HD23	1.74	0.69
1:A:4:LYS:HE3	1:A:5:LYS:N	2.07	0.69
1:B:132:GLY:O	1:B:133:LYS:O	2.10	0.68
1:B:83:GLU:OE1	1:B:83:GLU:HA	1.91	0.67
1:B:151:ARG:NH1	1:B:151:ARG:HG3	2.08	0.67
1:A:4:LYS:HE3	1:A:4:LYS:HA	1.76	0.67
1:B:8:VAL:HB	1:B:75:THR:CG2	2.25	0.66
1:B:46:GLU:HG3	1:B:50:GLN:HE22	1.58	0.66
1:B:228:LEU:HD22	1:B:236:VAL:HG21	1.75	0.66
1:B:134:GLY:O	1:B:136:VAL:N	2.28	0.66
1:B:153:PRO:HG3	1:B:214:LEU:O	1.96	0.66
1:B:220:THR:HG22	1:B:222:GLU:N	2.09	0.66
1:A:66:GLU:O	1:A:67:LEU:HB2	1.95	0.65
1:B:78:VAL:HG12	1:B:80:ASN:H	1.62	0.65
1:A:296:PHE:O	1:A:298:LEU:N	2.30	0.65
1:B:57:GLY:HA3	1:B:64:ILE:HD13	1.80	0.64
1:B:155:TYR:CG	1:B:190:VAL:HG22	2.32	0.64
1:B:102:ARG:HD2	1:B:143:ILE:HG23	1.80	0.64
1:B:272:ILE:HG13	1:B:273:GLU:N	2.11	0.64
1:B:10:PHE:CD2	1:B:77:ILE:HG22	2.32	0.64
1:A:11:GLY:CA	2:A:3698:NAP:O3B	2.41	0.63
1:A:216:THR:HG21	1:A:284:THR:HA	1.81	0.63
1:A:284:THR:HG22	1:A:287:GLN:H	1.63	0.62
1:A:13:THR:HG21	1:A:41:LYS:NZ	2.14	0.62
1:B:151:ARG:HB2	1:B:213:GLY:HA2	1.82	0.61
1:B:77:ILE:HD11	1:B:111:TYR:CD2	2.35	0.61
1:B:143:ILE:HG22	1:B:145:VAL:HG23	1.83	0.60
1:A:117:ILE:O	1:A:121:THR:HB	2.02	0.60
1:B:153:PRO:CG	1:B:214:LEU:O	2.50	0.60
1:A:4:LYS:CA	1:A:4:LYS:HE3	2.32	0.60
1:A:126:ALA:H	1:A:259:ASN:HD22	1.49	0.60
1:B:231:HIS:CE1	1:B:290:GLU:HG2	2.37	0.59
1:B:232:THR:HG22	1:B:234:LYS:HB2	1.84	0.59
1:B:243:PRO:O	1:B:244:GLU:HB2	2.03	0.59
1:B:151:ARG:HH11	1:B:151:ARG:HG3	1.66	0.59
1:A:36:THR:O	1:A:56:GLN:HA	2.02	0.59
1:A:10:PHE:HZ	1:A:69:LEU:HD21	1.68	0.59
1:A:27:ASP:OD2	1:A:29:THR:OG1	2.21	0.58
1:B:151:ARG:HH11	1:B:151:ARG:CG	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:HG21	1:B:90:GLU:HG2	1.83	0.58
1:B:133:LYS:HD2	1:B:133:LYS:N	2.19	0.58
1:B:157:GLU:H	1:B:157:GLU:CD	2.05	0.58
1:A:121:THR:HG21	1:A:125:LEU:HD12	1.85	0.58
1:B:131:ASP:HA	1:B:133:LYS:HZ2	1.69	0.58
1:B:69:LEU:HD12	1:B:100:LEU:HD23	1.85	0.58
1:B:153:PRO:HD2	1:B:188:MET:CE	2.34	0.57
1:B:81:TYR:HD2	1:B:114:LEU:HB2	1.67	0.57
1:B:36:THR:HG22	1:B:38:ASN:N	2.20	0.57
1:B:131:ASP:CG	1:B:132:GLY:H	2.07	0.57
1:A:126:ALA:H	1:A:259:ASN:ND2	2.03	0.57
1:A:6:LEU:HD23	1:A:7:VAL:N	2.20	0.57
1:A:178:LEU:O	1:A:180:THR:N	2.38	0.56
1:B:4:LYS:O	1:B:31:LYS:HE2	2.06	0.56
1:A:4:LYS:HG3	1:A:31:LYS:HD3	1.86	0.56
1:B:168:ALA:CB	1:B:169:PRO:CD	2.73	0.56
1:A:121:THR:HG21	1:A:125:LEU:H	1.71	0.56
1:A:4:LYS:HE3	1:A:5:LYS:H	1.70	0.56
1:A:284:THR:HB	1:A:287:GLN:OE1	2.05	0.56
1:B:170:ASP:HA	1:B:235:VAL:O	2.06	0.55
1:A:4:LYS:CE	1:A:4:LYS:HA	2.31	0.55
1:A:294:GLY:O	1:A:297:ASN:ND2	2.38	0.55
1:B:39:PRO:HG3	1:B:56:GLN:HB3	1.88	0.55
1:B:231:HIS:HE1	1:B:290:GLU:HG2	1.71	0.55
1:A:121:THR:CG2	1:A:125:LEU:H	2.19	0.55
1:B:133:LYS:CE	1:B:151:ARG:HH21	2.19	0.55
1:B:131:ASP:CG	1:B:132:GLY:N	2.59	0.55
1:B:172:LYS:NZ	1:B:228:LEU:HD13	2.22	0.55
1:A:65:MET:HG2	1:A:97:LEU:HD21	1.89	0.55
1:B:82:TRP:NE1	1:B:260:MET:HG2	2.22	0.55
1:B:79:THR:O	1:B:79:THR:HG22	2.07	0.54
1:A:16:GLN:HG3	2:A:3698:NAP:O1N	2.07	0.54
1:B:12:GLY:HA3	1:B:34:VAL:CG1	2.38	0.54
1:B:189:SER:HB3	1:B:192:ASP:OD2	2.08	0.54
1:A:41:LYS:HE3	1:B:62:GLN:OE1	2.08	0.54
1:B:56:GLN:N	1:B:56:GLN:CD	2.55	0.53
1:A:168:ALA:HB2	1:A:175:LEU:CD1	2.37	0.53
1:B:257:LEU:O	1:B:260:MET:HB2	2.09	0.53
1:B:115:GLU:OE2	1:B:151:ARG:NH1	2.41	0.53
1:A:66:GLU:OE2	1:A:103:ARG:NH2	2.42	0.53
1:A:284:THR:HG23	4:A:3744:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:O	1:B:232:THR:HB	2.09	0.53
1:A:36:THR:HG23	2:A:3698:NAP:O3X	2.09	0.53
1:B:37:ARG:O	1:B:39:PRO:HD3	2.08	0.53
1:B:134:GLY:O	1:B:135:GLU:C	2.47	0.52
1:B:111:TYR:O	1:B:149:SER:HA	2.10	0.52
1:B:187:GLY:O	1:B:216:THR:HG22	2.10	0.52
1:B:40:ARG:HH11	1:B:40:ARG:HG2	1.73	0.52
1:A:203:MET:N	1:A:204:PRO:HD3	2.25	0.52
1:A:57:GLY:HA2	1:A:64:ILE:HG21	1.93	0.51
1:B:134:GLY:O	1:B:137:GLU:N	2.43	0.51
1:B:131:ASP:C	1:B:133:LYS:H	2.13	0.51
1:B:175:LEU:N	1:B:175:LEU:CD2	2.71	0.51
1:B:79:THR:HG21	1:B:90:GLU:CG	2.41	0.51
1:B:69:LEU:HD21	1:B:75:THR:CG2	2.41	0.51
1:B:66:GLU:OE1	1:B:103:ARG:NH2	2.43	0.51
1:B:16:GLN:NE2	1:B:152:LEU:HD13	2.26	0.50
1:B:128:ALA:HB1	1:B:130:PHE:H	1.76	0.50
1:A:296:PHE:C	1:A:298:LEU:HD12	2.32	0.50
1:A:13:THR:HG21	1:A:41:LYS:HZ3	1.73	0.50
1:B:91:VAL:CG1	1:B:135:GLU:HG2	2.41	0.50
1:B:153:PRO:HD2	1:B:188:MET:HE1	1.94	0.50
1:A:90:GLU:OE2	1:A:133:LYS:HE2	2.12	0.49
1:B:123:GLY:C	1:B:128:ALA:HB2	2.33	0.49
1:A:117:ILE:HG23	1:A:125:LEU:CD1	2.43	0.49
1:B:291:GLN:O	1:B:291:GLN:HG3	2.13	0.49
1:B:10:PHE:HB3	1:B:59:GLN:HG2	1.95	0.49
1:B:175:LEU:CD1	1:B:260:MET:HB2	2.42	0.48
1:B:133:LYS:HE2	1:B:151:ARG:HH21	1.79	0.48
1:B:232:THR:HG22	1:B:234:LYS:CB	2.44	0.47
1:B:169:PRO:O	1:B:235:VAL:O	2.31	0.47
1:B:37:ARG:HG3	1:B:37:ARG:HH11	1.79	0.47
1:A:65:MET:HG2	1:A:97:LEU:CD2	2.43	0.47
1:B:243:PRO:CG	1:B:261:PHE:CD1	2.97	0.47
1:A:34:VAL:HG21	1:A:47:LEU:HD13	1.96	0.47
1:A:80:ASN:HA	2:A:3698:NAP:O3D	2.15	0.47
1:A:164:LEU:HD11	1:A:298:LEU:HD13	1.95	0.47
1:A:4:LYS:NZ	1:A:29:THR:O	2.36	0.47
1:A:41:LYS:NZ	2:A:3698:NAP:O1X	2.47	0.47
1:A:41:LYS:HE2	1:B:96:LEU:HD22	1.96	0.47
1:B:214:LEU:O	1:B:270:ARG:HD2	2.14	0.47
1:A:10:PHE:CZ	1:A:69:LEU:HD21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASP:O	1:A:240:LYS:HG2	2.15	0.47
1:B:263:PHE:O	1:B:266:LEU:HB2	2.14	0.47
1:A:180:THR:HG21	1:A:221:ALA:N	2.25	0.46
1:B:16:GLN:HE21	1:B:152:LEU:HD13	1.80	0.46
1:A:178:LEU:HD22	1:A:185:MET:HE1	1.96	0.46
1:B:153:PRO:HD2	1:B:188:MET:HE2	1.96	0.46
1:B:257:LEU:C	1:B:257:LEU:HD23	2.36	0.46
1:B:8:VAL:O	1:B:75:THR:HG22	2.16	0.46
1:B:216:THR:HG21	1:B:283:LEU:O	2.16	0.46
1:A:1:MET:HA	1:A:1:MET:CE	2.45	0.46
1:A:216:THR:HG23	1:A:284:THR:HA	1.95	0.46
1:B:61:ASP:O	1:B:65:MET:HG3	2.14	0.46
1:A:141:ARG:NH2	1:A:211:ASN:OD1	2.48	0.46
1:B:166:GLN:O	1:B:167:LYS:HB2	2.16	0.46
1:A:96:LEU:HD13	1:A:96:LEU:C	2.37	0.46
1:A:4:LYS:HG3	1:A:31:LYS:CD	2.46	0.45
1:B:91:VAL:HG11	1:B:135:GLU:HG2	1.98	0.45
1:B:39:PRO:O	1:B:44:ALA:HB3	2.17	0.45
1:A:111:TYR:O	1:A:149:SER:HA	2.16	0.45
2:A:3698:NAP:C7N	3:A:2647:GOL:H2	2.47	0.45
1:B:82:TRP:HH2	1:B:263:PHE:HB2	1.81	0.45
1:B:77:ILE:HG13	1:B:77:ILE:O	2.16	0.45
1:A:197:VAL:O	1:A:201:LEU:HD22	2.16	0.45
1:B:7:VAL:O	1:B:7:VAL:HG13	2.17	0.45
1:B:220:THR:HB	1:B:223:GLU:HG3	1.99	0.45
1:B:132:GLY:C	1:B:133:LYS:O	2.54	0.45
1:B:56:GLN:NE2	1:B:56:GLN:H	2.15	0.45
1:B:157:GLU:CD	1:B:190:VAL:HG23	2.37	0.45
1:B:205:GLU:H	1:B:205:GLU:CD	2.19	0.45
1:B:87:GLN:OE1	1:B:117:ILE:HG23	2.16	0.45
1:B:11:GLY:O	1:B:17:GLY:HA3	2.17	0.44
1:B:13:THR:HB	1:B:36:THR:HG23	1.99	0.44
1:A:31:LYS:NZ	1:A:31:LYS:HB3	2.33	0.44
1:B:131:ASP:O	1:B:133:LYS:N	2.49	0.44
1:B:215:SER:O	1:B:272:ILE:HA	2.18	0.44
1:B:241:MET:HB3	1:B:246:TYR:CZ	2.52	0.44
1:B:123:GLY:O	1:B:128:ALA:HB2	2.18	0.44
1:B:131:ASP:HB2	1:B:133:LYS:HZ3	1.83	0.44
1:A:13:THR:HG23	1:A:43:ALA:HB3	1.99	0.43
1:B:246:TYR:CD2	1:B:257:LEU:HD21	2.53	0.43
1:A:22:ARG:HD3	4:A:3726:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:PHE:HD2	1:B:77:ILE:HG22	1.81	0.43
1:A:121:THR:HG21	1:A:125:LEU:N	2.34	0.43
1:A:174:TYR:CE2	1:A:234:LYS:HD3	2.53	0.43
1:A:25:LEU:HD11	1:A:52:ALA:HB2	2.00	0.43
1:A:11:GLY:C	1:A:17:GLY:HA3	2.38	0.43
1:A:4:LYS:C	1:A:4:LYS:HE3	2.38	0.43
1:A:56:GLN:NE2	1:B:63:VAL:HG21	2.34	0.43
1:B:175:LEU:HD11	1:B:260:MET:HB2	2.01	0.43
1:A:288:TRP:O	1:A:292:HIS:HB2	2.19	0.42
1:B:232:THR:O	1:B:234:LYS:HG3	2.19	0.42
1:A:234:LYS:HZ2	1:A:298:LEU:C	2.22	0.42
1:B:243:PRO:O	1:B:244:GLU:CB	2.67	0.42
1:A:130:PHE:CE1	1:A:260:MET:HG3	2.54	0.42
1:B:63:VAL:O	1:B:67:LEU:HG	2.19	0.42
1:A:117:ILE:CG2	1:A:125:LEU:CD1	2.98	0.42
1:A:113:GLY:O	1:A:114:LEU:HD13	2.19	0.42
1:A:180:THR:HG23	1:A:181:GLY:O	2.20	0.42
1:A:81:TYR:CD2	1:A:129:HIS:HB3	2.54	0.42
1:B:155:TYR:CD1	1:B:190:VAL:HG22	2.55	0.42
1:B:207:TYR:O	1:B:210:GLN:HB2	2.20	0.42
1:A:285:LEU:HD22	1:A:289:LEU:CD1	2.50	0.42
1:B:220:THR:CG2	1:B:221:ALA:N	2.83	0.42
1:B:7:VAL:HG11	1:B:24:LEU:CD2	2.46	0.41
1:B:157:GLU:CG	1:B:190:VAL:HG23	2.51	0.41
1:B:112:SER:HA	1:B:150:VAL:O	2.20	0.41
1:B:126:ALA:O	1:B:127:ALA:HB3	2.20	0.41
1:A:115:GLU:HG3	1:A:263:PHE:CZ	2.55	0.41
1:A:41:LYS:CE	1:B:96:LEU:HD22	2.49	0.41
1:B:290:GLU:OE2	1:B:293:LYS:NZ	2.54	0.41
1:A:198:LEU:O	1:A:202:LYS:HG2	2.21	0.41
1:A:38:ASN:O	1:A:41:LYS:HB2	2.20	0.41
1:B:271:ASP:OD2	1:B:274:LEU:HB2	2.20	0.41
1:A:115:GLU:HB2	1:A:120:LEU:HD21	2.02	0.41
1:A:36:THR:HG22	1:A:37:ARG:N	2.36	0.41
1:B:232:THR:HG22	1:B:234:LYS:HG3	2.03	0.41
1:B:272:ILE:CG1	1:B:273:GLU:N	2.82	0.41
1:B:77:ILE:HD11	1:B:111:TYR:HD2	1.80	0.41
1:B:81:TYR:OH	1:B:152:LEU:HG	2.21	0.41
1:B:36:THR:HG22	1:B:38:ASN:H	1.86	0.41
1:B:7:VAL:HG12	1:B:31:LYS:O	2.20	0.41
1:A:61:ASP:CG	1:A:64:ILE:HG12	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:THR:HG22	1:B:234:LYS:CG	2.51	0.40
1:B:133:LYS:NZ	1:B:151:ARG:NH2	2.69	0.40
1:B:257:LEU:HD23	1:B:258:ALA:N	2.37	0.40
1:A:133:LYS:NZ	2:A:3698:NAP:H1D	2.36	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	303/306 (99%)	295 (97%)	5 (2%)	3 (1%)	19	28
1	B	273/306 (89%)	249 (91%)	13 (5%)	11 (4%)	4	3
All	All	576/612 (94%)	544 (94%)	18 (3%)	14 (2%)	7	7

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	297	ASN
1	B	128	ALA
1	B	133	LYS
1	B	135	GLU
1	B	169	PRO
1	B	244	GLU
1	B	168	ALA
1	B	39	PRO
1	A	179	PRO
1	B	80	ASN
1	B	170	ASP
1	B	157	GLU
1	B	134	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	255/256 (100%)	230 (90%)	25 (10%)	10	14
1	B	235/256 (92%)	209 (89%)	26 (11%)	8	10
All	All	490/512 (96%)	439 (90%)	51 (10%)	9	12

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

Mol	Chain	Res	Type
1	A	-5	TYR
1	A	4	LYS
1	A	6	LEU
1	A	29	THR
1	A	32	VAL
1	A	65	MET
1	A	80	ASN
1	A	100	LEU
1	A	114	LEU
1	A	116	ASN
1	A	121	THR
1	A	125	LEU
1	A	141	ARG
1	A	147	MET
1	A	180	THR
1	A	196	VAL
1	A	200	LEU
1	A	201	LEU
1	A	205	GLU
1	A	208	VAL
1	A	216	THR
1	A	233	ARG
1	A	274	LEU
1	A	284	THR
1	A	285	LEU
1	B	13	THR
1	B	26	GLU

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Mol	Chain	Res	Type
1	B	37	ARG
1	B	58	ASP
1	B	60	ASP
1	B	75	THR
1	B	83	GLU
1	B	90	GLU
1	B	93	GLN
1	B	97	LEU
1	B	117	ILE
1	B	118	LYS
1	B	120	LEU
1	B	125	LEU
1	B	129	HIS
1	B	133	LYS
1	B	147	MET
1	B	151	ARG
1	B	162	HIS
1	B	174	TYR
1	B	175	LEU
1	B	203	MET
1	B	242	THR
1	B	257	LEU
1	B	266	LEU
1	B	269	ASP

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

Mol	Chain	Res	Type
1	A	16	GLN
1	A	56	GLN
1	A	59	GLN
1	A	80	ASN
1	A	87	GLN
1	A	93	GLN
1	A	116	ASN
1	A	259	ASN
1	A	297	ASN
1	B	16	GLN
1	B	50	GLN
1	B	89	GLN
1	B	116	ASN
1	B	292	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	GOL	A	2647	-	5,5,5	0.63	0	5,5,5	0.71	0
2	NAP	A	3698	-	42,52,52	1.38	6 (14%)	54,80,80	3.05	18 (33%)

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
3	GOL	A	2647	-	-	0/4/4/4	0/0/0/0
2	NAP	A	3698	-	-	0/27/67/67	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3698	NAP	PA-O2A	-2.01	1.46	1.54
2	A	3698	NAP	C6N-N1N	2.50	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3698	NAP	C4A-N3A	2.57	1.39	1.35
2	A	3698	NAP	C2A-N3A	3.35	1.38	1.32
2	A	3698	NAP	O4B-C1B	3.60	1.45	1.41
2	A	3698	NAP	C4N-C3N	3.74	1.45	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3698	NAP	O3X-P2B-O1X	-8.12	84.44	110.58
2	A	3698	NAP	O3-PN-O5D	-6.20	86.48	102.94
2	A	3698	NAP	O5D-PN-O1N	-6.04	86.19	109.62
2	A	3698	NAP	C4B-O4B-C1B	-5.95	103.18	109.72
2	A	3698	NAP	O3-PA-O5B	-5.56	88.19	102.94
2	A	3698	NAP	O3X-P2B-O2X	-5.26	87.36	107.38
2	A	3698	NAP	O2N-PN-O5D	-5.02	83.15	108.46
2	A	3698	NAP	N3A-C2A-N1A	-4.55	125.41	128.89
2	A	3698	NAP	C2A-N1A-C6A	2.03	122.39	118.77
2	A	3698	NAP	O2A-PA-O3	2.29	115.49	105.09
2	A	3698	NAP	O2N-PN-O3	2.52	116.52	105.09
2	A	3698	NAP	O2A-PA-O1A	2.65	126.91	112.53
2	A	3698	NAP	O2N-PN-O1N	2.69	127.10	112.53
2	A	3698	NAP	O2X-P2B-O1X	4.40	124.74	110.58
2	A	3698	NAP	PN-O3-PA	5.07	146.97	132.73
2	A	3698	NAP	O4D-C1D-N1N	5.18	113.83	108.13
2	A	3698	NAP	O4B-C4B-C5B	5.71	129.76	109.32
2	A	3698	NAP	O2B-P2B-O1X	6.25	122.71	107.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2647	GOL	1	0
2	A	3698	NAP	9	0

## 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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	305/306 (99%)	0.01	2 (0%) 89 88	10, 23, 40, 54	0
1	B	279/306 (91%)	0.45	20 (7%) 18 18	14, 33, 61, 77	0
All	All	584/612 (95%)	0.22	22 (3%) 44 45	10, 28, 54, 77	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	PHE	9.9
1	B	168	ALA	5.3
1	B	174	TYR	5.0
1	B	81	TYR	4.9
1	B	38	ASN	4.3
1	B	131	ASP	4.0
1	B	246	TYR	3.5
1	B	175	LEU	3.2
1	B	132	GLY	3.0
1	B	129	HIS	3.0
1	B	41	LYS	2.9
1	B	36	THR	2.8
1	B	60	ASP	2.5
1	B	257	LEU	2.5
1	B	133	LYS	2.4
1	B	128	ALA	2.3
1	A	298	LEU	2.1
1	A	-6	LEU	2.1
1	B	247	GLU	2.1
1	B	82	TRP	2.1
1	B	40	ARG	2.0
1	B	167	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	2647	6/6	0.85	0.21	3.75	20,27,29,30	0
2	NAP	A	3698	48/48	0.94	0.17	0.77	14,26,32,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.